Dewetting and spreading transitions for active matter on random pinning substrates

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We show that sterically interacting self-propelled disks in the presence of random pinning substrates exhibit transitions among a variety of different states. In particular, from a phase separated cluster state, the disks can spread out and homogeneously cover the substrate in what can be viewed as an example of an active matter wetting transition. We map the location of this transition as a function of activity, disk density, and substrate strength, and we also identify other phases including a cluster state, coexistence between a cluster and a labyrinth wetted phase, and a pinned liquid. Convenient measures of these phases include the cluster size, which dips at the wetting-dewetting transition, and the fraction of sixfold coordinated particles, which drops when dewetting occurs. *Published by AIP Publishing.* [<http://dx.doi.org/10.1063/1.4983344>]

I. INTRODUCTION

A wide class of systems exhibit pinning-induced order-disorder transitions in the presence of quenched disorder, including vortices in type-II superconductors,^{1,2} two-dimensional (2D) electron crystals,^{3,4} charged colloids,^{5–7} soft matter systems with core-softened potentials,⁸ and hard disks.⁹ When the ordered state is crystalline, increasing the substrate strength or decreasing the particle density can produce a transition to a disordered state through the proliferation of topological defects. In addition to these equilibrium phases, distinct phases can emerge under nonequilibrium conditions in active matter or self-driven particle systems,^{10,11} including biological systems such as run-and-tumble bacteria¹² or artificial swimmers such as self-motile colloids.^{11,13,14} One of the simplest models of active matter is monodisperse sterically interacting disks undergoing active Brownian motion or run and tumble dynamics, which can transition from a uniform liquid state to a clump or phase separated state with increasing disk density, persistence length,^{15–20} or run length.^{21–23} In the phase separated regime, which appears even in the absence of an attractive component in the disk-disk interactions, large clumps of densely packed disks are separated by a low density gas of active disks. Monodisperse disks exhibit crystalline or polycrystalline ordering within the high density regions inside the clumps.¹⁶ A natural question to ask is how robust these cluster phases are in the presence of quenched disorder and whether pinning-induced transitions can occur as a function of increasing substrate strength.

Obstacle arrays, which have been considered in several studies of swarming models^{24,25} and run and tumble disks,²³ produce quite different effects from the collective behavior

that can arise in pinning arrays. The distinction between a pin and an obstacle is that it is possible for particles to pass through a pinning site either individually or collectively, while obstacles present an impenetrable barrier. The dynamics of many physically relevant active matter systems, such as particles moving over rough substrates, are better described in terms of an effective pinning landscape instead of in terms of obstacle avoidance. Studies of modified Vicsek models in the presence of obstacles showed that swarming was optimized at a particular noise value,²⁴ while in other studies, increasing the disorder strength caused a phase transition from a swarming to a non-swarming state.²⁶ In studies of self-propelled disks interacting with obstacle arrays, the mobility of the disks was a non-monotonic function of the running length, since disks with long running times spend more time trapped behind obstacles.²³

Here we consider self-propelled disks interacting with a substrate composed of randomly placed pinning sites. A transition from a pin-free phase separated state to a homogeneous state can be induced by increasing the substrate strength. This transition can be viewed as an active matter version of a wetting-dewetting or spreading transition,²⁷ where the active particles spread out to cover the surface when the pinning is strong. We also show that a variety of different states can occur as a function of disk density, substrate strength, and activity, including cluster phases, coexisting clustered and wetted states, a wetted percolating state, and a pinned liquid state. These different states can be characterized by the size of the clusters and the amount of sixfold ordering of the disks.

II. SIMULATION

We numerically simulate a 2D system of $N_s = 8000$ – $20\,000$ self-propelled disks using graphics processing unit (GPU) based computing. The disk radius is $R = 1.0$ and the system size is $L \times L$ with $L = 300$, giving a filling factor of

