Molecular dynamics simulation of synchronization in driven particles

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Abstract

We study synchronization of interacting particles confined to a narrow channel driven by an externally applied force. Using 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. The molecular dynamics simulations model the particle dynamics using overdamped equations of motion suitable for a viscous suspension of microscopic particles. We observe particle synchronization under a variety of conditions, including static and dynamic patterns formed on periodic and quasiperiod substrates and the propagation of high density kinks. 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 also explore the limits of applied force that cause the dynamics to transition to chaotic behavior. We include sample code and exercises for students that include opportunties to reproduce our results and propose new numerical experiments. With only a few particles in two-dimensions, the simulation runs quickly, making this an appropriate model for undergraduates to explore.

I. INTRODUCTION

Numerical simulations of confined, driven particles can be used to model a variety of physical phenomena. Particles which interact over long distances include colloids, magnetic beads, superconducting vortices, dusty plasmas, electron gases. [more detail and references] Particles which interact over short distances include bubble arrays/emulsions [more systems and references].

Synchronization is a universal phenomena. Christiaan Huygens is credited with its discovery with his 1665 observation of in-phase oscillation of pendulum clocks[?] . Huygens explanation that the clocks vibrations are coupled through the supporting wall has since been rigorously demonstrated by 20th century researchers[?] . Examples of synchronization occur in many naturally oscillating systems, from fireflies syncing with a pulsed LED, to simultaneous flapping of birds wings, to neuronal firing cardiac muscle and brain tissue.

Dynamical mode locking is a controlled synchronization phenomena in which an external driving force causes the syncing of natural oscillation frequencies in weakly coupled oscillators. Mode locking is often observed in quantum electronic devices such as Josephson junctions and phase-locked loops. Instead of ohmic current-voltage (IV) relationships, such devices exhibit stepped regions such as Shapiro steps [explain].

Recently studies of colloidal particles confined in optical traps have been used to examine the microscopic dynamics of mode-locking when subject to external driving force[1].

Particles in confined geometries behave differently than free particles. Stabilized charged particles form patterns due to the interplay of the confining environment and particle interactions. Narrow channels studies are useful to provide insights of how particles move through systems such as wires and microchannels. Biological systems such as neuron axons and capillaries can also be studied with these models [more detail and references]. Many such systems execute local oscillations about stable points [elaborate]. An applied external force increases the diversity of behaviors, and can cause particles to flow in a variety of non-linear complex behaviors including synchronized, aperiod, or chaotic dynamical patterns. The presence of a modulating surface can modify these patterns in a variety of ways, changing the onset of dynamical flows, and the overall flow patterns.

Colloidal particles trapped in light fields have proven a particularly useful medium for studying these behaviors. The relatively large size of the colloids and ease in control has lead to a rich array of experimental results. Such studies are considered model systems for experimental systems relatively hard to access and visualize, such as cold atoms or electron gases.

Acoustic tweezers and surface acoustic wave (SAW)

Disordered chaotic dynamics are also possible, where irregular, unpredictable time evolution of nonlinear systems and occurs in mechanical oscillators[?] .

In the following paper we describe our molecular dynamics model in Section II. We include code to simulate and visualize the dynamics in this section and supplementary material. In Section III we summarize our results, including synchronized motion of a single confined particle driven across a periodic landscape in Section III A and multiple interacting particles in Section III B, including stationary propagation of high density kinks in Sec. III C. We present these results using standard tools of non-linear oscillators such phase diagrams of particle velocity versus position. In Section IV, we show how an aperiodic landscape modifies the particle dynamics. Finally we explore the transition to chaotic dynamics in Section V and conclude in Section VII. In each section we suggest exercises for interested students, and summarize our suggestions in Section VI.

II. MOLECULAR DYNAMICS MODEL

We use a classical two-dimensional model for studying the dynamics of N interacting particles. Particles are confined in a two-dimensional (2D) simulation of area $A = L \times L$ where $L = 36.5$. An individual particle i has position $\vec{r}_i = x_i\hat{x} + y_i\hat{y}$. Particles are subject to periodic boundary conditions such that a particle leaving the edges of the system is mapped back to a position within the simulation by the rules $x_i + L = x_i$ and $y_i + L = y_i$.

Particles are subject an external time-dependent driving force $\vec{F}_D(t)$ applied parallel to the y-direction. We model this force as

$$\vec{F}_D(t) = [F_{DC} + F_{AC}\sin(\omega t)]\hat{y}, \tag{1}$$

with modifiable parameters including a constant component F_{DC}, and a time dependent component with amplitude F_{AC} and frequency $\omega = 2\pi f$. The frequency is scaled in time units, where [finish]. We demonstrate how a single particle (Sec. III A) and many particles move (Sec. III B) in response to this applied force in a variety of light fields. In Sec. III C we set F_{DC} to zero and track the motion of a high density area of a particle chain (i.e. kink dynamics).

