Reversible to Irreversible Transitions for Cyclically Driven Particles on Periodic Obstacle Arrays

C. Reichhardt and C. J. O. Reichhardt

Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA

(*Electronic mail: cjrx@lanl.gov)

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We examine the collective dynamics of disks moving through a square array of obstacles under cyclic square wave driving. Below a critical density we find that system organizes into a reversible state in which the disks return to the same positions at the end of every drive cycle. Above this density, the dynamics are irreversible and the disks do not return to the same positions after each cycle. The critical density depends strongly on the angle $\theta$ between the driving direction and a symmetry axis of the obstacle array, with the highest critical densities appearing at commensurate angles such as $\theta = 0^\circ$ and $\theta = 45^\circ$ and the lowest critical densities falling at $\theta = \arctan(0.618)$, the inverse of the golden ratio, where the flow is the most frustrated. As the density increases, the number of cycles required to reach a reversible state grows as a power law with an exponent near $\nu = 1.36$, similar to what is found in periodically driven colloidal and superconducting vortex systems.

I. INTRODUCTION

The transition from reversible to irreversible dynamics was first studied in cyclically sheared dilute colloidal systems where the particles undergo only contact interactions with each other. For small shear amplitudes, the particles return to the same positions at the end of each shearing cycle, while for larger shear amplitudes or higher particle densities, the particles do not come back to the same positions but move irreversibly, with diffusion occurring both parallel and perpendicular to the shearing direction. Additional studies demonstrated that such systems are generally always in an irreversible state initially, but can organize to a reversible state after a number of cycles which diverges near the critical shear amplitude or density, suggesting that the reversible (R) to irresistible (IR) transition is an example of a nonequilibrium phase transition. For dilute particles, the transition to the reversible state is called random organization since the system forms a disordered configuration in which collisions between particles do not occur. In additional studies of periodically driven dilute colloidal particles, it was argued that these randomly organized states exhibit hyperuniformity. Transitions to irreversible states have also been studied in other periodically driven systems including granular matter and amorphous solids, where the particles are always in contact and the transition occurs for a critical shear amplitude. Such systems can also display reversibility spanning multiple cycles, as well as a variety of memory effects.

In another class of systems of collectively interacting particles that is cyclically driven over quenched disorder, such as vortices in type-II superconductors, magnetic skyrmions, and colloidal particles, the drive is applied uniformly to all the particles, and in the absence of quenched disorder, the assembly moves back and forth uniformly in a reversible manner. When quenched disorder is present, however, plastic deformations can occur that permit particles to move relative to one another from cycle to cycle. In vortex systems, studies of R-IR transitions in simulation and experiment, show that diverging time scales appear near critical drive amplitudes and critical densities with critical exponents similar to those observed in the dilute colloidal systems. Stoop et al. applied backward and forward pulse driving to hard sphere colloids moving over random obstacle arrays and obtained a variety of different dynamical phases as a function of obstacle density. R-IR transitions can also occur for particles moving over a periodic array of obstacles or a periodic substrate. The dynamics of particles coupled to periodic substrates has been explored for superconducting vortices, magnetic skyrmions, and colloidal systems. A key aspect of systems with periodic substrates is that the dynamics depend strongly on the direction $\theta$ of drive relative to a substrate symmetry direction. For example, in a square obstacle array, at $\theta = 0^\circ$ the particles can flow easily between the obstacles without collisions. Similarly, other drive angles such as $\theta = 45^\circ$ and $\theta = 90^\circ$ are also aligned with easy flow direction. At incommensurate angles, particles cannot easily travel in a straight line without encountering an obstacle, and the flow is more disordered. As the direction of a dc drive is changed relative to the substrate, a series of directional or symmetry locking effects appear in which the particle motion becomes locked to certain symmetry directions of the substrate even when the drive is not aligned precisely along those directions. This directional locking effect has been studied as a method for particle separation and in the context of transitions from ordered to disordered flow. In previous work on dc driven disks moving though square obstacle arrays, it was shown that the system is susceptible to jamming for flow along certain non-symmetry angles. Particles cyclically driven over a periodic substrate array provide a convenient system in which to study reversible to irreversible transitions since the effective frustration of the array can be tuned simply by changing the orientation of the drive relative to the symmetry directions of the array. In this work we examine a monodisperse assembly of disks interacting with a square obstacle array under periodic square wave
driving. When the drive is applied along $\theta = 0^\circ$ or $\theta = 45^\circ$, the system readily organizes to a reversible pattern forming state in which the particles return to the same positions after each drive cycle. For driving at incommensurate angles with a fixed drive amplitude, we find that there is a critical disk density above which an irreversible state forms that exhibits diffusive dynamics. Below this density, the number of cycles required to reach a reversible state varies with density as as a power law with the same exponents found for periodically sheared colloidal particles and driven superconducting vortex systems. In general we find that the disks form a disordered or fluid like state under irreversible flow, while a pattern forming or ordered configuration appears when the system reaches a reversible state. The critical density for the R-IR transition is nonmonotonic as a function of $\theta$, reaching maximum values for commensurate driving angles and showing a global minimum near the arctangent of the inverse of the golden ratio. Our results could be tested in a variety of systems such as colloidal particles, superconducting vortices, or magnetic skyrmions under periodic driving coupled to a periodic array of obstacles or a periodic substrate.

