Active Matter Shepherding and Clustering in Inhomogeneous Environments

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We consider a mixture of active and passive run-and-tumble disks in an inhomogeneous environment where only half of the sample contains quenched disorder or pinning. The disks are initialized in a fully mixed state of uniform density. We identify several distinct dynamical phases as a function of motor force and pinning density. At high pinning densities and high motor forces, there is a two step process initiated by a rapid accumulation of both active and passive disks in the pinned region, which produces a large density gradient in the system. This is followed by a slower species separation process where the inactive disks are shepherded by the active disks into the pin-free region, forming a non-clustered fluid and producing a more uniform density with species phase separation. For higher pinning densities and low motor forces, the dynamics becomes very slow and the system maintains a strong density gradient. For weaker pinning and large motor forces, a floating clustered state appears and the time averaged density of the system is uniform. We illustrate the appearance of these phases in a dynamic phase diagram.

Active matter, or self-motile particles or agents, arise in a variety of contexts including biological as well as designed systems such as self-propelled colloids and artificial swimmers ¹⁴⁻¹⁵. Due to their intrinsic non-equilibrium nature, such systems exhibit collective behaviors which are absent in systems with only thermal or Brownian motion. One of the best known examples of such an effect is the motility induced phase separation found for a collection of interacting disks. In the Brownian limit, at lower densities the disks form a uniform liquid phase; however, if the disks are active, there can be a transition to a self-clustered or phase separated state composed of regions of high density or solid clusters co-existing with a low density active gas ¹²⁻¹⁶. This phase separation can occur even when all the pairwise interactions between particles are repulsive.

Active matter can also exhibit a variety of other effects when it is coupled to complex environments ²⁻⁷, such as clustering along walls ⁹⁻¹³, activity induced depletion forces ¹⁴⁻¹⁵, ratchet behavior or spontaneous directed motion through funnels or asymmetric shapes ¹⁶⁻²⁸, novel transport in maze geometries ²¹⁻²⁹, and avalanches or activity induced clogging phenomena in constricted geometries ²⁶⁻²⁸. Active matter systems with random quenched disorder can undergo activity induced jamming ²⁷, trapping ³⁰⁻³², non-monotonic mobility ²⁸⁻³⁵, ³⁷, and different types of motion under external drift forces ³⁸⁻⁴².

The quenched disorder can take the form of obstacles which act as repulsive barriers or pinning sites which behave as localized traps. For dense pinning sites, the activity induced clustering effect can be suppressed when the active particles remain spread out due to trapping in the pinning sites ³¹. In contrast, obstacles can promote activity induced clustering ²⁹ by acting as nucleation sites ⁴³. The enhancement or reduction of activity included clustering by random disorder depends on the density and strength of the disorder. In addition to random disorder, there have been a variety of studies examining active matter coupled to periodic substrates which reveal directional locking effects ⁴⁴⁻⁴⁶, nonlinear transport ⁴⁷⁻⁵⁰, and commensuration effects ⁵¹⁻⁵².

In non-active matter systems with quenched disorder, such as vortices in superconductors ⁵³⁻⁵⁴, colloidal particles ⁵⁵⁻⁵⁶, and skyrmions ⁵⁷, it is known that the dynamics of the system can be modified strongly if the quenched disorder is inhomogeneous. An example of such disorder is a sample containing extended regions of strong pinning coexisting with regions where the pinning is weak or absent. Here, under an applied drive or increasing temperature, the system exhibits high mobility in the unpinned regions and reduced mobility in the pinned regions ⁵³⁻⁵⁵. Also, as the temperature is decreased from a high value, a glass or solid state first begins to form in the pinned region, with glassy behavior gradually spreading into the non-pinned regions ⁵⁴⁻⁵⁵. In inhomogeneous pinning environments, application of an external drive can produce an accumulation of particles along the interface between the pinned and pin-free regions ⁵⁷. These behaviors suggest that active matter moving in a sample containing coexisting pinned and non-pinned regions should also show significantly different behavior from active systems in uniform pinning.

In this work, we numerically examine a bidisperse assembly of run-and-tumble disks interacting with a substrate that is populated on only one half by quenched disorder in the form of pinning sites or obstacles. Half of the disks are active while the other half are passive. We vary the number of pinning sites and the active motor force, and initialize the system in a fully mixed state with a uniform density across the sample. For high motor forces and low pinning densities, the system forms an active mobile cluster phase in which the clusters contain both active and passive disks. These clusters spend equal amounts of time in the pinned and non-pinned regions, and the clusters act as large scale objects which over-
come the pinning effects to form what we call a floating cluster state with a uniform time-averaged density. At high motor forces and high pinning densities, we observe a two step dynamical process involving a transition from the uniform state to a density phase separated state followed by a coarsening process in which the different disk species segregate. In the first stage, a large build up of both species of disks into low mobility clusters occurs in the pinned region, producing a large density gradient between the pinned and non-pinned regions. The second stage is a slower species phase separation process in which active disks gradually shepherd the non-active disks out of the pinned regions, producing a phase separated state with a more uniform density in the long time limit. For other parameters, clusters can start to form along the edge of the pinned region, followed by the slow motion of a well defined density front into the pinned region. This process becomes slower as the motor force decreases. For the case of obstacles instead of pinning sites, we observe similar dynamics; however, the floating clustered state is lost and the shepherding behavior appears at much lower obstacle densities. When all the disks are active and the pinning is strong, the system only forms a low mobility clustered state in the pinned region and maintains a low density of active disks in the unpinned region.

