## Active matter shepherding and clustering in inhomogeneous environments

P. Forgács<sup>1</sup>, A. Libál<sup>1</sup>, C. Reichhardt, and C. J. O. Reichhardt<sup>2</sup>

<sup>1</sup>Mathematics and Computer Science Department, Babeş-Bolya University, Cluj 400084, Romania <sup>2</sup>Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

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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 phase separation process where the inactive disks are shepherded by the active disks into the pin-free region, forming a nonclustered 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.

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# I. INTRODUCTION

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 [1-3]. Due to their intrinsic nonequilibrium 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 coexisting with a low-density active gas [2,4-8]. 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], such as clustering along walls [9–13], activity-induced depletion forces [14–18], ratchet behavior or spontaneous directed motion through funnels or asymmetric shapes [19–23], novel transport in maze geometries [24,25], and avalanches or activity-induced clogging phenomena in constricted geometries [26–28]. Active matter systems with random quenched disorder can undergo activity-induced jamming [29], trapping [30–32], nonmonotonic mobility [29,33–37], 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 nonactive 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 [53,55,57]. 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 nonpinned 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 nonpinned 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 nonpinned regions, and the clusters act as large-scale objects which overcome 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 nonpinned regions. The second stage is a slower species phase separation process in which active disks gradually shepherd the nonactive 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 forms only 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 [58] 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.

Our results should be relevant to studies of the invasion of disordered or porous media by active particles. Our observation that the active particles can shepherd nonactive particles out of the pinned region could be useful for filtering with disordered media, separation techniques, microscale mining, active cargo transport in inhomogeneous environments, and understanding how active biological systems interact with inhomogeneous surroundings or transport cargo in such settings. Recent work using only active particles has focused on the invasion process in disordered media [59], where the self-propelled particles are adsorbed by the porous media. This is similar to the phase we observe in which the active particles accumulate strongly in the densely pinned region.

## **II. 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, 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



FIG. 1. Image of the substrate showing that the right half of the sample is empty and the left half contains  $N_p$  nonoverlapping pinning sites (dots).

a random uniform distribution of  $N_d$  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

$$\alpha_d \mathbf{v}_i = \mathbf{F}_i^{dd} + \mathbf{F}_i^m + \mathbf{F}_i^p. \tag{1}$$

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 interaction force is given by the harmonic repulsive potential  $\mathbf{F}_{i}^{dd}$  =  $\sum_{i\neq j}^{N_d} k(2r_a - |\mathbf{r}_{ij}|)\Theta(2r_a - |\mathbf{r}_{ij}|)\hat{\mathbf{r}}_{ij}$ , where  $\Theta$  is the Heaviside step function,  $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$ , and  $\hat{\mathbf{r}}_{ij} = \mathbf{r}_{ij}/|\mathbf{r}_{ij}|$ . 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  $\mathbf{F}_{i}^{m} = F_{M} \mathbf{\hat{m}}_{i}$  of magnitude  $F_{M}$  is exerted on the disk in a randomly chosen direction  $\hat{\mathbf{m}}$  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, giving  $l_r = 35$  to 800. For the disk densities we consider, the disks do not cluster in the absence of quenched disorder until  $l_r = 400$ , where strong clustering appears. At our choice of pinning density, self-clustering first occurs near  $l_r = 80$ . Our parameters are chosen such that we can cross from the motility-induced clustering state to a nonclustering state as a function of motor force [31,38]. Experimentally, our results should be relevant for driven diffusive colloids when the activity is large enough to produce self-clustering.

The substrate interaction term  $\mathbf{F}_i^p$  is the trapping force from randomly placed pinning sites modeled as harmonic traps with  $\mathbf{F}_i^p = \sum_{i}^{k} F_p(r_{ik}/r_p)\Theta(r_{ik} - r_p)\hat{\mathbf{r}}_{ik}$ , where  $F_p$  is the maximum pinning strength,  $\mathbf{r}_k$  is the location of pinning site  $k, r_{ik} = |\mathbf{r}_i - \mathbf{r}_k|$ , and  $\hat{\mathbf{r}}_{ik} = (\mathbf{r}_i - \mathbf{r}_k)/r_{ik}$ . In this work we fix  $F_p = 2.5$  and the pinning radius  $r_p = 0.5$ , such that a single pinning site can capture at most one disk. Since our motor forces  $F_M \leq 2.0$ , a disk that has been captured by a pinning site generally remains there unless strong collective effects occur in which the many body interactions of multiple disks pushing on each other become strong enough to force the trapped disk out of the pinning site. In the latter portion of this work we replace the pinning sites by obstacles in the form of immobile disks. The obstacle repulsion is strong enough that motor forces are incapable of pushing a disk through an obstacle.