II. SIMULATION

We consider a two dimensional system of size $L \times L$ containing a square array of $N_{\text{obs}} = 81$ circular obstacles of lattice spacing $a$ and radius $r_{\text{obs}}$. We impose periodic boundary conditions in the $x$ and $y$-directions and place $N_d$ monodisperse repulsive disks in the sample. The dynamics of disk $i$ is governed by the following overdamped equation of motion:

$$\alpha_d \dot{\mathbf{v}}_i = \mathbf{F}^{dd}_i + \mathbf{F}^{obs}_i + \mathbf{F}^D.$$  

(1)

The velocity of the disk at position $\mathbf{r}_i$ is $\mathbf{v}_i = d\mathbf{r}_i/dt$ and we set the damping constant $\alpha_d$ to unity. The first term on the right is the disk-disk interaction force $\mathbf{F}^{dd}_i$ represented by a short-range harmonic repulsive potential with radius $r_d$. In this work we fix $r_d = 0.55$. The disk-obstacle force $\mathbf{F}^{obs}_i$ is also modeled as a repulsive harmonic interaction. In our work we choose harmonic spring constants that are large enough to prevent the overlap between disks from becoming larger than one percent for the densities and driving forces we consider.

The density $\phi$ is defined to be the area covered by the obstacles and mobile disks, $\phi = N_{\text{obs}} \pi r_{\text{obs}}^2 / L^2 + N_d \pi r_d^2 / L^2$. The square wave driving force remains constant for a fixed period of time in the forward direction prior to reversing, and has the form $\mathbf{F}_D = A \cos(\theta) \hat{x} + A \sin(\theta) \hat{y}$, where $A$ is the drive amplitude and $\theta$ is the direction of the drive relative to the $x$-axis of the periodic array. This model was previously employed to study locking and clogging effects for dc driven disk systems. We fix the duration of the drive to $T/2 = 2 \times 10^5$ simulation time steps spent on each half cycle, and we vary the density $\phi$ and the drive amplitude $A$. We can characterize the system by measuring the change in the position of the disks from one cycle to the next, $R(n) = \sum_{i=1}^{N_d} \left[ \mathbf{r}_i(t_0 + nT) - \mathbf{r}_i(t_0 + (n-1)T) \right]$, where $t_0$ is an initial reference time. If the motion is reversible, $R_n = 0$. We also measure the total net displacement $d(n)$ as a function of cycle $n$, $d(n) = \sum_{i=1}^{N_d} [\mathbf{r}_i(t_0 + nT) - \mathbf{r}_i(t_0)]$. In an irreversible state, $d(n)$ grows continuously, while for a reversible state, $d(n)$ saturates to a finite value.

III. RESULTS

In Fig. 1(a) we show a snapshot of the obstacle locations and mobile disks for a system with $r_{\text{obs}} = 1.0$, $A = 0.031623$ and a driving angle of $\theta = 18.435^\circ$ for $N_d = 269$, giving an overall system density of $\phi = 0.3962$. Even after 1500 ac drive cycles, the system remains in an irreversible or fluctuating state. When the number of mobile disks is reduced to $N_d = 239$, giving $\phi = 0.3716$, the system organizes into a reversible state with an ordered structure, as illustrated in Fig. 1(b).