We note that Chepizhko and Peruani have also considered individual active particles interacting with quenched disorder in the form of obstacles placed in only half of the sample. They found that for sufficiently high obstacle densities, the active particle could become locally trapped. This model differs significantly from the present work, where we focus on strong collective interactions between the active particles.

I. SIMULATION

We consider a two-dimensional system of size $L_x = 400$ and $L_y = 200$ with periodic boundary conditions in the $x$ and $y$-directions. As illustrated in Fig. [1](a), the system is divided into two regions. The right region has no substrate, while the left region contains $N_p$ nonoverlapping pinning sites that are modeled as attractive wells. We initialize the system with a random uniform distribution of $N_p$ disks with radius $r_a$. The disk-disk interactions are represented by a stiff harmonic repulsion and the disk density is $\phi = N_d \pi r_a^2 / L_x L_y$. The disks are divided into two populations, A and B, where $N_A$ of the disks are active and experience self propulsion, while the remaining $N_B = N_d - N_A$ disks are passive and can move only in response to other disks or the pinning sites. The equation of motion of disk $i$ is

$$\alpha_d \mathbf{v}_i = \mathbf{F}_{\text{dd}}^{i} + \mathbf{F}_i^{m} + \mathbf{F}_i^{\text{obs}}. \tag{1}$$

The disk velocity is $\mathbf{v}_i = d\mathbf{r}_i / dt$, where $\mathbf{r}_i$ is the disk position and the damping constant $\alpha_d = 1.0$. The disk-disk force is given by the harmonic repulsive potential $\mathbf{F}_{\text{dd}} = \sum_{i \neq j} N_d k (2r_a - |\mathbf{r}_{ij}|) \Theta (2r_a - |\mathbf{r}_{ij}|) \mathbf{r}_{ij}$, where $\Theta$ is the Heaviside step function, $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$, and $\mathbf{r}_{ij} = \mathbf{r}_j / |\mathbf{r}_{ij}|$. We set $k = 20$ and $r_a = 1.0$ for both species $A$ and $B$. The active disks obey run-and-tumble dynamics in which a motor force $F_M$ is exerted on the disk in a randomly chosen direction during a run time of $\tau_l$ before instantaneously changing to a new randomly chosen direction during the next run time. We define the run length $l_r$ as the distance a disk would travel in the absence of pinning sites or disk-disk collisions, $l_r = F_M \tau_l \delta t$, where $\delta t = 0.005$ is the simulation time step. We vary $\tau_l$ over the range $\tau_l = 40.000$ to $80.000$ time steps and the motor force $F_M$ over the range $F_M = 0.175$ to $2.0$. For the non-active disks, the equation of motion is the same except $F_M = 0$. We use a total simulation time of $2 \times 10^7$. We fix the total number of disks to give a system density of $\phi = 0.55$. The pinning sites are modeled as harmonic traps with strength $F_p = 2.5$ and radius $r_p = 0.5$, such that a single pinning site can capture at most one disk. After initialization, we measure the time evolution of the local disk density $\phi(x,y)$ as a function of $x$ averaged over $y$ for all disks ($\phi_x$), only the active disks ($\phi_x^a$), and only the passive disks ($\phi_x^p$). We also measure the ratio of the average disk density in the unpinned, $\phi_u$, and pinned, $\phi_p$, portions of the sample, giving the density ratio of all disks $R_k = \phi_k^u / \phi_k^p$, of the active disks $R_a = \phi_a^u / \phi_a^p$, and of the passive disks $R_p = \phi_p^u / \phi_p^p$.

II. RESULTS

In Fig. [2](a) we plot the positions of the active and passive disks for a system with $F_M = 1.5$, $N_p = 9000$, and $l_r = 600$. The initial disk configuration in Fig. [2](a) has a uniform density with a uniform distribution of both disk species. At time $t = 3.9 \times 10^4$ in Fig. [2](b), a large density build up of both active and passive disks appears at the pinning interface and begins to move into the pinned region. The active and passive disks form patches of denser clusters with six-fold ordering in the pinned area, while in the non-pinned region a more uniform fluid like state appears. In Fig. [2](c) at $t = 5 \times 10^5$, there is a strong density...
mixed and have a uniform density. (b) At time $t = 0$, the initial configuration in which the disk species are well mixed and have a uniform density. (b) At time $t = 3.9 \times 10^4$, a dense front of mixed species moves into the pinned region from both sides. (c) At $t = 5 \times 10^5$, there is a strong density imbalance and the unpinned region contains a low density of mostly passive disks while the pinned region contains a dense mixed state. (d) At $t = 2 \times 10^7$, the phase separation is more pronounced but the density difference between the pinned and unpinned regions is diminished.

FIG. 3. Local densities $\phi^a_l$ as a function of $x$ for the sample in Fig. 2 with $F_M = 1.5$, $N_p = 9000$, and $l_r = 600$ at times $t = 0.0$ (blue) where all the densities are uniform, $t = 5 \times 10^5$ (orange), $t = 5 \times 10^6$ (green), and $t = 2 \times 10^7$ (red). (a) The local density of all disks $\phi^l_l$ versus $x$. (b) The local density of active disks $\phi^a_l$ versus $x$. (c) The local density of passive disks $\phi^p_l$ versus $x$.