We create several model light fields, creating a landscape of potential minima and maxima that modify the local force on a particle as a function of position $\vec{F}_{l,i} = \vec{F}_l(\vec{r}_i)$. The landscape potential $V(\vec{r})$ are static, generating a conservative force $\vec{F}_l = -\nabla V_l(\vec{r})$ with fixed minima and maxima that are periodic or quasi-periodic, as described in Sec. III. One example of a periodic light field is where

$$V_l(y) = V_0 \cos\left(N_p \pi y/L\right) \tag{2}$$

where N_p are the number of troughs in the landscape, and V_0 is an adjustable parameter to set the depth of the troughs.

In multi-particle simulations, we confine the particles along the $x-$direction with a quasi-one-dimensional geometry using a periodic function.

$$V_{q1D}(x) = V_0 \cos\left(\pi x/L\right) \tag{3}$$

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We model particle interactions with the Yukawa potential $\vec{F}_{ij} = -\nabla V_{ij}(r_{ij})$,

$$V_{ij}(r_{ij}) = \frac{E_0}{r_{ij}} e^{-\kappa r_{ij}}, \tag{4}$$

where $r_{ij} = |\vec{r}_i - \vec{r}_j|$. This is a screened Coulomb potential $E_0 = 2$ scales strength of repulsion where $E_0 = kq_1q_2$ [CHECK scaling/units]. $\kappa = 1/R_0$ is the screening parameter that accounts for the lengthscale at which many particle interactions and local environment that reduces the interaction range of individual particles. We fix R_0 to be unity in our simulation units.

The simulation is controlled by a $for()$ loop which runs from an intial to maximum *time* integer. Each time step represents a simulation time of $\Delta t = 0.001$. At each timestep we evaluate the net force on each particle as a function of its position $\vec{r}_i(t)$ and then use the equation of motion to move particles to an updated position $\vec{r}_i(t + \Delta t)$. We model the particle dynamics with an overdamped equation of motion integrated with the Verlet method. Here the suspending fluid is highly viscous and exerts a damping force on the particles equivalent to a linear drag force. The damping comes from a viscous fluid model providing a nonconservative force, modeled as a linear friction $\vec{F}_{drag} = -\eta \vec{v}_i$ sufficient so that the acceleration of the particle is zero. Such a model is appropriate when the particles are small and the viscosity is high [finish... reference...]

A single particle has the equation of motion

$$\eta \vec{v}_i = \vec{F}_{l,i} + \sum_{i \neq j}^{N} \vec{F}_{ij} + \vec{F}_D(t). \tag{5}$$

where $\eta = 1$. The equation of motion provides a direct calculation of the velocity of an individual particle from its location. Since we model the acceleration $\vec{a}$ as zero, the Verlet method simplifies to the Euler method, which is used to calculate the position at subsequent time steps.

$$\vec{r}_i(t + \Delta t) = \vec{v}_i(t)\Delta t + \vec{r}_i(t). \tag{6}$$

III. RESULTS

A. Single particle system

We place a single particle in a periodic landscape with corrugations along the y-direction

$$V_l(y) = V_{0y} \cos\left(N_p \pi y / L\right) \tag{7}$$

where $N_p = 20$ are the number of troughs in the landscape, and $V_{0x} = 2$ and $V_{0x} = 2$. This is illustrated in Fig. 1(a) where the red regions show local maxima and the blue local minima. The code for generating a two dimensional colored plot of the potential landscape is calculated by evaluating the analytic function in Eq. 7 for a grid of values (x_n, y_n).

We apply an external applied force, with a constant F_{AC} with frequency $\omega = 2\pi f$ then slowly increase F_{DC}. The particle hops between troughs in the energy landscape when the superposition of F_{AC} and F_{DC} is large enough to overcome the barrier height. By modifying F_{DC} we achieve a variety of oscillation 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}. We illustrate mode-locking in the velocity-force plot in Fig. 1(b). Here $\bar{v}_y$ is increasing in non-uniform steps, with a quantized height of $\bar{v}_y = n\lambda f$, where n is an integer, $\lambda = S_Y/N_p = 36.5/20 = 1.825$ is the spatial period, or wavelength of the landscape, and $f = 0.01$ cycles per time unit.

Our simulations reproduce results presented in Juniper *et al.*[1] which demonstrated mode locking in experiments of driven colloids on a optical periodic landscape.

We illustrate the hopping pattern in Fig. 1(c) and show the dynamics in supplementary materials[2].

