Molecular dynamics simulation of synchronization in driven particles

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Abstract

We study synchronization of interacting particles driven by an externally applied force while confined to a narrow channel. With numerical simulations, we control the particle interactions, external force and particle environment in order to mimick experimental studies of driven colloidal particles confined by light-fields. We use molecular dynamics simulations to model the particle dynamics, using overdamped equations of motion suitable for a viscous suspension of microscopic particles. We study particle synchronization under a variety of conditions, including static and dynamic patterns formed on periodic and quasiperiod substrates, kink propagation on these surfaces, and the limits of applied force that cause the particles to transition to chaotic behavior. We demonstrate the transition from trapped to sliding dynamics in quasiperiodic landscapes differs from that of a periodic landscape by [TBD], and that kinks of high density propagate [more/less ?] when [what?]. We include sample code and opportunties for students to reproduce our results and propose new numerical experiments.

I. INTRODUCTION

Synchronization is one of the most diverse fundamental physical phenomena. Synchronization has been studied for over three centuries, from Huygens pendulum clocks to the rhythmic beats of the flapping wings in a flock of birds. It is a goal of physicists to discover synchronization in different forms and learn how to control the phenomenon that occurs when weakly coupled competing oscillators adjust rhythms to match each other. A synchronization phenomenon that the physics community is particularly interested in is dynamic phase locking, which occurs when naturally oscillating motions are driven by an external modulation[1]. Another interest of ours is to study the transition from ordered, synchronized dynamics, to disordered, chaotic dynamics. Chaotic dynamics is the irregular, unpredictable time evolution of nonlinear systems and occurs in mechanical oscillators[?] . Here, we analyze the microscopic dynamics of phase locking in a colloidal model system using molecular dynamics (MD).

II. MOLECULAR DYNAMICS MODEL

The simulations use overdamped dynamics with Euler's method in a classical two-dimensional model for particles confined to a periodic potential. With only a few particles in two-dimensions, the simulation runs quickly, making this an appropriate model for undergraduates to explore.

Particles interact by the Yukawa potential.

A single particle has the equation of motion

$$\eta\vec{v_i} = \vec{F}_{landscape,i} + \textstyle\sum_j \vec{F}_{ij} + \vec{F}_{Drive}(t).$$

This includes the force of the landscape, inter-particle interactions $\vec{F}_{ij} = -\nabla V(\vec{r}_{ij})$, and a driving force $\vec{F}_{Drive}(t) = [F_{DC} + F_{AC}\sin(\omega t)]\hat{y}$, where $\omega = 2\pi f$. The landscape is a sine function that is position dependent and calculate the landscape force on the particle directly from its location. The driving force does add energy into the system, and some of it is lost. The damping comes from the viscous fluid providing a nonconservative force.

Overdamped dynamics is a common assumption in models of colloid particles. This is an assumption that the suspending fluid is highly viscous and exerts a damping force on the particles equivalent to a linear drag force $F_{drag} = -\eta v$ and the acceleration of the particle is zero. The equation of motion we include makes both assumptions and is rearranged to reflect that. The equation of motion is not integrated for the velocity, instead it provides a direct calculation of the velocity.

In this model the Verlet method is equivalent to the Euler method. Euler's method is then used to calculate the position. Most undergraduate students learn the Euler method in Computational Physics and Differential Equations, but don't encounter the Verlet method. It is a nice opportunity to teach an extension of a method they know.

III. MD SIMULATIONS

A. Single particle system

We used our model to generate a system, Fig. 1a), where the particle hops between troughs in the energy landscape. In the attached movie, Figure1.mp4, we apply a constant F_{AC} with frequency f then slowly increase F_{DC} to achieve a variety of modes. A mode is a periodic pattern of hops with a constant average particle velocity, $\bar{v}_y$ over a range of driving forces F_{DC}. In the velocity-force plot in Fig. 1b) $\bar{v}_y$ is increasing non-uniformly, with steps, indicating mode locking. A related experiment[1] revealed the microscopic dynamics of mode locking by driving colloids across a periodic landscape generated by optical tweezers.

B. Multi-particle system

We also simulated a twenty particle system confined to a narrow channel, as shown in Fig. 2a). The interparticle forces of neighboring particles cause the system to form a buckled chain when the system is annealed. When a single particle is driven, the neighboring particles act similarly to a periodic landscape to impede its motion. A driven particle can exhibit mode locking with a well-chosen AC drive and frequency. In the attached movie, Figure2.mp4, we show the complex dynamics of mode locking, where the driven particle leap-frogs past the other particles.