To get a better picture of the time evolution, in Fig. 3(a) we plot the local density of all disks $\phi^l_l$ versus $x$ for the system in Fig. 2 at three different times, while in Fig. 3(b,c) we show the local densities $\phi^a_l$ and $\phi^p_l$ of the active and passive disks, respectively, versus $x$. Pinning is present in the region with $x < 200$. At $t = 0$, the density is uniform throughout the system. For $t = 5 \times 10^5$, $\phi^a_l$ increases in the pinned region until the ratio of densities in the pinned and unpinned regions is $2 : 1$. The local density of active disks $\phi^a_l$ has a much stronger increase in the pinned region, with a ratio of close to $15 : 1$ for the density of active particles in the pinned and unpinned regions. At $t = 5 \times 10^6$ and $t = 2 \times 10^7$, $\phi^a_l$ in the pinned region remains fixed while the local density of passive disks $\phi^p_l$ in the pinned region drops. This occurs when the active particles shepherd the passive particles out of the pinned area, and causes the local density of all disks $\phi^l_l$ to become more uniform across the system.

As shown in Fig. 2, the initial buildup of active disks in the pinned region and show pronounced clustering, while the unpinned region contains mostly passive disks being pushed around by a small number of active disks. The overall density of the system is more uniform compared to Fig. 2(c). The clusters in the pinned region generally have low mobility, while weaker clustering of the passive disks in the unpinned region occurs when the active disks push the passive disks together.
the pinned region occurs through the formation of a dense front that moves into the pinned portion of the sample. This is more clearly illustrated in Fig. 4 where we plot a heat map of $\phi_a^p$ as a function of $x$ position versus time. At $t = 0$, $\phi_a^p$ is initially uniform, and then local maxima develop at the edges of the pinned region. These high density areas become fronts of active disks which move into the pinned region from either side and gradually merge at the center of the pinned region over time. For $t < 5 \times 10^4$, in the pinned region there are bands of higher density which appear as horizontal lines, indicating that the active disks have formed immobilized dense clusters in these locations, while in the unpinned region, the lines denoting high density areas run at angles, indicating that the active disks are in mobile clusters.

In Fig. 5(a), we plot the ratio $R_t = \phi_a^u/\phi_p^u$ of the density $\phi_a^u$ of all disks in the unpinned region to the density $\phi_p^u$ of all disks in the pinned region for the system in Fig. 3 at different values of $F_M$. Figure 5(b) shows the ratio $R_a = \phi_a^u/\phi_p^u$ of the density of active disks in the unpinned and pinned regions, while in Fig. 5(c) we plot the corresponding ratio $R_p = \phi_a^p/\phi_p^p$ for the passive disks. At initialization, we have $R_t = R_a = R_p = 1.0$. We first focus on the case of $F_M = 1.5$, which matches the system shown in Fig. 2. There is an initial rapid drop in $R_t$ from $R_t = 1.0$ to $R_t = 0.4$ which is accompanied by an even more rapid drop in the active particle ratio from $R_a = 1.0$ to $R_a \approx 0.1$. As the active disks enter the pinned region, they drag along a portion of the passive disks, as indicated by the small drop in $R_p$ for $t < 0.05 \times 10^7$ in Fig. 5(c). In Fig. 6 we show a blow up of Fig. 5 over the range $t < 0.1 \times 10^7$ in order to illustrate more clearly the initial invasion of the active and passive disks into the pinned region. A portion of the passive disks are dragged into the pinned region by the active disks, causing $R_p$ to decrease. For $t > 0.05 \times 10^7$, there is a crossover to the second stage in which $R_p$ remains fixed but $R_a$ gradually increases due to the shepherd-
FIG. 6. A blow up of the density ratio versus time curves from Fig. 5 over the range $t < 1.0 \times 10^6$. Here $N_p = 9000$, $l_r = 600$, and $F_M = 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3, 1.4,$ and $1.5$, from top left to bottom left. (a) Density ratio for all disks $R_t = \phi_u / \phi_p$. (b) Active disk density ratio $R_a = \phi_a^u / \phi_p$. (c) Passive disk density ratio $R_p = \phi_p^u / \phi_p$. The invasion of active disks into the pinned region is accompanied by the dragging of some of the passive disks into the pinned region. This is followed by a crossover to passive particle shepherding out of the pinned region, indicated by an increase in $R_p$.

FIG. 7. Linear-log plot of the active disk density ratio $R_a$ versus time for the system in Fig. 5 with $N_p = 9000$, $l_r = 600$, and varied $F_M$. For lower motor forces the curves decay approximately as $R_a \propto A - B \log(t)$, as indicated by the upper solid line.

FIG. 8. Density ratios for the unpinned to pinned regions for a system with $N_p = 6000$ and $l_r = 600$ at varied $F_M$. (a) The density ratio of all disks $R_t = \phi_u^t / \phi_p$. (b) The active disk density ratio $R_a = \phi_a^t / \phi_p$. (c) The passive disk density ratio $R_p = \phi_p^t / \phi_p$. At high $F_M$, the system saturates to a state with $R_t = 0.75$.

observed in vibrated granular matter [59] where there is a gradual compaction to a denser state. In our system the equivalent of the compaction dynamics is the build up of the active disks in the pinned region.