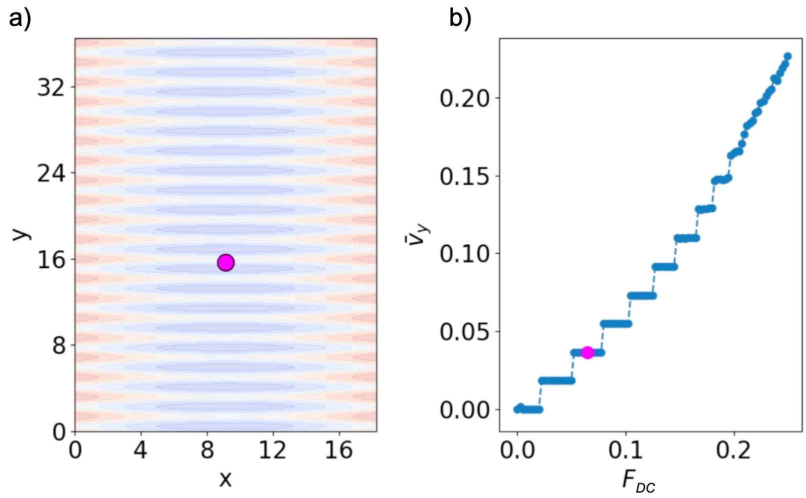

FIG. 1: **(a)** The particle is driven with a constant amplitude F_{AC} and frequency ω through a periodic spatial potential landscape. The landscape is represented with a colormap where blue are minima and red are maxima in the potential. **(b)** An average particle velocity in the y-direction $\bar{v}_y$ as a function of a constant driving force F_{DC}. In the animation available in Ref.[2] the magenta dot represents the average velocity of the particle $\bar{v}_y$ at which the particle in Fig. 1(a) is moving.

B. Synchronization in multi-particle systems

We simulated a twenty particle system confined to a narrow channel, as shown in Fig. 2a). We create the confining channel with a sinusoidal function with a single period.

$$V_l(x) = V_{0x} \cos(\pi x/L) \tag{8}$$

where the trough heights is larger V_{0x}, and the associated force

$$\vec{F} = -\nabla V(x) = -\frac{dV}{dx}\hat{x} = -\frac{V_{0x}\pi}{L}\sin(\pi x/L)\hat{x} \tag{9}$$

restores particles to the center of a long narrow region of the simulation. The landscape is illustrated in Fig. 2(a) where red regions are high potential and blue regions are low potential.

The initial configuration of the system is shown in Fig. 2(a). We annealed the system into a ground-state configuration by raising the system to a high temperature T, and slowly lowering the temperature in steps of $dT = -0.01$ until the particles form a buckled chain in the low region of the channel due to the competition between particle repulsion and channel confinement. The interparticle forces between neighboring particles cause the system to form a buckled chain. The molecular dynamics of simulated annealing is described in Ref. **??**, and presented simulations begin with particle configurations that result from the annealing process, as listed in Appendix [ref] and available in supplementary material.

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.

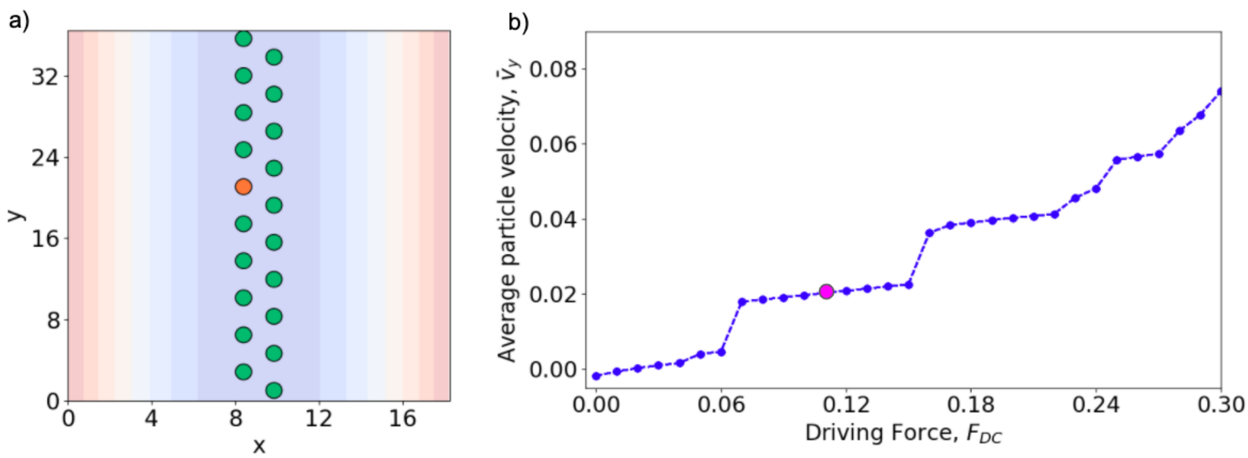

FIG. 2: **(a)** The orange particle is driven with a constant F_{AC} and f through 19 particles, colored green, confined by a quasi one-dimensional channel. The landscape is colored as in Fig. 1. **(b)** $\bar{v}_y$ versus F_{DC}, where $\bar{v}_y$ is the average particle velocity of the driven particle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

C. Kinked system

We confine N particles to $N-1$ troughs to create a local high density region. $F_{DC}/F_{AC} = 1$ [CHECK!]

IV. QUASIPERIODIC SUBSTRATE

V. CHAOTIC DYNAMICS

VI. ASSOCIATED PROBLEMS

VII. CONCLUSION

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[1] M. P. N. Juniper, A. V. Straube, R. Besseling, D. G. A. L. Aarts, and R. P. A. Dullens, Microscopic dynamics of synchronization in driven colloids. Nat. Commun. 6, 7187 (2015).

[2] See Figure1.mp4 in appropriate