For the nonactive disks, the equation of motion is the same as Eq. (1) except  $F_M = 0$ . We use a total simulation time of  $2 \times 10^7$ , and fix the total number of disks to give a system density of  $\phi = 0.55$ . After initialization, we measure the time evolution of the local disk density  $\phi_l$  as a function of *x* averaged over *y* for all disks  $(\phi_l^t)$ , the active disks only  $(\phi_l^a)$ , and the passive disks only  $(\phi_l^p)$ . 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  $R_l = \phi_u^t / \phi_p^t$ , of the active disks  $R_a = \phi_u^a / \phi_p^a$ , and of the passive disks  $R_p = \phi_p^u / \phi_p^p$ .

#### **III. RESULTS**

In Fig. 2 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 sixfold ordering in the pinned area, while in the nonpinned region a more uniform fluid-like state appears. In Fig. 2(c) at  $t = 5 \times 10^5$ , there is a strong density build-up in the pinned region, while the nonpinned region contains a small density of mostly passive disks, with a density ratio of close to 2:1 in the pinned and unpinned regions. At longer times, a coarsening process occurs in which the passive disks are gradually shepherded out of the pinned region by the active disks. At  $t = 2 \times 10^7$ in Fig. 2(d), the majority of the active disks have collected 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.

To get a better picture of the time evolution, in Fig. 3(a) we plot the local density of all disks  $\phi_l^t$  vs x for the system in Fig. 2 at three different times, while in Figs. 3(b) and 3(c) we show the local densities  $\phi_l^a$  and  $\phi_l^p$  of the active and passive disks, respectively, vs x. Pinning is present in the region with x < 200. At t = 0, the density is uniform throughout the system. For  $t = 5 \times 10^5$ ,  $\phi_l^t$  increases in the pinned regions is 2:1. The local density of active disks  $\phi_l^a$  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  $t = 2 \times 10^7$ ,  $\phi_l^a$  in the pinned region remains fixed while the local density of passive disks  $\phi_l^p$  in the pinned region drops. This occurs when



FIG. 2. Images of the active disks (blue) and passive disks (red) for a system with  $F_M = 1.5$ ,  $N_p = 9000$ , and  $l_r = 600$ . (a) 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.

the active particles shepherd the passive particles out of the pinned area, causing the local density of all disks  $\phi_l^t$  to become more uniform across the system.



FIG. 3. Local densities  $\phi_l$  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  $\phi_l^t$  vs x. (b) The local density of active disks  $\phi_l^a$  vs x. (c) The local density of passive disks  $\phi_l^p$  vs x.

As shown in Fig. 2, the initial build-up of active disks in 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  $\phi_l^a$  as a function of x position vs time. At t = 0,  $\phi_l^a$  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



FIG. 4. Heat map of the local active disk density  $\phi_l^a$  as a function of position *x* vs time for the system in Fig. 3 with  $F_M = 1.5$ ,  $N_p = 9000$ , and  $l_r = 600$ . The active disks move into the pinned regime, which is the region from x = 0 to x = 200, in the form of a front of higher density.



FIG. 5. Ratios *R* of the average density  $\phi_u$  in the unpinned region to the average density  $\phi_p$  in the pinned region vs time for the system in Fig. 3 with  $N_p = 9000$  and  $l_r = 600$  at varied  $F_M = 0.5$ , 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 ratio  $R_t = \phi_u^t / \phi_p^t$  of the density of all disks. (b) The ratio  $R_a = \phi_a^a / \phi_p^a$  of the active disk density. (c) The ratio  $R_p = \phi_u^p / \phi_p^p$  of the passive disk density. We find a two-stage evolution. In the first stage, the active disks invade the pinned region, while in the second stage, the active particles shepherd the passive particles out of the pinned region and into the unpinned region. The duration of the first stage increases as  $F_M$  decreases.

