Active Matter Commensuration and Frustration Effects on Periodic Substrates

C. Reichhardt and C. J. O. Reichhardt
Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

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We show that self-driven particles coupled to a periodic obstacle array exhibit novel active matter commensuration effects that are absent in the Brownian limit. As the obstacle size is varied for sufficiently large activity, a series of commensuration effects appear in which the motility induced phase separation produces commensurate crystalline states, while for other obstacle sizes we find frustrated or amorphous states. The commensuration effects are associated with peaks in the amount of six-fold ordering and the maximum cluster size. When a drift force is added to the system, the mobility contains peaks and dips similar to those found in transport studies for commensuration effects in superconducting vortices and colloidal particles.

Commensuration effects arise in a variety of hard and soft matter systems when an assembly of particles is coupled to a periodic substrate with a spacing that matches the average interparticle spacing. Such effects occur for the ordering of atoms or molecules on surfaces [1, 3], vortices in superconductors or Bose-Einstein condensates with periodic pinning arrays [4, 5], colloidal particles on optical trap arrays [6, 10], or patterned surfaces [11], and cold atoms on optical lattices [12]. Conversely, if the particle assembly cannot fit within the constraints imposed by the substrate, then frustration can cause the disordering of the system or the formation of localized defects such as kinks or anti-kinks [13, 14]. Commensuration effects also strongly modify the transport properties under an applied drive in these systems, producing reduced transport or enhanced pinning when a commensuration occurs and generating a series of peaks or dips in the transport coefficients as the parameters are varied [3, 6, 13, 17].

Coupling of active matter or self-driven particles to a substrate [18, 19] has been realized in numerous experiments [18–22]. Many active particles have only short range repulsive interactions, so the system forms a uniform liquid at lower densities in the non-active or Brownian limit; however, when activity is present, the particles undergo a self-clustering or motility induced phase separation into a high density crystalline phase surrounded by a low density gas [20, 21, 23–25]. Although there have been various methods proposed for coupling an active matter system to random [19, 22, 20, 22] or periodic obstacle arrays [33, 35], the possible commensuration effects that could occur on a periodic substrate in active systems have not been considered before now. For a two-dimensional (2D) system of disks in the Brownian or zero activity regime, commensuration effects do not arise until the disk density \( \phi \) is high enough for all of the disks to touch each other, so for a nonactive system at \( \phi < 0.8 \), commensuration effects should be absent. Additionally, since thermal effects typically wash out commensuration effects [15], it might be expected that active matter systems would not exhibit commensuration effects.

Here we examine a 2D active matter system of self-propelled run-and-tumble disks interacting with a square array of obstacles. For certain obstacle sizes, we find that the system can undergo a strong motility-induced phase transition into a crystalline state that is commensurate with the obstacle lattice and that coexists with a low density gas. For other obstacle sizes, the motility-induced phase separation produces an amorphous crystal due to a frustration effect caused by a mismatch between the active disk spacing and the obstacle spacing. The spacing of the disks in the motility-induced dense phase is key in determining whether commensurate or incommensurate behavior occurs. The commensuration effects produce peaks in the size of the largest cluster and in the amount of sixfold ordering. A variety of different commensurate states appear, including states with local square ordering, aligned states, and sliding crystalline states. Under an applied drift force, the transport is a strongly nonmonotonic function of the obstacle size and exhibits dips at commensurate states as well as peaks at incommensurate or frustrated states. These commensuration effects are absent in the Brownian limit and become stronger for increasing activity or longer run times.

**Simulation and System**— We model a 2D system of active run-and-tumble disks of density \( \phi_a \) interacting with a periodic array of obstacles composed of posts of diameter \( d \) and lattice constant \( a \). The overdamped equation of motion for an active disk \( i \) is given by

\[
\alpha_d \dot{\mathbf{v}}_i = \mathbf{F}^{dd}_i + \mathbf{F}^m_i + \mathbf{F}^{obs}_i + \mathbf{F}^D_i, 
\]

where the damping constant \( \alpha_d = 1.0 \), and \( \mathbf{v}_i = d\mathbf{r}_i/dt \) are the position and velocity of disk \( i \). For the disk-disk interaction force \( \mathbf{F}^{dd}_i \), we use a harmonic repulsion with spring constant \( k_a \) and disk radius \( r_a \), so that the disk diameter is \( d_a = 2r_a \). We set \( k_a = 150 \), which is large enough to keep the disk-disk overlap in our study below one percent. The disk-obstacle force
We show two run length values: $l_C$ and $l_6$.