In Fig. 8 we plot $R_t$, $R_a$, and $R_p$ versus time for a system with a lower number of pinning sites $N_p = 6000$ at different values of $F_M$. The overall behavior is similar to that found for the $N_p = 9000$ sample. When $F_M > 0.8$ we find the two step process of an initial active disk invasion of the pinned region and the later passive disk shepherding out of the pinned region. For $F_M > 1.2$, the system reaches a steady state with $R_t = 0.75$, indicating a higher overall density in the pinned region compared to the unpinned region.

In Fig. 9 we plot $R_t$, $R_a$, and $R_p$ versus time for a system with an even lower number of pinning sites $N_p = 2000$. For $F_M < 0.8$ we find the usual two stage behavior of a rapid advancement of active disks into the pinned region followed by a slow species phase separation at longer times. For $F_M > 0.8$, the behavior changes and there are strong oscillations in $R_t$, $R_a$, and $R_p$. These oscillations result when a large scale motility induced clustering state forms, as shown in Fig. 10(a) at $t = 2 \times 10^7$ for the system in Fig. 9 at $F_M = 1.5$. In the pinned region, there is a background of pinned disks coexisting with a much larger cluster composed of both active and inactive disks. The density ratio oscillations in Fig. 9 are correlated with each other, indicating that there is
FIG. 9. Density ratios for the unpinned to pinned regions versus time for a system with \( N_p = 2000 \) and \( l_r = 600 \) at \( F_M = 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.1, 1.2, 1.3, 1.4, \) and \( 1.5 \), from top left to bottom left. (a) The density ratio of all disks \( R_t = \phi_t^u / \phi_t^p \). (b) The active disk density ratio \( R_a = \phi_a^u / \phi_a^p \). (c) The passive disk density ratio \( R_p = \phi_p^u / \phi_p^p \). For \( F_M > 0.8 \), we find strong density oscillations due to motility induced clustering, as illustrated in Fig. 10(a).

FIG. 10. Images of the active disks (blue) and passive disks (red) for the system in Fig. 9 with \( N_p = 2000 \) and \( l_r = 600 \) at \( t = 2 \times 10^7 \). (a) For \( F_M = 1.5 \), the system forms a motility induced cluster state. (b) At \( F_M = 0.5 \), there is a liquid like state with some species phase separation.

FIG. 11. Dynamic phase diagram as a function of motor force \( F_M \) versus number of pinning sites \( N_p \) obtained from the value of the passive disk density ratio \( R_p \) at a time \( t = 2 \times 10^7 \). Green: strong shepherding with species separation. Yellow: Weak or no shepherding. Red: large density oscillations occur due to the formation of the motility induced cluster state illustrated in Figs. 9 and 10(a).

Based on the behavior of the density ratios and our determination of whether density oscillations of the type shown in Fig. 9 are present, we can construct a dynamic phase diagram of the different behaviors as a function of \( F_M \) versus \( N_p \), as shown in Fig. 11 using the value of the passive disk density ratio \( R_p \) at a time \( t = 2 \times 10^7 \). In the green region, we find strong shepherding effects and the sample reaches a saturated state, while in the yellow region, the shepherding is weak or absent. The motility induced cluster state of the type illustrated in Fig. 10(a) appears in the red region. We find that shepherding can only occur for a sufficiently large number of pinning sites and a sufficiently high motor force.
motility induced cluster state grows in extent as $F_M$ increases. When the number of pins is large but $F_M$ is small, the pinned portion of the sample is in a disordered or glassy state. In this study we fix $F_p = 2.5$ and consider only the regime $F_M < F_p$, but we expect that when $F_M > F_p$, the motility induced cluster state will dominate the phase diagram.

At intermediate motor forces and larger $N_p$, near the phase boundary between shepherding (green) and absence of shepherding (yellow) in Fig. 11, a frozen invasion front can appear, as illustrated in Fig. 12 for a sample with $N_p = 8500$ and $F_M = 0.7$. Here the initial invasion of the active front occurs slowly enough that as the front starts to penetrate the pinned region, the front itself becomes pinned, forming a crystallized state near the edge of the pinned region. This pinned dense front makes it difficult for the passive disks to escape into the unpinned region. Figure 12(b) shows that at a much later time of $t = 2 \times 10^7$, the dense front has become better defined and has failed to penetrate further into the pinned region. The effective drive experienced by the dense front is proportional to $F_M$. In other systems where an interface moves over quenched disorder, it is known that there is a minimum critical force $F_c$ at the point where $F_M$ drops below the effective $F_c$ for interface depinning.

There have been several studies examining bidisperse mixtures of passive and active particles which have shown that both motility induced phase separation and species separation can occur [61–64]. It has also been demonstrated that active particles can move passive particles and organize them into particular states even when there are only a small number of active particles present, which is known as active doping [65–68]. This is similar to the shepherding phenomenon we observe. Our results show that quenched disorder could be used to achieve both density and species phase separation. For example, it should be possible to create a patterned state with pinning where the active particles could accumulate and gradually move the inactive particles in order to create a tailored self-assembled arrangement of active and passive particles.