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$\phi = \pi R^2/L^2 = 0.279$ to 0.698 . The disks obey the following overdamped equation of motion:

$$\eta \frac{d\mathbf{r}_i}{dt} = \mathbf{F}_{\text{inter}}^i + \mathbf{F}_m^i + \mathbf{F}_p^i, \quad (1)$$

where $\eta = 1$ is the drag coefficient, $\mathbf{F}_{\text{inter}}^i = \sum_{i \neq j}^{N_s} \Theta(d - 2R)k(d - 2R)\hat{\mathbf{d}}$ is the repulsive disk-disk interaction force, $d = |\mathbf{r}_i - \mathbf{r}_j|$, $\hat{\mathbf{d}} = (\mathbf{r}_i - \mathbf{r}_j)/d$, $k = 20$ is the harmonic spring contact force, and $\Theta(x)$ is the Heaviside function. The motor force $\mathbf{F}_m^i = F_m \hat{\mathbf{m}}_i$ with fixed $F_m = 1.0$ acts on each disk in a direction $\hat{\mathbf{m}}_i$ that changes randomly via a run and tumble protocol every t_r simulation time steps. The time step used in the simulations is $dt = 0.001$. We characterize the activity of the disks by $\tilde{l}_r = F_m t_r dt$, which is the distance a disk would travel in a single running time in the absence of disk-disk interactions or pinning, and take $\tilde{l}_r$ to be uniformly distributed over the range $[l_r, 2l_r]$. $\mathbf{F}_p^i$, the pinning force exerted by the substrate, is modeled by an array of N_p randomly placed circular parabolic traps with a finite radius of $R_p = 0.5$, with $\mathbf{F}_p^i = \sum_{k=1}^{N_p} F_p(r_p^{ik}/R_p)\Theta(r_p^{ik} - R_p)\hat{\mathbf{r}}_p^{ik}$ where F_p is the maximum pinning force exerted at the edge of the trap, $r_p^{ik} = |\mathbf{r}_i - \mathbf{r}_k^{(p)}|$ is the distance from the center of disk i to the center of pinning site k , and $\hat{\mathbf{r}}_p^{ik} = (\mathbf{r}_i - \mathbf{r}_k^{(p)})/r_p^{ik}$. Since $R_p < R$, a given pinning site can trap no more than one disk at a time.

III. RESULTS

In Fig. 1 we show four representative images of the phases that appear for active disks moving over a quenched pinning

FIG. 1. The disk positions (open circles) and pinning site positions (dots) for run and tumble disks interacting with a random pinning substrate in samples with $l_r = 300$ and $N_p/N_s = 0.5$. Colors indicate the largest clusters in the system. (a) A dewetted state (phase I) at $F_p = 1.0$ and $\phi = 0.55$. (b) A partially wetted state (phase II) at $F_p = 2.25$ and $\phi = 0.55$. (c) At $F_p = 8.0$ and $\phi = 0.55$, the disk density is uniform and the system forms a wetted state with disordered clusters (phase III). (d) At $F_p = 8.0$ and $\phi = 0.349$, there is a pinned liquid state (phase IV).

landscape in a sample with $l_r = 300$ and $N_p/N_s = 0.5$. The coloring highlights the largest individual clusters of disks, identified using the algorithm of Luding and Herrmann.²⁸ In the absence of a substrate, $F_p = 0.0$, the disks form a phase separated state for these parameters. For $F_p = 1.0$ in Fig. 1(a), a phase separated state containing a single high density cluster is still present. Disks in the surrounding low density gas state can be temporarily pinned since $F_m = F_p$, but overall the morphology is similar to that of the pin-free state. We term this the active dewetted state or phase I. At $F_p = 2.25$ in Fig. 1(b), a large cluster is still present but numerous smaller clusters have nucleated due to the trapping of gas phase disks by the pinning sites. As a result, the large cluster is smaller than that shown in Fig. 1(a), while the gas phase density is higher. This partially wetted state, called phase II, can be viewed as a coexistence of the dewetted state, consisting of the large cluster, and a wetted state in which the particles coat the entire substrate. At $F_p = 8.0$ in Fig. 1(c), the single large cluster has vanished and the system adopts a uniform labyrinth morphology which we refer to as the wetted state or phase III. In general we observe a similar sequence of phases at lower disk densities but find that the wetted state becomes less labyrinthine when the disks contact each other less frequently, as shown in Fig. 1(d) for $F_p = 8.0$ and $\phi = 0.349$ where the system forms a pinned liquid state called phase IV.