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  $R_t = \phi_u^t / \phi_p^t$  of the density  $\phi_u^t$ of all disks in the unpinned region to the density  $\phi_p^t$  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  $R_a = \phi_u^a / \phi_p^a$  of the density of active disks in the unpinned and pinned regions, while in Fig. 5(c) we plot the corresponding ratio  $R_p = \phi_u^p / \phi_p^p$  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  $R_a$  remains fixed but  $R_p$  gradually increases due to the shepherding process in



FIG. 6. A blow-up of the density ratio vs 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  $R_t = \phi_u^t/\phi_p^t$ . (b) Active disk density ratio  $R_a = \phi_u^a/\phi_p^a$ . (c) Passive disk density ratio  $R_p = \phi_u^p/\phi_p^p$ . 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  $R_p$ .

which the active disks eject the passive disks from the pinned region. Figure 5 shows that  $R_p$  increases from  $R_p = 0.9$  to  $R_p \approx 2.5$ . At the same time, the density ratio for all disks  $R_t$  increases and approaches  $R_t = 0.75$  at the longest times. This suggests that for even longer times, the system should gradually approach a state with nearly uniform total density in which the active and passive disks are phase separated in the pinned and unpinned regions. In Fig. 5 we find that the time needed to reach a species-separated state increases with decreasing  $F_M$ . The duration of the initial invasion of the active particles into the pinned region also increases with decreasing  $F_M$ , and for  $F_M < 0.9$  we resolve only the initial invasion stage.

In Fig. 7 we plot  $R_a$  vs time on a linear-log scale to show more clearly the slowing of the initial invasion stage with decreasing motor force. The curves for  $F_M < 1.0$  can be described as having three parts. In the first part for  $t < 2 \times 10^5$ , there is an initial sharp decrease in  $R_a$  corresponding to the moving front of active disks. This is followed by a slower relaxation of the form  $R_a \propto A - B \log(t)$ , and finally by an eventual saturation close to a ratio  $R_a = 0.1$ . Logarithmic relaxation has been observed in vibrated granular matter [60] 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 the granular compaction studies, the logarithmic behavior can be mapped to a simplified one-dimensional version of a parking



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.

lot model of adsorption-desorption [60,61], giving a density time evolution which obeys  $1 + B \ln(1 + t/\tau)$ , where B and  $\tau$  are parameters associated with the acceleration from the driving of the granular matter. In our case, the active disks can be viewed as the cars, while the pinning sites assume the role of the parking spots. As more and more spots are filled, it becomes more difficult for the last remaining active disks to find a pinning site to occupy. By comparison to the granular system, the acceleration terms could be associated with the activity. This suggests that a similar analytical approach using an adsorption-desorption parking lot-inspired model [61] could be applied to the asymmetric behavior of our system. There are several differences between the two models. Strong diskdisk interactions are present in our system, and in addition to direct pinning by the pinning sites, there is a secondary pinning process in which a disk that has been trapped by a pinning site can block the motion of other unpinned disks. A more reasonable approach could be to consider multiple coupled parking lot models, since there are likely several different regimes in our system. Such analytic approaches can be considered elsewhere for a more simplified version of our system.

In Fig. 8 we plot  $R_t$ ,  $R_a$ , and  $R_p$  vs 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 twostep 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  $R_p$  vs 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 large density fluctuations in  $R_t$ ,  $R_a$ , and  $R_p$ . These fluctuations result when a large-scale



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  $R_t = \phi_u^t / \phi_p^t$ . (b) The active disk density ratio  $R_a = \phi_u^a / \phi_p^a$ . (c) The passive disk density ratio  $R_p = \phi_u^p / \phi_p^p$ . At high  $F_M$ , the system saturates to a state with  $R_t = 0.75$ .



FIG. 9. Density ratios for the unpinned to pinned regions vs 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  $R_t = \phi_u^t / \phi_p^t$ . (b) The active disk density ratio  $R_a = \phi_u^a / \phi_p^a$ . (c) The passive disk density ratio  $R_p = \phi_u^p / \phi_p^p$ . For  $F_M > 0.8$ , we find strong density fluctuations 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.

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 fluctuations in Fig. 9 are correlated with each other, indicating that there is either no species phase separation or at most only very weak separation. In the snapshot, the large cluster is located in the pinned region, but the cluster is mobile and spends an equal amount of time in the pinned and unpinned regions, producing the density ratio fluctuations and giving a time-averaged density that is close to uniform. The motility-induced cluster in Fig. 10(a) differs from the clustering found in the pinned region at higher  $N_p$ , since the latter clusters are mostly frozen in time and have little to no mobility. In contrast, the cluster shown in Fig. 10(a) gradually drifts through the entire sample over time. In Fig. 10(b) we illustrate the disk configurations for the system in Fig. 9 for  $F_M = 0.5$  at  $t = 2 \times 10^7$ , where the clustering is lost but there is still some phase separation. We have constructed a series of plots similar to those shown in Fig. 9 and find that motility-induced clustering always occurs in samples with  $N_p < 4500$  at the larger motor forces. We note that the large fluctuations are not periodic in time since the clusters move in and out of the pinned and unpinned regions at random.

