Molecular dynamics simulation of a driven synchronized particle

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(Dated: March 30, 2021)

Abstract

Synchronization plays an important role in many physical processes. We discuss a molecular dynamics simulation of a single particle moving through a viscous liquid while being driven across a washboard potential energy landscape. Our results show many dynamical patterns as the landscape and driving force are altered. For certain conditions, the particle velocity and location are synchronized or phase-locked, forming closed orbits in phase space. Quasi-periodic motion is common, for which the dynamical center of motion shifts the phase space orbit. This synchronized motion is observed in simulations and table-top experiments, and can be used to isolate complex natural behaviors.

I. INTRODUCTION

Synchronization is a universal phenomena in which individual oscillators change frequency due to external stimuli.[1] The flickering patterns of candle flames [DM - the air molecules are oscillating xx is a flame an oscillator? xx] mediated by temperature fluctuations,[2] the vibrations of singing wine glasses interacting through sound waves,[3] and metronomes vibrating through a supporting platform[4] are examples of in-phase coupled oscillations. Biological systems benefit from cooperative synchronization – birds coordinate wing flaps to optimize energy use during flight,[5] frogs alternate croaking patterns,[6] humans clap in time with music,[7] and at a cellular level, neurons simultaneously fire in cardiac muscle[8] and brain tissue.[9] External forcing can cause or regulate synchronization. For example, an electrical pacemaker regulates a heart beat and a pulsed light modifies the flashing pattern of fireflies.

Synchronized phase-locking or mode-locking first appeared in the scientific literature with Huygens' 1665 experiments on the motions of synchronized pendula in wall-mounted clocks.[10] A locked-mode is an integer frequency ratio. In Huygens clocks, the pendula were observed to swing at the same rate in the same direction (1:1 mode) or opposite directions (-1:1 mode). A 2:1 mode occurs when a simple pendulum four times the length of another swings with twice the period.

Complex dynamics such as synchronized mode-locking can be studied with colloid particles in experiments. Typical colloids are plastic spheres suspended in de-ionized water or silica beads suspended in organic solvent. Because colloids are large and move slowly, the particle positions can be measured in real time with an optical camera.[11] Experimental measurements of the step-by-step dynamics of colloids performing phase-locked motions are useful for understanding synchronization at a single particle level.[12,13]

Light is a tool for manipulating the colloidal environment to alter synchronization patterns. Colloids can be trapped with radiation pressure from a laser beam.[14] A colloid centered in an optical trap is uniformly bombarded by photons. Off-center colloids experience a net force due to uneven photon collisions across the particle surface. Depending on the location of the particle in the trap, the radiation pressure either moves colloids toward the center or ejects it from the trap. Diffraction gratings can create more complex light environments, such as periodic patterns of minima suitable for synchronization studies.[15]

The model discussed in this paper resembles an overdamped driven pendulum. A single

particle oscillator in a potential well is like a skateboarder in a half-pipe or a child on a swing. A confined oscillator may synchronize its location to the periodic pattern of the external drive, moving back and forth in time with the beat, or moving between substrate minima. When a constant or dc drive is applied, the particle velocity is modulated by the potential energy landscape exerted on the particle. [DM swapped "seen by" for "exerted on" xx check added wording xx] Below some threshold the dc force is not strong enough to push the particle across a potential maximum so the average velocity is zero, a phenomena referred to as pinning.[16] Above the pinning threshold, a particle subject to a constant drive force increases its speed at a rate proportional to the external drive. When the applied force varies periodically, the ac drive can cause the particle to hop back and forth across the landscape minima. Many synchronized patterns occur, controlled by the substrate period, leading to mode-locking, where the average particle velocity is fixed for a range of dc drive forces.[17]

In this paper we discuss numerical simulations of the synchronized dynamics of a confined particle driven over a washboard shaped potential energy landscape. We describe our molecular dynamics model in Sec. II. The model is easy to simulate yet relevant to condensed matter systems. We summarize our results including the synchronized motion of a single confined particle driven across a periodic landscape in Sec. III.