In Fig. 2(a), we plot the fraction of particles in the largest cluster C_l/N_s versus F_p for the system in Fig. 1 at a fixed run length of $l_r = 300$ for varied ϕ . Figure 2(b) shows the corresponding fraction P_6 of sixfold coordinated disks obtained using the CGAL library.²⁹ For $\phi > 0.315$, we find $C_l/N_s > 0.8$ and $P_6 > 0.8$ at low F_p since the system forms a single large clump with strong sixfold ordering. In the range $0.315 < \phi < 0.5$, there is a pronounced drop in both C_l/N_s and P_6 with increasing F_p as the system transitions from the clump phase illustrated in Fig. 1(a) to a pinned liquid phase of the type shown in Fig. 1(d). For $\phi > 0.5$, just before C_l/N_s reaches a minimum value at $F_p \approx 2.5$, the system enters

FIG. 2. (a) The fractional size of the largest cluster C_l/N_s vs F_p at $l_r = 300$ and $N_p = 8000$ for $N_s = 8000$ – $20\,000$ corresponding to $\phi = 0.279$ – 0.698 . The letters **a**, **b**, **c**, and **d** indicate the points at which the images in Figs. 1(a)–1(d) were obtained. The dip near $F_p = 2.5$ occurs at the transition from the dewetted phase I or the partially wetted phase II to the wetted phase III. (b) The corresponding fraction of sixfold coordinated particles P_6 vs F_p shows a drop as the system enters phase III.

a partially wetted state similar to that shown in Fig. 1(b). As F_p increases further, C_l/N_s increases again but P_6 continues to decrease, indicating that clusters with disordered structure have emerged, as illustrated in Fig. 1(c) at $F_p = 8.0$ where the system forms a labyrinth state and the disk density becomes uniform. The morphology of the large cluster is different in the two high C_l/N_s regimes, with a compact cluster forming in the dewetted state for $F_p < 2.5$ and a much more porous, extended, and branching cluster appearing in the wetted state for $F_p > 2.5$. For $\phi < 0.5$ at high F_p , interconnections between small branching clusters can no longer percolate across the sample, so there is no giant branching cluster and C_l/N_s remains low. Overall, we find that for the dewetted cluster (I), C_l/N_s and P_6 are both large and the disk density is heterogeneous. In the partially wetted phase (II), C_l/N_s is low and P_6 has an intermediate value while the disk density remains heterogeneous. The wetted labyrinth phase (III) has high C_l/N_s and high P_6 along with a homogeneous disk density. Finally, in the pinned liquid phase (IV), C_l/N_s and P_6 are both low and the disk density is homogeneous.

In Fig. 3(a), we show a heat map³⁰ based on C_l/N_s values as a function of ϕ versus F_p indicating the locations of phases I through IV. For $\phi < 0.35$, the system is too dilute to form clusters, so C_l/N_s remains low at all values of F_p . A dewetting-wetting transition from phase I to phase III occurs for $\phi \geq 0.35$, with the dashed line indicating the sliver of the partially wetted phase (II) that exists close to this transition. The transition from phase I to phase II is not sharply defined. For the clump-forming densities $\phi \geq 0.35$, over the range $0.0 < F_p < 2.75$ the radius R_{cl} of the compact clump decreases with increasing F_p while the density of the gaslike phase surrounding the clump increases. A direct measurement of R_{cl} in the $\phi = 0.55$ sample gives $R_{cl} \propto (F_c - F_p)^\alpha$ with $\alpha = 1.0$ and $F_c = 2.75$. In the dewetted phase I, there is a coexistence between a high density phase inside the clumps in which the local density ϕ_h is close to the monodisperse packing limit of $\phi_h \approx 0.9$, along with a low density phase with local density $\phi_l \ll \phi_h$. As F_p increases, more disks become trapped by pinning sites, so that the spatial extent of the dense phase decreases while ϕ_h remains constant.

FIG. 3. A heat map of C_l/N_s showing the locations of the different phases as a function of ϕ vs F_p for fixed $l_r = 300$ and $N_p = 8000$. Red areas for $F_p < 2.75$ indicate the formation of large compact clumps, while in the green areas for $F_p \geq 2.75$, large branching clumps appear. I: dewetted phase; II: partially wetted phase (along dashed line); III: wetted phase; IV: pinned liquid. The letters **a**, **b**, **c**, and **d** indicate the values of ϕ and F_p at which the images in Fig. 1 were obtained.