In Fig. 2(a) we plot $R_n$ versus cycle number $n$ for the system in Fig. 1 for increasing total densities of $\phi = 0.335, 0.3496, 0.3569, 0.36427, 0.36867, 0.3716, 0.3789, 0.3862, \text{ and } 0.3962$. For $\phi < 0.3789$, $R_n$ goes to zero, indicating that after an initial transient of some length, the disks return to the same positions after every driving cycle and the system behaves reversibly. As $\phi$ increases, the number of cycles $\tau$ required to reach a reversible state also increases. For example, at $\phi = 0.3716$ it takes $\tau = 1360$ cycles to reach the reversible state illustrated in Fig. 1(b), while at lower densities such as $\phi = 0.335, \tau = 12$. Figure 2(b) shows the corresponding $d$ versus $n$. For $\phi > 0.3962$, $d$ continues to grow as a function of time, while below this density it saturates to a finite value. The dashed line indicates a fit to $d \sim n^{1/2}$. Since $n$ also corresponds to an elapsed time, this implies that the displacements are growing as $n^{1/2}$ and thus have Brownian characteristics, similar to the behavior of the displacement found in the irreversible states of sheared colloidal systems.

In Fig. 3 we plot the trajectories of the disks from the system in Fig. 2 to illustrate more clearly the difference between the irreversible and reversible dynamics. Figure 3(a) shows that the trajectories in the irreversible state at $\phi = 0.3962$ fill space, and the disks are translating in both the $x$ and $y$ directions. In Fig. 3(b), the reversible state at $\phi = 0.3496$ contains
much more ordered trajectories and the motion is always confined between rows of obstacles with no hopping from row to row. If the trajectory plot in the reversible state is extended over a larger number of cycles, exactly the same same trajectory pattern appears.

In Fig. 4 we plot the the number of cycles $\tau$ required to reach the reversible state as a function of $\phi - \phi_c$, where we have assumed a critical density of $\phi_c = 0.3726$, for the system from Fig. 2 with $r_{obs} = 1.0$, $A = 0.031623$, and $\theta = 18.435^\circ$. The line is a fit to $\tau = (\phi - \phi_c)^{-\nu}$ with $\nu = 1.36$.

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FIG. 2. (a) $R_n$ versus cycle number $n$ for the system in Fig. 1 with $r_{obs} = 1.0$ for increasing total density $\phi = 0.335, 0.3496, 0.3569, 0.36427, 0.36867, 0.3716, 0.3789, 0.3862,$ and $0.3962$, from top to bottom. Here $A = 0.031623$ and $\theta = 18.435^\circ$. For $\phi < 0.3789$, $R_n$ goes to zero, indicating the system has reached a reversible state. (b) The corresponding $d$ versus $n$. For $\phi > 0.3962$, $d$ grows continuously, while at densities smaller than this, $d$ saturates to a finite value. The dashed line is a fit to $d \propto n^{1/2}$.

FIG. 3. Obstacle locations (red), mobile disks (blue), and mobile disk trajectories (brown) in a portion of the sample for the system in Fig. 2 with $r_{obs} = 1.0$, $A = 0.031623$, and $\theta = 18.435^\circ$. (a) An irreversible state at $\phi = 0.3962$, where the trajectories gradually fill all of space and the disks undergo long time diffusion. (b) A reversible state at $\phi = 0.3496$, where the disks repeatedly follow the same path and the motion is confined between the rows of obstacles.

FIG. 4. The number of cycles $\tau$ required to reach the reversible state versus $\phi - \phi_c$, where we have assumed a critical density of $\phi_c = 0.3726$, for the system from Fig. 2 with $r_{obs} = 1.0$, $A = 0.031623$, and $\theta = 18.435^\circ$. The line is a fit to $\tau = (\phi - \phi_c)^{-\nu}$ with $\nu = 1.36$.

FIG. 5. $R_n$ versus $n$ for the system in Fig. 2 with $r_{obs} = 1.0$ and $A = 0.031623$ but for driving along $\theta = 45^\circ$ or a commensurate angle. The total density is $\phi = 0.5124, 0.5183, 0.53295, 0.5402, 0.54319, 0.5446, 0.54612,$ and $0.56225$, from bottom to top. (b) The corresponding $\tau$ versus $\phi - \phi_c$ where we assume a critical density of $\phi_c = 0.54612$. The line is a fit to $\tau = (\phi - \phi_c)^{-\nu}$ with $\nu = 1.38$.

tems showed a similar divergence in the time to reach the reversible state with $\nu = 1.33_2$, while studies of superconducting vortices driven over random disorder gave exponents of $\nu = 1.38$ for critical drive amplitudes and $\nu = 1.32$ for critical densities. These exponents are close to those expected for 2D directed percolation, where $\nu = 1.295_{48}$.

The images in Fig. 3 clarify why the R-IR transition is connected to percolation. In a reversible state, the trajectories do not simultaneously percolate in both the $x$ and $y$ directions, while in an irreversible state, the trajectories are mixing. The percolation transition could be considered to occur at the point where the trajectories just begin to overlap in both the $x$ and $y$ directions.