In Sec. IV we describe how our results apply to physical systems, such as optically trapped colloids [DM rewrote to better align with conclusion xx added words is this correct? xx] and superconducting vortices in the presence of periodic pinning arrays. [DM resolved xx Josephson junctions not explicitly mentioned in conclusion, xx] We include problems for interested readers in Sec. V.

II. SIMULATION

We use a classical model for studying the dynamics, using the net force on a particle to calculate its trajectory. The particle is confined in a two-dimensional (2D) [DM singular] simulation of area $A = L \times L$, where $L = 46.\bar{6}\, a_0$ where a_0 is a dimensionless unit of length. [DM - yes. in the simulation we just use $L = 46.6$ and the a_0 is to satisfy readers unfamiliar with simulation units xx confused about the role of a_0 because it and hence L are dimensionless, Is it really the size of a colloid particle, which in the simulation you set

to unity? xx] The particle [DM resolved xx since we are doing non-interacting particles and thus only one particle is moving can we eliminate the subscript i? xx] has position $\vec{r} = x\hat{x} + y\hat{y}$ and velocity $\vec{v} = d\vec{r}/dt$. The edges of the system are treated by periodic boundary conditions, such that a particle leaving the edge of the system is mapped back to a position within the simulation boundaries by the transformation $x+L \rightarrow x$ and $y+L \rightarrow y$. We show a schematic of the system in Fig. 1(a). The units of the simulated variables are summarized in Table I.

We confine the particles using a position dependent potential energy, called a landscape or substrate. The landscape is modulated in the y-direction by the periodic function

$$U(y) = U_0 \cos(2\pi y/\lambda), \tag{1}$$

where $\lambda = L/N_p$, with N_p equal to the number of periods, and U_0 is a parameter that sets the depth of the minima with simulation units of energy E_0. We plot this function in Fig. 1 for $N_p = 3$. In Fig. 1(a) we show the x-y plane with a contour plot of $U(y)$ to illustrate the 2D potential energy landscape; the maxima are colored gray and the minima colored white. [DM - switch from red/blue to gray/white - xx make sure that all your figures make sense when printed in b/w xx]

The confining force on the particle [DM removed subscripts] i is given by

$$\vec{F}_\ell(\vec{r}) = -\vec{\nabla}U(\vec{r}).[DMremoved^\ell] \tag{2}$$

where ℓ denotes the landscape. In Fig. 1(b) we plot $U(y)$ to illustrate how the magnitude $|\vec{F}_\ell|$ is calculated from the particle position y. [DM - begrudingly changed - My collaborators and I usually use superscripts for these equations to separate the force superscripts from the particle index subscripts. This is consistent with the textbook I teach from. xx suggest that you use subscripts instead of superscripts. We can easily make that change in the next iteration of your manuscript. However, you would need to change the figures, e.g., $\vec{F}_\mathrm{d}$ F_dc F_ac. One of us didn't like superscripts where he was an undergraduate! xx]

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

$$\vec{F}_\mathrm{d}(t) = [F_\mathrm{dc} + F_\mathrm{ac}\sin(\omega t)]\hat{y}, \tag{3}$$

with a constant component F_dc and a time dependent component with amplitude F_ac with angular frequency $\omega = 2\pi f$.

The inertia of small particles is reduced by interactions with the fluid particles.[18] We assume colloids are overdamped so the particles do not accelerate, that is, they are suspended in a continuous viscous fluid that dissipates energy supplied externally. Newton's second law for an individual particle is simplified by the assumption that $\vec{a}$ is zero. The overdamped equation of motion for the velocity $\vec{v}$ of an isolated particle is

$$\eta\vec{v} = \vec{F}_\ell(\vec{r}) + \vec{F}_\mathrm{d}(t). \tag{4}$$

with friction coefficient $\eta = 1$ in units of v_0/F_0. The term $-\eta\vec{v}$ is a drag force, which models energy dissipation due to the fluid. We discuss models for spheres moving through fluids in Problem 3.

The equation of motion provides a direct calculation of the velocity of an individual particle at position $\vec{r}$ and simulation time t. The simulation is controlled by a loop which runs to a maximum integer time step. At each time step we evaluate the net force on each particle as a function of its position $\vec{r}(t)$ and then integrate the equation of motion to move particles to an updated position. Because the acceleration is zero, the integration of the equation of motion is performed via the simple first-order Euler method

$$\vec{r}(t + \Delta t) = \vec{v}(t)\Delta t + \vec{r}(t) \tag{5}$$

for a time step $\Delta t = 0.1\,\tau$. In Problem 1 we describe the numerical methods for solving differential equations.