### III. OBSTACLE ARRAYS

We have also considered samples in which the attractive pinning sites are replaced by repulsive obstacles in the form of immobile disks. In Fig. 13(a,b,c) we plot $R_t$, $R_a$, and $R_p$ as a function of time for a system with...
any cluster that forms, while the cluster can effectively
Fig. 10(a) for pinning site systems with low N_v
serve drifting or floating clusters of the type illustrated in
N_v not mobile. In our system with obstacles, we do not ob-
 ters which are induced by the presence of the obstacles
produced clusters break apart as the active particles spread
there can be a wetting transition in which mobility in-
we have also considered monodisperse systems in
N_v = 1500 obstacles and F_M = 1.5. The active disks
rapidly move into the obstacle region, followed by the
long time shepherding of the inactive disks into the un-
pinned region, similar to what we find for samples with
attractive pinning sites at much higher pinning densities
of N_p > 5000.
In Fig. 14(a) we show the positions of the active and
passive disks along with the obstacle locations for
the system in Fig. 13 at t = 0.05 × 10^7, where the active
and passive disks begin to cluster in the obstacle-filled
region. In Fig. 14(b), the same system at a later time of
t = 2.0 × 10^7 has a stronger species separation. In the
obstacle-filled region, the active disk density is higher
than in samples containing pinning sites. Previous work
for active matter on random pinning arrays showed that
there can be a wetting transition in which mobility in-
duced clusters break apart as the active particles spread
out and attempt to occupy as many pinning sites as pos-
able 31. On the other hand, it has also been shown
that repulsive obstacles can act as nucleation sites pro-
moting the clustering of active particles 33. The clusters
which are induced by the presence of the obstacles
remain pinned at the locations of the obstacles and are
not mobile. In our system with obstacles, we do not ob-
serve drifting or floating clusters of the type illustrated in
Fig. 10(a) for pinning site systems with low N_p and high
F_M, since even a small number of obstacles can pin down
any cluster that forms, while the cluster can effectively

FIG. 14. Images of the active disks (blue), passive disks
(red), and obstacle locations (black) for the system in Fig. 13
with repulsive obstacles instead of attractive pinning sites at
N_v = 1500, l_v = 600, and F_M = 1.5. (a) At t = 0.05 × 10^7,
there is an initial invasion into the region with obstacles. (b)
At t = 2 × 10^7, there is a stronger species separation.

float above the pinning sites if F_M is sufficiently large. In
the obstacle-free region we observe some weak clustering
due to the shepherding of the passive particles by a small
number of active particles, as shown in Fig. 14(b). We
find behavior similar to that illustrated in Figs. 13 and
14 for other obstacle densities.

IV. MONODISPERSE ACTIVE DISKS

We have also considered monodisperse systems in
which all of the disks are active and there are no pas-
sive disks. Here, we find only two generic phases. The
first is the accumulation of active disks in the pinned re-
gion, forming a large density gradient, and the second is
the formation of a large scale drifting cluster that floats
over the random pinning. In Fig. 15(a) we show the
initial uniform configuration for a monodisperse system

FIG. 15. Images of the active disks (blue) for a system with
N_p = 9000 pinning sites and no passive disks at l_v = 600
and F_M = 1.5. (a) The t = 0 initial uniform configuration.
(b) At t = 0.02 × 10^7, clusters form on both sides of the
pinned region. (c) The fully density phase separated state at
t = 2.0 × 10^7.
containing only active disks with \( N_p = 9000 \) pinning sites and \( F_M = 1.5 \). At \( t = 0.01 \times 10^7 \) in Fig. 15(b), mobile clusters have formed in the unpinned region while pinned clusters appear in the pinned region. In Fig. 15(c) at \( t = 2 \times 10^7 \), most of the disks are in the pinned region with a low density gas of active disks present in the unpinned region. For smaller \( F_M \), the same behavior occurs but the time required for the active disks to penetrate the pinned region fully increases.

If we place monodisperse active disks in a sample containing obstacles instead of pinning sites, we find behavior similar to that shown in Fig. 14 but the mobile cluster phase is absent since the clusters become pinned in the obstacle-filled region. In general, one might expect the active disks to accumulate in the unpinned region where they have more space to move; however, this is not what occurs due to a combination of effects. The first is the reduction of the mobility through direct interactions between the active disks and the pinning sites or obstacles. In a system where one region has a low diffusion coefficient and another region has a high diffusion coefficient, particles in the high diffusion region can rapidly explore space and reach the low diffusion region, whereas particles in the low diffusion region have reduced mobility and cannot reach the high diffusion region easily. The resulting flux imbalance causes the low diffusion region to accumulate a higher concentration of particles. In the case of active disks, the motility induced clustering effect which slows down the disks and is enhanced by the presence of pinning sites or obstacles. In a system where one region has a low diffusion coefficient and another region has a high diffusion coefficient, particles in the high diffusion region can rapidly explore space and reach the low diffusion region, whereas particles in the low diffusion region have reduced mobility and cannot reach the high diffusion region easily. The resulting flux imbalance causes the low diffusion region to accumulate a higher concentration of particles. In the case of active disks, the motility induced clustering state also produces a lower effective diffusion coefficient compared to freely moving non-interacting active disks. If a landscape structure could be identified which breaks apart the motility induced clusters only in the disordered region but not in the disorder-free region, it would be possible to achieve a higher effective diffusion coefficient in the disordered region, causing an accumulation of particles in the unpinned region, as opposed to what we observe, which is the opposite effect where the active disks accumulate in the pinned or obstacle-filled region.