We next consider the R-IR transition for driving at commensurate angles. In Fig. 5 we plot $R_n$ vs $n$ for the same system in Fig. 2 but at a driving angle of $\theta = 45^\circ$ for total
chains form that are aligned with the driving direction of $\phi = 45^\circ$. (b) An irreversible state at $\phi = 0.6$ where the configuration is disordered.

FIG. 7. Phase diagram as a function of total density $\phi$ versus driving angle $\theta$ showing regions where the system organizes to a reversible state (blue) or an irreversible state (orange) for the system in Fig. 2 with $r_{\text{obs}} = 1.0$ and $A = 0.031623$. Circles indicate the transition density $\phi_c$. The reversible region reaches maximum extents at $\theta = 0^\circ$, $\theta = 45^\circ$, and $\theta = 26.5^\circ = \arctan(1/2)$. The minimum width of the reversible region falls near $\theta = 31.0^\circ$ or close to $\theta = \arctan(0.618)$ where 0.618 is the inverse of the golden ratio.

FIG. 8. Snapshots of the obstacle locations (red) and mobile disks (blue) in a portion of the sample from Fig. 7 with $r_{\text{obs}} = 1.0$ and $A = 0.031623$. (a) A reversible state at $\theta = 0^\circ$ and $\phi = 0.577$, where the system forms a pattern of chains aligned along the $x$ direction. (b) A reversible state at $\theta = \arctan(1/2) = 26.5^\circ$ for $\phi = 0.4302$, where the repeating pattern is disordered.

densities of $\phi = 0.5124$ to 0.56225. When $\phi < 0.5446$, the system organizes to a reversible state in a time $\tau$ that grows with increasing $\phi$. In Fig. 4(b) we plot $\tau$ versus $\phi - \phi_c$ for a critical density of $\phi_c = 0.54612$, as well as a line indicating a fit to $\tau = (\phi - \phi_c)^{-\nu}$ with $\nu = 1.38$. This result indicates that the R-IR transition shown in Fig. 3 persists for driving along $\theta = 45^\circ$; however, the critical density $\phi_c$ is higher. In Fig. 6 we illustrate the disk configurations above and below the critical R-IR transition density. Figure 7(a) shows a reversible state at $\phi = 0.5036$ where the disks form ordered one-dimensional (1D) chains aligned with the drive along $\theta = 45^\circ$. In Fig. 8(b), the same system at $\phi = 0.577$ is in a irreversible state where the disk positions are disordered.

By conducting a series of simulations for fixed driving amplitude $A = 0.031623$ and varied $\theta$, we explore the dependence of $\phi_c$ on the driving angle $\theta$. We plot the reversible and irreversible regions as a function of $\phi$ versus $\theta$ in Fig. 7. Note that for symmetry reasons, the pattern shown in Fig. 7 repeats in an inverted fashion over the range $\theta = 45^\circ$ to $\theta = 90^\circ$. At $\theta = 0^\circ$, the system remains in a reversible state up to the largest values of $\phi$ we consider, $\phi = 0.61$. For larger densities, jamming effects become important and we would need to switch to a different disk initialization algorithm. It may be possible that additional R-IR transitions occur at higher disk densities when jammed states begin to appear; however, this is beyond the scope of the present work. For $0 < \theta < 7.5^\circ$, we find that the R-IR transition occurs near a critical density $\phi_c = 0.575$. There is a peak in $\phi_c$ near $\theta = 26.565^\circ$, which corresponds to a commensurate angle of $\theta = \arctan(1/2)$. When the driving angle is close to lattice symmetry directions such as 0, 1/2, or 1/1, which correspond to $\theta = 0^\circ$, 26.5$^\circ$, and 45$^\circ$, respectively, $\phi_c$ reaches its highest values. Under these commensurate angles, the disks can move easily along straight lines while avoiding collisions with the obstacles. There is no noticeable peak in $\phi_c$ at $\theta = \arctan(1/3)$ or $\theta = \arctan(2/3)$, and the disk dynamics for these driving angles are similar to what is found at incommensurate driving angles. A minimum in $\phi_c$ occurs near $\theta = 31^\circ$ or close to $\theta = \arctan(0.618)$, where 0.618 is the inverse of the golden ratio from the Fibonacci sequence. The incommensuration is maximized at the inverse golden ratio where the driven disk collides with the largest possible number of obstacles while moving through the system. The variations in the extent of the reversible regions should also depend on the radius $r_d$ of the mobile disk. If a smaller disk were used, other possible commensuration effects could appear depending on how many rows of mobile particles can fit along 45$^\circ$ or other commensurate angles.