III. MODE-LOCKING OF A SINGLE PARTICLE

Here we drive a single particle across the landscape. The numerical implementation of the landscape is calculated with Eqs. (1) and (2) [DM - right, two negative signs, one from the derivative, the other from the definition of force. I found the "mistakenly" dropped minus sign in the depths of january and added it. xx but you should get a + sign not a minus sign xx]

$$F_{\ell y}(y) = A_p \sin(2\pi y/\lambda), \tag{6}$$

where the force is scaled by the parameter $A_p = 2\pi U_0/\lambda$. In this section we fix the landscape parameters to $A_p = 0.1\,F_0$ with $N_p = 20$ minima, corresponding to a spatial period $\lambda = 2.3\,a_0$. The competition between the driving force and the landscape potential can produce

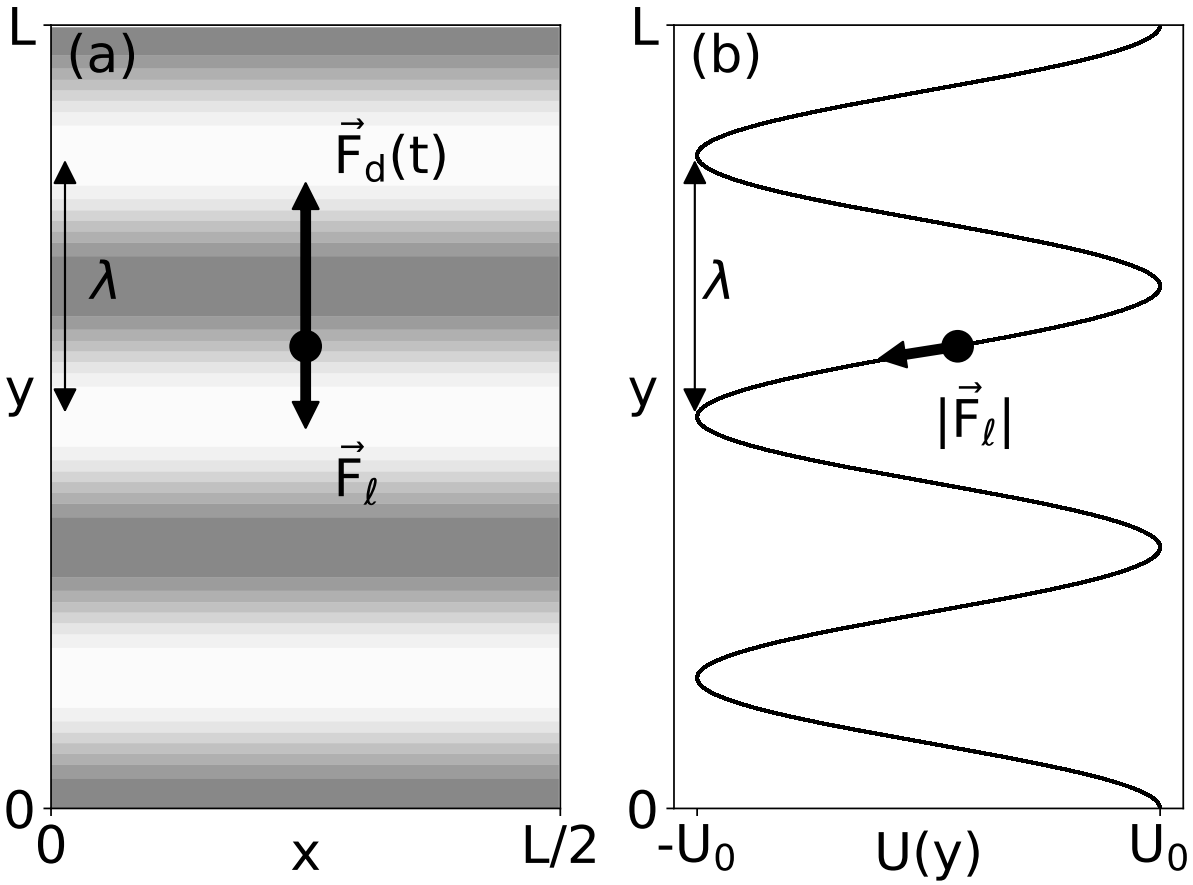

FIG. 1. Schematic of the simulation of a single particle driven across a washboard potential energy landscape. (a) View of the x-y plane. The time-dependent applied driving force $\vec{F}_{\rm d}$ is parallel to the y-axis. The landscape is shown with [DM changed color scheme from red/blue to gray/white for better BW conversion] maxima in the potential energy are gray and minima are white A particle is subject to competing forces of the landscape and applied driving force. (b) The potential energy function along the y-axis $U(y)$. [DM removed $_\ell$] The particle in (a) is shown at the same y-position. The slope of $U(y)$ [DM removed $_\ell$ use the subscripts with the potential, but will move to superscript xx used subscript here xx] is the magnitude of force $\vec{F}_\ell$.

a variety of hopping patterns in the particle motion. The relative values of $F_{\rm ac}$, $F_{\rm dc}$ and A_p control the rate and distance a particle moves forward and backward in the landscape. If $F_{\rm d}(t) > A_p$, a particle can overcome the barrier height of the landscape, and the particle hops between minima in the energy landscape. If the driving frequency is low, as in Fig. 2, the driven particle moves in a pattern with the same frequency as the time-dependent force