Based on the behavior of the density ratios and our determination of whether large density fluctuations of the type shown in Fig. 9 are present, we can construct a dynamic phase diagram of the different behaviors as a function of  $F_M$  vs  $N_p$ , as shown in Fig. 11 using the value of the passive disk



FIG. 11. Dynamic phase diagram as a function of motor force  $F_M$  vs 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 fluctuations occur due to the formation of the motility-induced cluster state illustrated in Figs. 9 and 10(a).

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 occur only for a sufficiently large number of pinning sites and a sufficiently high motor force. The motilityinduced 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 is a minimum critical force  $F_c$  which must be applied in order for the interface to depin [62], so the crossover from the shepherding regime to the nonshepherding glassy state can be viewed as occurring at the point where  $F_M$  drops below the effective  $F_c$  for interface depinning.





FIG. 12. Images of the active disks (blue) and passive disks (red) for a system with  $N_p = 8500$ ,  $l_r = 600$ , and  $F_M = 0.7$ , near the transition between the shepherding and nonshepherding states in Fig. 11. (a) At  $t = 5 \times 10^5$ , a dense interface of active disks has formed at the edge of the pinned region. (b) The image at a much later time of  $t = 2 \times 10^7$  shows that this interface is effectively pinned.

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 [63–66]. 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 [67–70]. 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.

#### **IV. 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 Figs. 13(a), 13(b), and 13(c) we plot  $R_t$ ,  $R_a$ , and  $R_p$  as a function of time for a system with  $N_{obs} = 1500$  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 unpinned 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  $t = 0.05 \times 10^7$ , where the active and passive disks begin to cluster in the obstacle-filled region. In Fig. 14(b) the



FIG. 13. Density ratios for the unpinned to pinned regions vs time for a system with  $N_{obs} = 1500$  repulsive obstacles and  $l_r = 600$ . (a) The density ratio of all disks  $R_t = \phi_u^t / \phi_p^t$ . (b) The active disk density ratio  $R_a = \phi_u^a / \phi_p^a$ . (c) The passive disk density ratio  $R_p = \phi_u^p / \phi_p^p$ . Here we find that the active disks move rapidly into the obstacle-filled region and then gradually shepherd the passive particles into the obstacle-free region.



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  $N_{\rm obs} = 1500$ ,  $l_r = 600$ , and  $F_M = 1.5$ . (a) At  $t = 0.05 \times 10^7$ , there is an initial invasion into the region with obstacles. (b) At  $t = 2 \times 10^7$ , there is a stronger species separation.

same system at a later time of  $t = 2.0 \times 10^7$  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-induced clusters break apart as the active particles spread out and attempt to occupy as many pinning sites as possible [31]. On the other hand, it has also been shown that repulsive obstacles can act as nucleation sites promoting the clustering of active particles [43]. 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 observe 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 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.

# V. MONODISPERSE ACTIVE DISKS

We have also considered monodisperse systems in which all of the disks are active and there are no passive disks. Here, we find only two generic phases. The first is the accumulation of active disks in the pinned region, 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 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 fully penetrate the pinned region 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, and the second is 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



FIG. 15. Images of the active disks (blue) for a system with  $N_p =$  9000 pinning sites and no passive disks at  $l_r = 600$  and  $F_M = 1.5$ . (a) The t = 0 initial uniform configuration. (b) At  $t = 0.02 \times 10^7$ , clusters form on both sides of the pinned region. (c) The fully density phase-separated state at  $t = 2.0 \times 10^7$ .

the case of active disks, the motility-induced clustering state also produces a lower effective diffusion coefficient compared to freely moving noninteracting active disks. If a landscape structure could be identified which breaks apart the motilityinduced 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 obstaclefilled region. The strong accumulation of the monodisperse active disks in the dense disordered region is also similar to recent results obtained for self-propelled particles in homogeneous obstacle arrays, where for large enough motility, most of the particles end up in the trapped region [59].

#### VI. 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 density fluctuations 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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