Dewetting and Spreading Transitions for Active Matter on Random Pinning Substrates

Cs. Sándor,1,2 A. Libál,∗1,2, C. Reichhardt,2, and C. J. Olson Reichhardt2

Received Xth XXXXXXXXXX 20XX, Accepted Xth XXXXXXXXXX 20XX
First published on the web Xth XXXXXXXXXX 20XX
DOI: 10.1039/b000000x

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. These phases can be identified using the cluster size, which dips at the wetting-dewetting transition, and the fraction of sixfold coordinated particles, which drops when dewetting occurs.

1 Introduction

A wide class of systems exhibit pinning-induced order-disorder transitions in the presence of quenched disorder, including vortices in type-II superconductors, two-dimensional (2D) electron crystal, charged colloid, soft matter systems with core-softened potentials, and hard disk. When the ordered state is crystalline, a transition to the disordered state as a function of increasing substrate strength or decreasing particle density occurs through the proliferation of topological defects. In addition to such equilibrium phases, distinct phases can emerge under nonequilibrium conditions in active matter or self-driven particle systems including biological systems such as run-and-tumble bacteria or artificial swimmers such as self-motile colloids. One of the simplest models of active matter is monodisperse sterically interacting disks undergoing active Brownian motion or run and tumble dynamics. These can transition from a uniform liquid state to a clump or phase separated state with increasing disk density, increasing persistence length or increasing run length. In the phase separated regime, which appears even in the absence of an attractive component in the particle-particle interactions, large clumps of densely packed disks are separated by a low density gas of active particles. Monodisperse disks exhibit crystalline or polycrystalline ordering within the high density regions inside the clumps. 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 and run and tumble disks, 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 while in other studies, increasing the disorder strength caused a phase transition from a swarming to a non-swarming state. 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.

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, 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 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
used in the simulations is \( dt \) the protocol every \( t \) in a direction \( \hat{m} \). A dewetted state (Phase I) at \( F_p = 2.25 \) 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).

clusters and the amount of sixfold ordering of the disks.

2 Simulation

We numerically simulate a 2D system of \( N_s = 8000 \) to 20,000 self-propelled disks using GPU based computing. The disk radius is \( R = 1.0 \) and the system size is \( L \times L \) with \( L = 300.0 \), giving a filling factor of \( \phi = \pi R^2 / L^2 = 0.279 \) to 0.698. The disks obey the following overdamped equation of motion:

\[
\eta \frac{dr_i}{dt} = F_{\text{inter}} + F_m^i + F_p^i, \tag{1}
\]

where \( \eta = 1 \) is the drag coefficient, \( F_{\text{inter}} = \sum_{j \neq i} \Theta(d - 2R/k(d - 2R)) \) \( \hat{d} \) is the repuls disk-disk interaction force, \( d = |r_i - r_j|, \hat{d} = (r_i - r_j)/d, k = 20.0 \) is the harmonic spring contact force, and \( \Theta(x) \) is the Heaviside function. The motor force \( F_m^i = F_m \hat{m} \) with fixed \( F_m = 1.0 \) acts on each disk in a direction \( \hat{m} \) 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 \( \tilde{I} = F_m r_i dt \), which is the distance a disk would travel in a single running time in the absence of disk-disk interactions or pinning, and take \( \tilde{I} \) to be uniformly distributed over the range \([I_1, 2I_1]\). \( F_p^i \), 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 \( R_p = 0.5 \), \( F_p^i = \sum_{k=1}^{N_p} F_p (r_{ik}^p / R_p) \Theta(r_{ik}^p - R_p) r_{ik}^p \) where \( F_p \) is the maximum pinning force exerted at the edge of the trap, \( r_{ik}^p = |r_i - r_{ik}^p| \) is the distance from the center of disk \( i \) to the center of pinning site \( k \), and \( r_{ik}^p = (r_i - r_{ik}^p) / r_{ik}^p \). Since \( R_p < R \), a given pinning site can trap no more than one disk at a time.