The fraction of six-fold coordinated particles $\phi_6$ vs $d$. The letters a-d in panel (a) indicate the points corresponding to the images in Fig. 2.

In Fig. 1(a) we show a snapshot of the active particles and the obstacles for the system in Fig. 1 at $l_r = 0.025$ and $\ell_r = 0.025$, where a uniform liquid state appears. By comparison, in Fig. 2(b) a sample with $l_r = 175$ at $d = 1.05$ forms a phase separated state of high density coexisting with a low density gas. This combination of parameters corresponds to the peak in $P_0$ and the dip in $M$ in Fig. 1. In Fig. 2(a) we show a blowup of the high density region from Fig. 2(b), indicating more clearly that the system forms a triangular lattice which is commensurate with the underlying square array. Figure 2(c) illustrates the system in Fig. 1 at $l = 175$ and $d = 1.3$, corresponding to a local minimum in $M$ and a drop in $P_0$. Although the system still shows clustering, the structure of the active disks in the dense region is now amorphous, as shown more clearly in Fig. 2(b). The disorder is produced by a frustration effect that arises when the natural spacing of the active crystal does not

$M_{\text{obs}}$ is also modeled as a harmonic potential. The active disk coverage is $\phi_a$ and the combined coverage of the disks and obstacles is $\phi_{\text{tot}}$. For the self-propulsion of the active disks $F_m$, a force $F_M$ is applied in a randomly chosen direction for a run time of $\tau_1$, after which the motor force instantaneously reorients to a new randomly chosen direction for the next run time. We characterize the system by the run length $\tau_1 = F_m \tau_1$, the distance an isolated active particle would move during the run time $\tau_1$. We also consider the effects of an external drive $F_D = F_D \hat{x}$ and measure the mobility $M$ using the average velocity in the driving direction, $\langle V_x \rangle = \sum_{i=1}^{N_d} v \cdot x$. We define $M = \langle V_x \rangle / V_{\text{free}}$, where $V_{\text{free}}$ is the average velocity that would appear under the same driving force in the absence of any obstacles. We fix $a = 3.0$ and $F_D = 0.2$, and vary $d_a$, $d$, and $\tau_1$.

Results. In Fig. 1(a,b,c) we plot the mobility $M$, the fraction of six-fold coordinated particles $\phi_6$, and the fraction of particles in the largest cluster $C$ versus the obstacle diameter $d$ for a system with $\phi_a = 0.32$ and $d_a = 0.9$. We show two run length values: $l_r = 0.025$, where the system is in the Brownian limit, and $l_r = 175$, the active limit where an obstacle free system would exhibit motility induced phase separation. For the short run length of $l_r = 0.025$, $M$ has an initial value near 1.0 and exhibits a monotonic decrease with increasing $d$, while $P_0$ is mostly flat and $C$ starts to increase once $d > 1.5$. For the active limit of $l_r = 175$, $M$ also has an initial value near 1.0 but changes nonmonotonically with increasing $d$, showing a pronounced dip near $d = 1.05$ which correlates with a peak in $P_0$ and a smaller peak in $C$. There is also a peak in $M$ near $d = 1.3$ that is associated with a drop in $P_0$ and a smaller dip in $C$. Additional features include a peak in $M$ near $d = 0.2$ and a smaller peak near $d = 1.75$.
match the spacing of the interstitial region between the obstacles. The dip in $M$ is similar to the drop in motion or decrease in the critical depinning force found in non-active commensurate systems at incommensurate densities [5, 6, 13–15]. In the non-active systems, the commensurate crystalline states have a higher shear modulus and can be more strongly pinned by the obstacles. In contrast, for the frustrated system the shear modulus is reduced, permitting the particles to move more easily and producing minima in the depinning force of the incommensurate state. Near $d = 0.2$ for the active system in Fig. 4(a) a peak in $M$ and a dip in $P_b$ appear at another incommensurate region where the disks are disordered, as shown in Fig. 4(b) for $d = 0.225$.

For $d > 1.5$, a distinctive type of active cluster appears which has local square short-range ordering within a single plaquette. These clusters are associated with a drop in $M$ and an increase in $C$. An example of the $d = 1.7$ clustered state appears in Fig. 4(c), where a single plaquette with local square ordering is highlighted. As $d$ increases further, other types of commensurate crystals can occur.

In the active system near $d = 0.15$, where there is a smaller peak in $C$, the disks form a sliding crystalline state where the commensuration effect is determined by the number of rows of active disks that can fit between adjacent rows of obstacles, as shown in Fig. 4(d) for four rows of disks. The sliding crystal exhibits intermittent jumping between crystal and disordered states, causing the value of $P_b$ to be reduced compared to the commensurate state which appears at higher $d$. If we consider a random array of obstacles, we do not observe any commensurate effects but instead find a monotonic decrease of the mobility with increasing $d$.