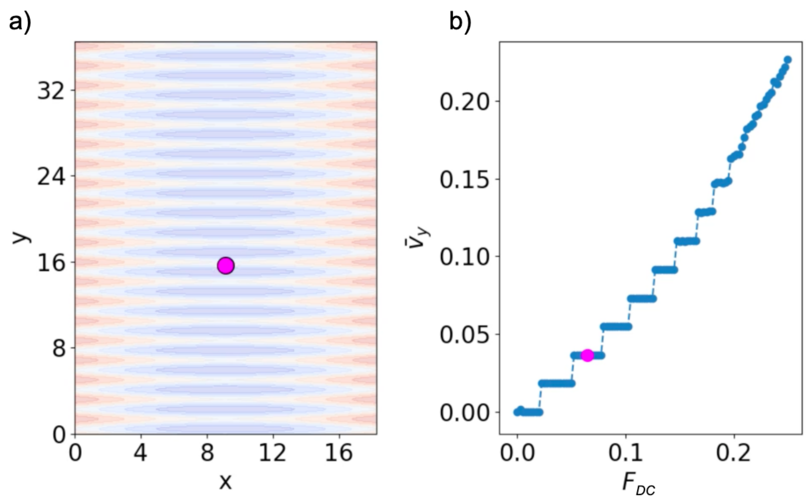

FIG. 1: **(a)** The particle is driven with a constant F_{AC} and f through a periodic potential landscape where blue are minima and red are maxima in the potential. **(b)** An average particle velocity in the y-direction $\bar{v}_y$ as a function of the driving force F_{DC}. In the animation the magenta dot represents the $\bar{v}_y$ at which the particle in Fig. 1a) is moving.

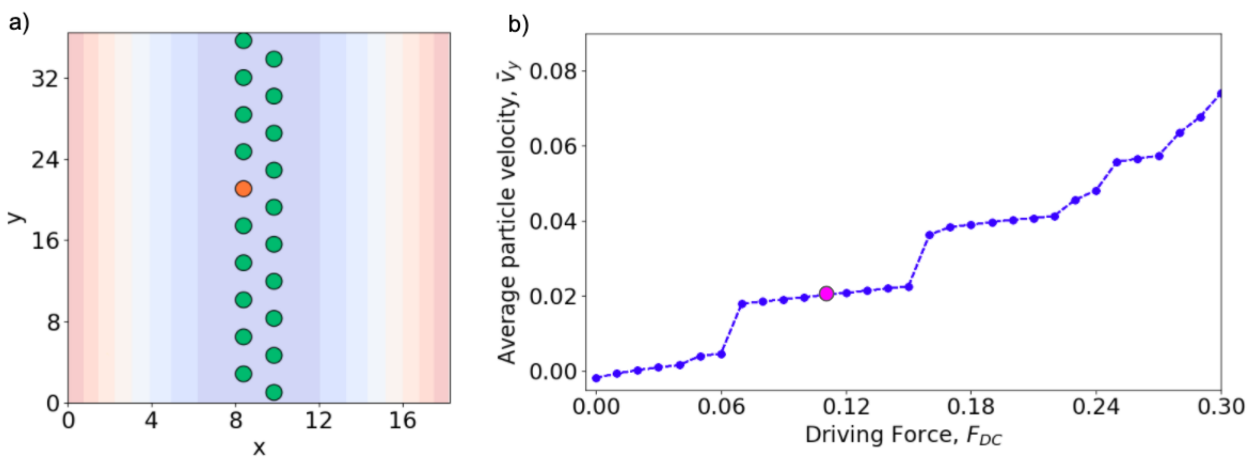

FIG. 2: **(a)** The orange particle is driven with a constant F_{AC} and f through 19 particles, colored green, confined by a quasi one-dimensional channel. The landscape is colored as in Fig. 1. **(b)** $\bar{v}_y$ versus F_{DC}, where $\bar{v}_y$ is the average particle velocity of the driven particle in the y-direction.

C. Kinked system

IV. QUASIPERIODIC SUBSTRATE

V. ASSOCIATED PROBLEMS

VI. CONCLUSION

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