3 Results

In Fig. 1 we show four representative images of the phases that appear for active disks moving over a quenched pinning landscape in a sample with \( l_s = 300 \) and \( N_p / N_s = 0.5 \). The coloring highlights the largest individual clusters of disks, identified using the algorithm of Luding and Herrmann.\(^{22}\) 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. 1a), 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. 1b), 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 as 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 phase 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 \( \phi \). Figure 2(b) shows the corresponding fraction \( P_s \) of sixfold coordinated disks obtained using the CGAL library. For \( \phi > 0.315 \), we find \( C_l/N_s > 0.8 \) and \( P_s > 0.8 \) at low \( F_p \). At high \( F_p \), 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 \( P_s \) 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 a partially wetted state similar to that shown in Fig. 1(b). As \( F_p \) increases further, \( C_l/N_s \) increases again but \( P_s \) 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 \( P_s \) are both large and the disk density is homogeneous. In the partially wetted phase (II), \( C_l/N_s \) is low and \( P_s \) has an intermediate value while the disk density remains heterogeneous. The wetted labyrinth phase (III) has high \( C_l/N_s \) and high \( P_s \) along with a homogeneous disk density. Finally, in the pinned liquid phase (IV), \( C_l/N_s \) and \( P_s \) are both low and the disk density is homogeneous.

In Fig. 3(a) we show a heat map based on \( C_l/N_s \) values as a function of \( \phi \) 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 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 $\phi_l$ is close to the monodisperse packing limit of $\phi_l = 0.9$, along with a low density phase with local density $\phi_l \ll \phi_l$. As $F_p$ increases, more disks become trapped by pinning sites, so that the spatial extent of the dense phase decreases while $\phi_l$ remains constant. At the same time, $\phi_l$ 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 Fig. 4(a,b) where we plot $C_1/N_s$ and $P_0$ versus $F_p$. For small $l_r < 20$, $C_1/N_s$ and $P_0$ 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 $C_1/N_s$ and a drop in $P_0$ at the dewetting-wetting transition. The overall behavior is very similar to that shown for varied $\phi$ and fixed $l_r$ in Fig. 2. The heat map diagram of $C_1/N_s$ values in Fig. 5 as a function of $l_r$ versus $F_p$ illustrates the locations of phases I through 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 other to form a cluster, and at large $N_p$ almost every disk is trapped, so $C_1/N_s$ drops nearly to zero.

In Fig. 6 we plot the changes in the local density $\phi_l$ inside the clusters (green) and $\phi_l$ in the gas phase (brown) at fixed $\phi = 0.55$. (a) $\phi_l$ and $\phi_l$ vs $F_p$ for $l_r = 300$ and $N_p/N_s = 0.5$. (b) $\phi_l$ and $\phi_l$ vs $l_r$ for $F_p = 2.0$ and $N_p/N_s = 0.5$. c) $\phi_l$ and $\phi_l$ 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.

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. 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. Since the disks in a cluster are less strongly coupled to the substrate than disks that are not part 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.
4 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. 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.

5 Acknowledgments

This work was carried out under the auspices of the NNSA of the U.S. DoE at LANL under Contract No. DE-AC52-06NA25396. Cs. Sándor and A. Libál thank the Nvidia Corporation for their graphical card donation that was used in carrying out these simulations.