FIG. 4. (a) The size of the largest cluster C_l/N_s vs F_p at fixed $\phi = 0.55$ and $N_p/N_s = 0.5$ for run lengths ranging from $l_r = 1$ to $l_r = 500$. (b) The corresponding fraction of sixfold coordinated particles P_6 vs F_p shows a drop as the system enters phase III.

At the same time, ϕ_l increases until, at the transition to the fully wetted phase III, $\phi_l = \phi$.

We have also considered the effect of the run length by fixing the disk density at $\phi = 0.55$ and increasing l_r , as shown in Figs. 4(a) and 4(b) where we plot C_l/N_s and P_6 versus F_p . For small $l_r < 20$, C_l/N_s and P_6 are both low and the system is in a pinned liquid state. For large $l_r \geq 20$, a clump phase appears for $F_p < 2.75$ and we observe a dip feature in C_l/N_s and a drop in P_6 at the dewetting-wetting transition. The overall behavior is very similar to that shown for varied ϕ and fixed l_r in Fig. 2. The heat map diagram of C_l/N_s values in Fig. 5 as a function of l_r versus F_p illustrates the locations of phases I to IV.

To test the effect of the pinning site density, we fix $l_r = 300$, $\phi = 0.55$, and $F_p = 2.0$ and increase the number of pinning sites N_p . We find that at low pinning densities, a dewetted clump phase appears that transitions to a wetted phase as N_p increases. One difference between sweeping F_p and sweeping N_p is that at the highest pinning densities, the percolating cluster phase disappears. Since overlapping of pinning sites is not allowed, trapped disks are not likely to come into contact with each

FIG. 5. A heat map of C_l/N_s showing the locations of the different phases as a function of l_r vs F_p for fixed $\phi = 0.55$ and $N_p/N_s = 0.5$. Red areas for $F_p < 2.5$ indicate the formation of large compact clumps, while in the green areas for $F_p \geq 2.5$, large branching clumps appear. I: dewetted phase; II: partially wetted phase (along dashed line); III: wetted phase; IV: pinned liquid.

FIG. 6. The local density ϕ_h inside the clusters (green) and ϕ_l in the gas phase (brown) at fixed $\phi = 0.55$. (a) ϕ_h and ϕ_l vs F_p for $l_r = 300$ and $N_p/N_s = 0.5$. (b) ϕ_h and ϕ_l vs l_r for $F_p = 2.0$ and $N_p/N_s = 0.5$. (c) ϕ_h and ϕ_l vs N_p/N_s for $l_r = 300$ and $F_p = 5.0$. Dashed lines indicate the point at which the large cluster disappears from the system.

other to form a cluster, and at large N_p almost every disk is trapped, so C_l/N_s drops nearly to zero.

In Fig. 6, we plot the changes in the local density ϕ_h inside the clusters and ϕ_l in the gas phase as a function of F_p , l_r , and N_p/N_s . In each case, ϕ_h decreases slightly from $\phi_h = 0.9$ before suddenly dropping to $\phi_h = 0$ when the cluster disappears and the system reaches a uniformly wetted state. At the same time, ϕ_l gradually increases as the transition to the fully wetted cluster-free state is approached. The gentle decrease in ϕ_h in the cluster state occurs since the effective pressure inside the cluster falls as the cluster shrinks. The increase in ϕ_l is caused by a simple conservation of mass; as disks leave the cluster they become part of the gas phase which fully wets the substrate once $\phi_l = \phi$.