In Fig. 8(a) we illustrate the disk positions in a reversible state at $\theta = 0^\circ$ and $\phi = 0.577$, where the disks form two nearly filled rows moving in the $x$ direction. We note that not all of the reversible states are associated with ordered disk arrangements. For example, at $\theta = \arctan(1/2)$, where a peak in $\phi_c$ appears in Fig. 7, the system forms the disordered but repeatable pattern shown in Fig. 8(b) for $\phi = 0.4302$ in the reversible
Irreversible state appears only for large values of $\phi$. Here, when $r_{\text{obs}} = 1.0$, $\phi = 0.041$. There is a reentrant R-IR transition as a function of $r_{\text{obs}}$ for all but the lowest values of $A$.

Up to this point we have concentrated on samples with $r_{\text{obs}} = 1.0$, but there can be a reentrant R-IR transition as $r_{\text{obs}}$ is varied. In a system with $\theta = 7.5^\circ$, Fig. 7 indicates that an irreversible state appears only for large values of $\phi$. In this case, a transition occurs from 1D reversible motion of disks along the $x$ direction to 2D irreversible motion. If we reduce $r_{\text{obs}}$, the transition to irreversible motion shifts to lower $\phi$ because the disks can more readily move in two dimensions instead of remaining locked in a 1D channel. If, however, $r_{\text{obs}}$ is reduced even further, collisions with the obstacles become less frequent and the system can once again organize into a reversible state. This is illustrated in Fig. 9, where we plot the locations of the reversible and irreversible regimes as a function of $r_{\text{obs}}$ versus $A$ for a system with $N_R = 279$ at $\theta = 7.5^\circ$. Here, when $r_{\text{obs}} = 2.0$, $\phi = 0.401$. For large $r_{\text{obs}} > 0.9$, the system is always in a reversible state regardless of the value of $A$, and the disks form 1D chains. Furthermore, for $A < 0.04$ the system is always in a reversible state since the disks do not move far enough during a single drive cycle to collide with the obstacles. When $A > 0.04$ and $0.4 < r_{\text{obs}} < 0.9$, irreversible behavior appears, while for $r_{\text{obs}} < 0.4$, there is a reversible state in which the disks are moving. The result is the appearance of a reentrant R-IR transition as a function of $r_{\text{obs}}$ for all but the smallest values of $A$. Similar reentrant transitions should occur near commensurate driving angles such as $\theta = 45^\circ$. In contrast, for incommensurate angles the system will remain in an irreversible state down to much smaller $r_{\text{obs}}$ since even relatively small moving disks continue to collide with the obstacles due to the driving direction. The existence of reentrance will also depend on the mobile disk density since for low mobile disk densities the system will generally be able to organize into a reversible state.

We can also observe a R-IR transition at fixed $\phi$ under increasing $A$, as illustrated in Fig. 10 for a system with $\phi = 0.549$ and $\theta = 45^\circ$. When $A = 0.03162$, this system is in an irreversible state. In Fig. 10(a) we plot $R_n$ versus $n$ for $A = 0.02846, 0.02767, 0.0268, 0.025247, 0.0253, 0.02435$, and 0.022136. The system organizes to a reversible state when $A < 0.02846$, and the number of cycles $\tau$ needed to reach the reversible state decreases with decreasing $A$. In Fig. 10(b) we plot $\tau$ versus $A - A_c$ where $A_c = 0.0285$. The line is a fit to $\tau = |A - A_c|^{-\nu}$ with $\nu = 1.4$.

IV. SUMMARY

We have numerically examined the reversible to irreversible transition for periodically driven disks moving through a two-dimensional square periodic obstacle array. For fixed ac drive amplitude, we find that there is a critical density at which the system is able to organize into a reversible state instead of remaining in an irreversible state. The number of cycles required to reach the reversible state diverges as a power law with an exponent $\nu \approx 1.36$. This is close to the value of $\nu$ observed for periodically sheared colloidal particles and periodically driven superconducting vortices, suggesting that the reversible-irreversible transitions of all of these systems fall into the same universality class. The critical density at which the transition occurs is non-monotonic as a function of the angle between the applied drive and a symmetry direction of the obstacle array. The highest critical densities appear for commensurate driving angles such as $\theta = 0^\circ$ and $\theta = 45^\circ$. We find the same power law exponents for both incommensurate and commensurate angles. We obtain the lowest critical density for $\theta = \arctan(0.618)$, which is the inverse of the golden ratio. This frustrated driving direction produces the highest
frequency of collisions between disks and obstacles.

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DATA AVAILABILITY STATEMENT

Data available on request from the authors.

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