References

1 E.H. Brandt, Rep. Prog. Phys. 1995, 58, 1465.
2 S.C. Ganguli, H. Singh, G. Saraswat, R. Ganguly, V. Bugwe, P. Shirage, A. Thamizhavel, and P. Raychaudhuri, Sci. Rep. 2015, 5, 10613.
3 M.-C. Cha and H.A. Fertig, Phys. Rev. Lett. 1995, 74, 4867.
4 D. Carpentier and P. Le Doussal, Phys. Rev. Lett. 1998, 81, 1881.
5 A. Pertsinidis and X.S. Ling, Phys. Rev. Lett. 2008, 100, 028303.
6 C. Reichhardt and C.J. Olson, Phys. Rev. Lett. 2002, 89, 078301.
7 S. Deutschländer, T. Horn, H. Löwen, G. Maret, and P. Keim, Phys. Rev. Lett. 2013, 111, 098301.
8 E.N. Tsiok, D.E. Dudalov, Yu.D. Fomin, and V.N. Ryzhov, Phys. Rev. E 2015, 92, 032110.
9 W. Qi and M. Dijkstra, Soft Matter 2015 11, 2852.
10 M.C. Marchetti, J.F. Joanny, S. Ramaswamy, T.B. Liverpool, J. Prost, M. Rao, and R.A. Simha, Rev. Mod. Phys. 2013, 85, 1143.
11 C. Bechinger, R. Di Leonardo, H. Löwen, C. Reichhardt, G. Volpe, and G. Volpe, Rev. Mod. Phys., in press (2016).
12 H.C. Berg, Random Walks in Biology (Princeton University Press, Princeton, 1983).
13 J.R. Howe, R.A.L. Jones, A.J. Ryan, T. Gough, R. Vafabakhsh, and R. Golestanian, Phys. Rev. Lett. 2007, 99, 048102.
14 G. Volpe, I. Buttinoni, D. Vogt, H.-J. Kümmerer, and C. Bechinger, Soft Matter 2011, 7, 8810.
15 Y. Fily and M.C. Marchetti, Phys. Rev. Lett. 2012, 108, 235702.
16 G.S. Redner, M.F. Hagan, and A. Baskaran, Phys. Rev. Lett. 2013, 110, 055701.
17 J. Palacci, S. Sacanna, A.P. Steinberg, D.J. Pine, and P.M. Chaikin, Science 2013, 339, 936.
18 I. Buttinoni, J. Bialk´e, F. K¨ummel, H. Löwen, C. Bechinger, and T. Speck, Phys. Rev. Lett. 2013, 110, 238301.
19 C. Tung, J. Harder, C. Valeriani, and A. Cacciuto, Soft Matter 2016, 12, 555.
20 J. Bialk´e, J.T. Siebert, H. Löwen, and T. Speck, Phys. Rev. Lett. 2015, 115, 098301.
21 J. Tailleur and M.E. Cates, Phys. Rev. Lett. 2008, 100, 218103.
22 A.G. Thompson, J. Tailleur, M.E. Cates, and R.A. Blythe, J. Stat. Mech.: Theor. Exp. 2011, 2011, P02029.
23 C. Reichhardt and C. J. Olson Reichhardt, Phys. Rev. E 2014, 90, 012701.
24 O. Chepizhko, E.G. Altmann, and F. Peruani, Phys. Rev. Lett. 2013, 110, 238101.
25 O. Chepizhko and F. Peruani, Phys. Rev. Lett. 2013, 111, 160604.
26 D. Quint and A. Gopinathan, Phys. Biol. 2015, 17, 046008.
27 D. Bonn, J. Eggers, J. Indekeu, J. Meunier, and E. Rolley, Rev. Mod. Phys. 2009, 81, 739.
28 S. Luding and H.J. Herrmann, Chaos 1999, 9, 673.
29 M. Karavelas, “2D Voronoi diagram adaptor” in CGAL User and Reference Manual (2016).
30 J.D. Hunter, Comput. Sci. Eng. 2007, 9, 90.
31 M Paoluzzi, R Di Leonardo, and L Angelani, J. Phys.: Condens. Matter 2014, 26, 375101.
32 E. Pince, S.K.P. Velu, A. Callegari, P. Elahi, S. Gigan, G. Volpe, and G. Volpe, Nature Commun. 2015, 7, 10907.
33 M.E. Cates and J. Tailleur, Europhys. Lett. 2013, 101, 20010.