We can also characterize the different regimes by measuring the mean square particle displacements as a function of time, $\Delta r^2(t) = \sum_i^N |(\mathbf{r}_i(t) - \mathbf{r}_i(t_0))|^2$. In Fig. 7(a) we plot Δr^2 versus time for a sample from Fig. 5 with $l_r = 1.0$ and $\phi = 0.55$ at $F_p = 0$ and $F_p = 5.0$. In the substrate-free limit of $F_p = 0$, the

FIG. 7. The mean square displacement Δr^2 vs time in simulation time steps from the system in Fig. 5 at $\phi = 0.55$. (a) For $l_r = 1$ at $F_p = 0$ (purple) and $F_p = 1.0$ (dark blue), we can fit $\delta r^2 \propto t^\alpha$. At long times, $\alpha = 1.0$ for $F_p = 0$ (blue dashed line), consistent with diffusive motion, while for $F_p = 1.0$ we find subdiffusive behavior with $\alpha = 0.7$ (green dashed line) due to the particle trapping. (b) Δr^2 vs time for $l_r = 300$ at $F_p = 1.0$ (blue), 1.5 (green), 4.0 (orange), and 6.0 (red). For $F_p = 1.0$ and $F_p = 1.5$, in phase I and phase II, the system is superdiffusive at short and intermediate times with $\alpha = 1.7$ (blue dashed line) and diffusive or slightly subdiffusive at long times with $\alpha = 0.85$ (purple dashed line). For $F_p = 4.0$ and $F_p = 5.0$, the crossover to subdiffusion occurs at earlier times in phase III.

disks behave like a collection of diffusing Brownian particles and $\Delta r^2 \propto t^\alpha$ with $\alpha = 1.0$ for long times, while at shorter times $\alpha > 1.0$ indicating superdiffusion due to the activity of the disks. For $F_p = 5.0$, we find $\alpha = 0.7$ at long times, indicating subdiffusion due to the strong trapping of disks by the pinning sites. At time scales longer than what is shown in the figure, the system exhibits regular diffusion so that there is a crossover to $\alpha = 1.0$. In Fig. 7(b), we plot Δr^2 versus time for samples with $l_r = 300$ at $F_p = 1.0, 1.5, 4.0$, and 6.0 . At $F_p = 1.0$ the system is in the dewetted phase I and exhibits superdiffusive behavior with $\alpha = 1.7$ for short and intermediate times due to the activity of the disks. In the weak pinning regime, for large l_r the particles can move ballistically for long times, giving rise to the superdiffusive exponent; however, at longer times when the particle can change its running direction, there is a crossover to diffusive behavior with $\alpha = 1.0$. A similar behavior appears for $F_p = 1.5$ near the partially wetted phase II, where the crossover from superdiffusion to subdiffusion occurs at an earlier time. For $F_p = 4.0$ in the wetted phase III, superdiffusive behavior occurs at short times due to the disk activity but a crossover to diffusive behavior occurs at much earlier times than was the case for phases I and II, while deeper into the wetted phase III at $F_p = 6.0$, the long time behavior is weakly subdiffusive with $\alpha \approx 0.85$ to 0.9 due to the strong pinning effects. We also observe similar behavior for varied ϕ in the different phases.

We can also characterize the different phases based on the distribution of local disk density ϕ_{loc} , measured by partitioning the system into a grid array and obtaining the distribution of the disk density in individual grid elements. In Fig. 8(a), we plot $P(\phi_{loc})$ for a system from Fig. 3 in the phase I cluster state at $l_r = 300$, $\phi = 0.55$, and $F_p = 1.0$. There is a strong bimodal distribution of ϕ_{loc} with a peak near $\phi_{loc} = 0.1$ corresponding to the low density region and a second peak near $\phi_{loc} = 1.0$ produced by the dense regions. In the partially wetted phase II at $\phi = 0.55$ and $F_p = 2.25$, Fig. 8(b) shows that $P(\phi_{loc})$ also

FIG. 8. Distributions $P(\phi_{loc})$ of the local density ϕ_{loc} for the system in Fig. 3 for $l_r = 300$. (a) The dewetted phase I at $\phi = 0.55$ and $F_p = 1.0$ has a bimodal distribution of ϕ_{loc} . (b) The partially wetted phase II at $\phi = 0.55$ and $F_p = 2.25$ has a bimodal distribution with increased weight at lower ϕ_{loc} . (c) The dewetted phase III at $\phi = 0.55$ and $F_p = 8.0$ has a single broad peak in $P(\phi_{loc})$ centered at $\phi_{loc} = \phi$. (d) The pinned liquid phase IV at $\phi = 0.349$ and $F_p = 8.0$ has a single peak centered at $\phi_{loc} = \phi$.