V. SUMMARY

We have examined a bidisperse mixture of active and passive disks interacting with inhomogeneous disorder in which half of the sample contains randomly distributed pinning sites and the other half is free of disorder. We consider active disks obeying run-and-tumble dynamics, and vary the magnitude of the motor force and the density of pinning sites. For dense pinning and high motor forces, we observe a two step process in which active and passive particles accumulate in the pinned region, producing a large density gradient, followed by a slower shepherding process in which the passive disks are pushed into the unpinned region, producing a state that is more uniform in density but is phase separated. For lower motor forces, the initial invasion process becomes slower, and if the motor force is below a critical value, the invasion front entering the pinned region becomes pinned. For larger motor forces and lower pinning density, we find large scale drifting clusters containing a mixture of active and passive disks which effectively float over the pinning sites, leading to large oscillations in the density on either side of the sample but giving a uniform time averaged density across the entire sample. If we replace the attractive pinning sites by repulsive obstacles, the drifting cluster phase is lost and we observe an expanded shepherding region with the formation of much more compact clusters in the disordered portion of the sample. For a monodisperse system containing only active disks and no passive disks, the disks accumulate in the pinned region for higher pinning density and form a drifting motility induced cluster state at low pinning densities. Our results indicate that active particles could be used to move passive particles though complex landscapes or to control the invasion of active fluids into disordered media.

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[1] M. C. Marchetti, J. F. Joanny, S. Ramaswamy, T. B. Liverpool, J. Prost, M. Rao, and R. A. Simha, “Hydrodynamics of soft active matter,” Rev. Mod. Phys. 85, 1143–1189 (2013).

[2] C. Bechinger, R. Di Leonardo, H. Löwen, C. Reichhardt, G. Volpe, and G. Volpe, “Active particles in complex and crowded environments,” Rev. Mod. Phys. 88, 045006 (2016).

[3] G. Gompper, R. G. Winkler, T. Speck, A. Solon, C. Nardini, F. Peruani, H. Löwen, R. Golestanian, U. Benjamin Kaupp, L. Alvarez, T. Kissboe, E. Lauga, W. C. K. Poon, A. DeSimone, S. Muiños-Landin, A. Fischer, N. A. Söker, F. Chichos, R. Kapral, P. Gaspard, M. Ripoll, F. Sagues, A. Doostmohammadi, Y. M. Yeomans, I. S. Aranson, C. Bechinger, H. Stark, C. K. Hemelrijk, F. J. Nedelec, T. Sarkar, T. Aryaksama, M. Lacroix, G. Duc-
10

los, V. Yashunsky, P. Silberzan, M. Arroyo, and S. Kale, “The 2020 motile active matter roadmap,” J. Phys.: Condens. Matter 32, 193001 (2020).

[4] Y. Fily and M. C. Marchetti, “Athermal phase separation of self-propelled particles with no alignment,” Phys. Rev. Lett. 108, 235702 (2012).

[5] G. S. Redner, M. F. Hagan, and A. Baskaran, “Structure and dynamics of a phase-separating active colloidal fluid,” Phys. Rev. Lett. 110, 055701 (2013).

[6] J. Palacci, S. Sacanna, A. P. Steinberg, D. J. Pine, and P. M. Chaikin, “Living crystals of light-activated colloidal surfers,” Science 339, 936–940 (2013).

[7] I. Buttinioni, J. Bílaké, F. Kümmel, H. Löwen, C. Bechinger, and T. Speck, “Dynamical clustering and phase separation in suspensions of self-propelled colloidal particles,” Phys. Rev. Lett. 110, 238301 (2013).

[8] M. E. Cates and J. Tailleur, “Motility-induced phase separation,” Annual Review of Condensed Matter Physics 6, 219–244 (2015).

[9] Y. Fily, A. Baskaran, and M. F. Hagan, “Dynamics of self-propelled particles under strong confinement,” Soft Matter 10, 5609–5617 (2014).

[10] F. Sartori, E. Chiarello, G. Jayaswal, M. Pierno, G. Mishto, P. Brun, A. Tiribocchi, and E. Orlandini, “Wall accumulation of bacteria with different motility patterns,” Phys. Rev. E 97, 022610 (2018).

[11] T. Speck, “Collective forces in scalar active matter,” Soft Matter 16, 2652 (2020).

[12] S. Das, S. Ghosh, and R. Chelakkot, “Aggregate morphology of active Brownian particles on porous, circular walls,” Phys. Rev. E 102, 032619 (2020).

[13] Z. Fazli and A. Naji, “Active particles with polar alignment in ring-shaped confinement,” Phys. Rev. E 103, 022601 (2021).

[14] D. Ray, C. Reichhardt, and C. J. Olson Reichhardt, “Casimir effect in active matter systems,” Phys. Rev. E 90, 013019 (2014).

[15] R. Ni, M. A. Cohen Stuart, and P. G. Bolhuis, “Tunable long range forces mediated by self-propelled colloidal hard spheres,” Phys. Rev. Lett. 114, 018302 (2015).

[16] L. R. Leite, D. Lucena, F. Q. Potiguar, and W. P. Ferreira, “Depletion forces on circular and elliptical obstacles induced by active matter,” Phys. Rev. E 94, 062602 (2016).