In Fig. 4(a) we plot $M$ vs $d$ for the system in Fig. 1 with fixed $d_o = 0.9$ at varied $l_r = 0.00025$, 0.1, 0.025, 0.25, 40, 175, and 1750, from top to bottom. (b) $M$ vs $d$ for $l_r = 175$ at $d_o = 0.7$, 0.8, 0.9, and 1.0, from top to bottom, corresponding to $\phi_o = 0.195$, 0.254, 0.32, and 0.4. For clarity, the first three curves are shifted up by 0.915, 0.61, and 0.305, respectively, on the $M$ axis. (c) $M$ vs $d$ for samples with $d_o = 0.8$ and $l_r = 175$ at varied disk density $\phi_o = 0.00212$, 0.09, 0.17, 0.254, and 0.332, from top to bottom. (d) The corresponding fraction of particles in the largest cluster $C$ vs $d$ for the system in panel (c).
locally square commensurate state shifts to lower values of $d$ with increasing $d_a$. The drop in $M$ near $d = 1.0$ in the $\phi_a = 0.254$ system is due to the appearance of a different type of commensurate clustering state where the ordering is triangular rather than square, similar to what is shown in Fig. 2(b) and Fig. 3(a). The triangular commensurate state persists up to $d = 1.1$ for the $\phi_a = 0.254$ system and appears over a slightly higher range of $d$ in the $\phi_a = 0.32$ system. The peak near $d = 1.1$ for $\phi_a = 0.254$ is the result of the formation of a frustrated state of the type illustrated in Fig 2(c) and Fig. 3(b). For $\phi_a = 0.4$, the triangular commensurate state is present near the dip in $M$ at $d = 0.7$. In general, as $\phi_a$ increases, the overall magnitude of $M$ drops.

The behavior of $M$ versus $d$ for samples with $l_r = 175$ where we hold the active disk diameter fixed at $d_a = 0.8$ but consider different disk densities $\phi_a = 0.00212, 0.09, 0.17, 0.254$, and 0.332 is shown in Fig. 4(c). Since the disk radius is fixed, the locally square commensuration dip in $M$ at $d = 1.85$ does not shift with changing $\phi_a$. For $\phi_a = 0.00212$, the system is in the single particle limit, there are no commensurate peaks or dips, and $M$ drops to zero for $d > 2.25$ when the obstacles form a percolating barrier to motion. For $\phi_a = 0.09$ and $0.17$, the triangular commensuration dip at $d = 1.0$ and the incommensuration peak at $d = 1.1$ found for larger $\phi_a$ are absent; however, there is a high density incommensuration peak at $d = 1.95$. When $\phi_a = 0.332$, the overall value of $M$ decreases and additional incommensuration peak forms at $d = 1.5$. Here, $M$ drops to zero for $d > 1.9$ when the system enters an active clogged state.

In Fig. 4(d) we plot the largest cluster size $C$ versus $d$ for the system in Fig. 4(c) with varied $\phi_a$. When $\phi_a = 0.00212$, $C$ remains small indicating the lack of any clustering in the single particle limit, while for $\phi_a = 0.09$ and $\phi_a = 0.18$, $C$ approaches $C = 1.0$ for $d > 2.25$ and has a peak at $d = 1.8$ corresponding to the formation of local square ordering in individual substrate plaquettes. At $\phi_a = 0.254$, there are three peaks in $C$ corresponding to the commensuration effects at $d = 1.0, 1.35$, and 1.85, as well as a dip produced by a frustrated state at $d = 1.1$. For $\phi_a = 0.332$, a clustered state appears for all values of $d$ which develops crystalline ordering at the three commensuration values of $d$.

Summary—We have examined run-and-tumble active matter disks interacting with a periodic obstacle array and find novel active matter commensuration and frustration effects. These arise when the active matter undergoes motility-induced phase separation into a dense crystalline phase which has a natural disk spacing. When this spacing is commensurate with the lattice constant of the obstacle array, a large crystalline phase separated state can appear, whereas for other obstacle spacings, the crystalline phase cannot fit on the substrate and we instead find a frustrated state in which the clusters are amorphous and not as large. The commensuration and incommensuration effects produce peaks and dips in the mobility, six-fold order, and cluster size as a function of changing obstacle diameter. The commensurate crystal states can have long range triangular ordering or local square ordering. At low activity or in the Brownian limit, the commensuration effects are lost.

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