has a bimodal distribution with one peak near $\phi_{\text{loc}} = 0.4$ from the lower density regions containing individually pinned particles, and a second peak near $\phi_{\text{loc}} = 0.95$ corresponding to the dense cluster. In Fig. 8(c), the wetted phase III at $\phi = 0.55$ and $F_p = 8.0$ exhibits a single broad peak centered at $\phi_{\text{loc}} = \phi = 0.55$ with weight extending up to $\phi_{\text{loc}} = 0.75$ and down to $\phi_{\text{loc}} = 0.4$. Figure 8(d) shows that in the pinned liquid phase IV at $\phi = 0.349$ and $F_p = 8.0$, there is again a single peak centered close to $\phi_{\text{loc}} = \phi = 0.349$, but the distribution is narrower than it was in phase III.

Another question is how robust these results are in the presence of different types of substrates, such as repulsive pinning sites or obstacles. In Fig. 9 we plot the cluster sizes C_l/N_s as well as P_6 versus F_p for the same system as in Fig. 2 but with repulsive pinning sites for $R_l = 300$, $N_p = 8000$, and $N_s = 8000$ –20 000 corresponding to $\phi = 0.279$ to 0.698 . In this case, for $\phi < 0.349$ the system is homogeneous for all F_p , while for $\phi \geq 0.349$ a cluster state appears at $F_p = 0$. At $\phi = 0.349$ there is a transition from a cluster state at low F_p to a pinned liquid state for $F_p \geq 2.0$, while at $\phi = 0.419$ the transition to the pinned liquid state is shifted up to $F_p = 5.0$. In general the features in C_l/N_s and P_6 are similar to those found for attractive pinning sites in Fig. 2, and we find the same four phases; however, the values of F_p at which transitions between these phases occur are shifted to higher values of F_p for the repulsive pinning sites compared to the system with attractive pinning sites. These results indicate that the general features of the phase diagram in Fig. 3 remain robust for either attractive or repulsive pinning sites. Recent experiments on flocking systems of active rolling colloids show that as a function of increasing obstacle number, a transition occurs from a flocking state to a disordered state.^{34,35} In our system, for a fixed repulsive pinning strength, we also find a transition from a cluster state to a homogeneous state when the ratio of the number active disks to the number of pinning sites is varied, as shown in Fig. 9.

FIG. 9. Results for repulsive pinning sites in a sample with $l_r = 300$, $N_p = 8000$, and ϕ ranging from 0.279 to 0.698. (a) The size of the largest cluster C_l/N_s vs F_p . (b) The fraction of six-fold coordinated particles P_6 vs F_p . We find the same general trends as for the attractive pinning case; however, the transition from the cluster phase to the pinned liquid or labyrinth phase is shifted to higher values of F_p .

Our results could be tested using active matter systems in the presence of a rough substrate. One method that can be used to create such a substrate is optical trapping, which allows the substrate strength to be tuned by varying the light intensity. There has already been some work examining the behavior of run and tumble bacteria in optical trap arrays.^{31,32} Although we focus on run and tumble systems, our results should be general to driven Brownian particle systems in which similar clustering transitions occur due to the density dependence of the particle motility.³³ Since the disks in a cluster are less strongly coupled to the substrate than the disks that are not part of a cluster, the onset of clustering may be a useful strategy that could be exploited by living active matter to collectively escape from a disordered environment.

In summary, we have numerically examined run and tumble disks interacting with a random pinning substrate where we find that there can be active matter wetting-dewetting transitions as a function of pinning strength, disk density, and run length. In regimes where the pin-free system forms a cluster state, we find that increasing the substrate strength causes the size of the cluster to shrink gradually until the disk density becomes homogeneous. Here, the cluster phase can be viewed as a dewetted state, while the homogeneous phase is like a wetted state. We show that the system exhibits different phases including a clump state, a partially wetted state in which clumps coexist with a gas of pinned disks, a fully wetted labyrinth state, and a pinned liquid state. Transitions between these states can be identified by measuring the size of the largest cluster and the fraction of sixfold coordinated particles. Our results indicate that pinning can induce transitions in the behavior of active matter systems that are similar to the pinning-induced order-disorder transitions in equilibrium condensed matter systems.

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