[17] S. A. Mailory, C. Valeriani, and A. Cacciuto, “An active approach to colloidal self-assembly,” Ann. Rev. Phys. Chem. 69, 59 (2018).

[18] C. M. Kjeldbjerg and J. F. Brady, “Theory for the Casimir effect and the partitioning of active matter,” Soft Matter 17, 523 (2021).

[19] P. Galajda, J. Keymer, P. Chaikin, and R. Austin, “A wall of funnels concentrates swimming bacteria,” J. Bacteriol. 189, 8704–8707 (2007).

[20] J. Tailleur and M. E. Cates, “Sedimentation, trapping, and rectification of dilute bacteria,” EPL 86, 60002 (2009).

[21] B. Ai, “Ratchet transport powered by chiral active particles,” Sci. Rep. 6, 18740 (2016).

[22] C. J. Olson Reichhardt and C. Reichhardt, “Ratchet effects in active matter systems,” Ann. Rev. Condens. Matter Phys. 8, 51–75 (2017).

[23] A. D. Borba, Jorge L. C. Domingos, E. C. B. Moraes, F. Q. Potiguar, and W. P. Ferreira, “Controlling the transport of active matter in disordered lattices of asymmetrical obstacles,” Phys. Rev. E 101, 022601 (2020).

[24] M. Khatami, K. Wolff, O. Pohl, M. R. Ejtehadi, and H. Stark, “Active Brownian particles and run-and-tumble particles separate inside a maze,” Sci. Rep. 6, 37670 (2016).

[25] Y. Yang and M. A. Bevan, “Optimal navigation of self-propelled colloids,” ACS Nano 12, 10712 (2018).

[26] C. Reichhardt and C. J. O. Reichhardt, “Clogging and depinning of ballistic active matter systems in disordered media,” Phys. Rev. E 97, 052613 (2018).

[27] L. Caprini, F. Cecconi, C. Maggi, and U. Marini Bettolo Marconi, “Activity-controlled clogging and unclogging of microchannels,” Phys. Rev. Research 2, 043359 (2020).

[28] S. Shi, H. Li, G. Feng, W. Tian, and K Chen, “Transport of self-propelled particles across a porous medium: trapping, clogging, and the Matthew effect,” Phys. Chem. Chem. Phys. 22, 14052 (2020).

[29] C. Reichhardt and C. J. Olson Reichhardt, “Active matter transport and jamming on disordered landscapes,” Phys. Rev. E 90, 012701 (2014).

[30] M. Zeitz, K. Wolff, and H. Stark, “Active Brownian particles moving in a random Lorentz gas,” Eur. Phys. J. E 40, 23 (2017).

[31] Cs. Sándor, A. Libál, C. Reichhardt, and C. J. Olson Reichhardt, “Dewetting and spreading transitions for active matter on random pinning substrates,” J. Chem. Phys. 146, 204903 (2017).

[32] A. Morin, D. Lopes Cardozo, V. Chikkadi, and D. Bartolo, “Diffusion, subdiffusion, and localization of active colloids in random post lattices,” Phys. Rev. E 96, 042611 (2017).

[33] O. Chepizhko, E. G. Altmann, and F. Peruani, “Optimal noise maximizes collective motion in heterogeneous media,” Phys. Rev. Lett. 110, 238101 (2013).

[34] T. Bertrand, Y. Zhao, O. Bénichou, J. Tailleur, and R. Voituriez, “Optimized diffusion of run-and-tumble particles in crowded environments,” Phys. Rev. Lett. 120, 198103 (2018).

[35] O. Chepizhko and T. Franosch, “Ideal circle microswimmers in crowded media,” Soft Matter 15, 452–461 (2019).

[36] T. Bhattacharjee and S. S. Datta, “Confinement and activity regulate bacterial motion in porous media,” Soft Matter 15, 9920 (2019).

[37] D. Breoni, M. Schmedeberg, and H. Löwen, “Active Brownian and inertial particles in disordered environments: Short-time expansion of the mean-square displacement,” Phys. Rev. E 102, 062604 (2020).

[38] Cs. Sándor, A. Libál, C. Reichhardt, and C. J. Olson Reichhardt, “Dynamic phases of active matter systems with quenched disorder,” Phys. Rev. E 95, 032606 (2017).

[39] C. J. O. Reichhardt and C. Reichhardt, “Avalanche dynamics for active matter in heterogeneous media,” New J. Phys. 20, 025002 (2018).

[40] A. Morin, N. Desreumaux, J.-B. Cassini, and D. Bartolo, “Distortion and destruction of colloidal flocks in disordered environments,” Nature Phys. 13, 63–67 (2017).

[41] B. Bijnen and C. Maes, “Pushing run-and-tumble particles through a rugged channel,” J. Stat. Mech.: Theor. Exp. 2021, 033206 (2021).

[42] A. Chardac, S. Shankar, M. C. Marchetti, and D. Bartolo, “Emergence of dynamic vortex glasses in disordered polar active fluids,” Proc. Natl. Acad. Sci. (USA) 118, e2018218118 (2021).
[43] C. Reichhardt and C. J. Olson Reichhardt, “Absorbing phase transitions and dynamic freezing in running active matter systems,” Soft Matter 10, 7502–7510 (2014).

[44] G. Volpe, I. Buttinoni, D. Vogt, H.-J. Kümmerer, and C. Bechinger, “Microswimmers in patterned environments,” Soft Matter 7, 8810–8815 (2011).

[45] C. Reichhardt and C. J. O. Reichhardt, “Directional locking effects for active matter particles coupled to a periodic substrate,” Phys. Rev. E 102, 042616 (2020).

[46] M. Brun-Cosme-Bruny, A. Försch, W. Zimmermann, E. Bertin, P. Peyla, and S. Rafai, “Deflection of phototactic microswimmers through obstacle arrays,” Phys. Rev. Fluids 5, 093302 (2020).

[47] S. Pattanayak, R. Das, M. Kumar, and S. Mishra, “Enhanced dynamics of active Brownian particles in periodic obstacle arrays and corrugated channels,” Eur. Phys. J. E 42, 62 (2019).

[48] K. Schakenraad, L. Ravazzano, N. Sarkar, J. A. J. Wondervgem, R. M. H. Merks, and L. Giomi, “Topotaxis of active Brownian particles,” Phys. Rev. E 101, 042602 (2020).

[49] H. E. Ribeiro, W. P. Ferreira, and Fabrício Q. Potiguar, “Trapping and sorting of active matter in a periodic background potential,” Phys. Rev. E 101, 032126 (2020).

[50] C. Reichhardt and C. J. O. Reichhardt, “Active matter commensuration and frustration effects on periodic substrates,” Phys. Rev. E 103, 022602 (2021).

[51] H. Reinken, D. Nishiguchi, S. Heidenreich, A. Sokolov, M. Bär, S. H. L. Klapp, and I. S. Aranson, Commun. Phys. 3, 76 (2020).

[52] C. Reichhardt and C. J. O. Reichhardt, “Active matter commensuration and frustration effects on periodic substrates,” Phys. Rev. E 103, 022602 (2021).

[53] M. C. Marchetti and D. R. Nelson, “Patterned geometries and hydrodynamics at the vortex Bose glass transition,” Phys. Rev. B 59, 13624–13627 (1999).

[54] S. S. Banerjee, A. Soibel, Y. Myasoedov, M. Rappaport, E. Zeldov, M. Menghini, Y. Fasano, F. de la Cruz, C. J. van der Beek, M. Konczykowski, and T. Tamegai, “Melting of “porous” vortex matter,” Phys. Rev. Lett. 90, 087004 (2003).

[55] R. Seshadri and R. M. Westervelt, “Forced shear flow of magnetic bubble arrays,” Phys. Rev. Lett. 70, 234–237 (1993).

[56] K. H. Nagamanasa, S. Gokhale, A. K. Sood, and R. Ganapathy, “Direct measurements of growing amorphous order and non-monotonic dynamic correlations in a colloidal glass-former,” Nature Phys. 11, 403–408 (2015).

[57] C. Reichhardt and C. J. O. Reichhardt, “Shear banding, intermittency, jamming, and dynamic phases for skyrmions in inhomogeneous pinning arrays,” Phys. Rev. B 101, 054423 (2020).

[58] O. Chepizhko and F. Peruani, “Diffusion, subdiffusion, and trapping of active particles in heterogeneous media,” Phys. Rev. Lett. 111, 160604 (2013).

[59] E. R. Nowak, J. B. Knight, E. Ben-Naim, H. M. Jaeger, and S. R. Nagel, “Density fluctuations in vibrated granular materials,” Phys. Rev. E 57, 1971 (1998).

[60] C. Reichhardt and C. J. Olson Reichhardt, “Depinning and nonequilibrium dynamic phases of particle assemblies driven over random and ordered substrates: a review,” Rep. Prog. Phys. 80, 026501 (2017).

[61] J. Stehmann, R. Wittkowski, D. Marenduzzo, and M. E. Cates, “Activity-induced phase separation and self-assembly in mixtures of active and passive particles,” Phys. Rev. Lett. 114, 018301 (2015).

[62] B.-Q. Ai, Z.-G. Shao, and W.-R. Zhong, “Mixing and demixing of binary mixtures of polar chiral active particles,” Soft Matter 14, 4388–4395 (2018).

[63] T. Kolb and D. Kotsia, “Active binary mixtures of fast and slow hard spheres,” Soft Matter 16, 1067 (2020).

[64] D. R. Rodriguez, F. Alarcon, R. Martinez, J. Ramirez, and C. Valeriani, “Phase behaviour and dynamical features of a two-dimensional binary mixture of active/passive spherical particles,” Soft Matter 16, 1162 (2020).

[65] R. Ni, M. A. Cohen Stuart, M. Dijkstra, and P. G. Bolhuis, “Crystallizing hard-sphere glasses by doping with active particles,” Soft Matter 10, 6609 (2014).

[66] F. Kümmel, P. Shabestari, C. Lozano, G. Volpe, and C. Bechinger, “Formation, compression and surface melting of colloidal clusters by active particles,” Soft Matter 11, 6187–6191 (2015).

[67] S. Ramananarivo, E. Ducrot, and J. Palacci, “Activity-controlled annealing of colloidal monolayers,” Nature Commun. 10, 3380 (2019).

[68] A. K. Omar, Y. Wu, Z. G. Wang, and J. F. Brady, “Swimming to stability: Structural and dynamical control via active doping,” ACS Nano 13, 560 (2019).