$F_{\rm d}(t)$, but is modulated by the landscape period. We explore changes in the frequency and different values of $F_{\rm ac}$ in Problem 2. Here we vary $F_{\rm dc}$ while holding the remaining parameters fixed.

TABLE I. Simulation parameters and units with comparable experimental values.[12,13] The substrate is scaled by our force units, while an experimental landscape is scaled by the Brownian motion of the particles.

Quantity	Simulation Units	Experimental values
length	$a_0 = 1$	$a_0 \sim 1.5\mu m$
energy	$E_0 = 1$	
force	$F_0 = E_0/a_0$	
time	$\tau = \eta a_0/F_0$	$\tau \sim 3\,\mathrm{s}$
velocity	$v_0 = a_0/\tau$	$v \sim 5\,\mu\mathrm{m/s}$
substrate period	$\lambda = 2.3\,a_0$	$\lambda = 3.5\,\mu\mathrm{m}$
substrate amplitude	$A_p = 0.1\,F_0$	$U_0 = 25k_BT \sim 1\,\mathrm{J}$
temperature	$T_0 = 0$	$T \sim 290\,\mathrm{K}$

In Fig. 2(a) we plot $F_{\rm d}(t)$ as a function of time with the constants $F_{\rm dc} = 0.07$, $F_{\rm ac} = 0.07$ and $f = 0.01$ cycles per time unit τ. The temporal period of the driving force is $T = 1/f = 100\,\tau$. In Fig. 2(b) we show the y-position of the particle as a function of time, where we have normalized y by λ. The initial particle position is $y = 0$. The particle moves in the positive y-direction through a distance $\Delta y = \lambda$ in a time T, so that the average velocity $\langle v_y \rangle = \lambda f$. The inset of Fig. 2(b) shows y over one period $100\,\tau < t < 200\,\tau$ with the contour plot described in Fig. 1(a). The motion is synchronized such that the driving force is a maximum when the landscape force is minimum, as shown by the coincidence of the steep slope of y/λ and the maxima in $F_{\rm d}(t)$. When $F_{\rm d}(t)$ is large, the particle moves across the substrate maxima, [DM - color change] shown in gray with the contour plot.

To explore the possible hopping patterns, we sweep through a range of $F_{\rm dc}$ for fixed $F_{\rm ac}$ and A_p. In Fig. 3 we increase $F_{\rm dc}$ in increments of $0.001\,F_0$, and measure the average velocity $\langle v_y \rangle$ as a function of $F_{\rm dc}$. We also perform the sweep for a non-oscillatory drive $F_{\rm ac} = 0$. With no oscillating component of the driving force, the force-velocity relation

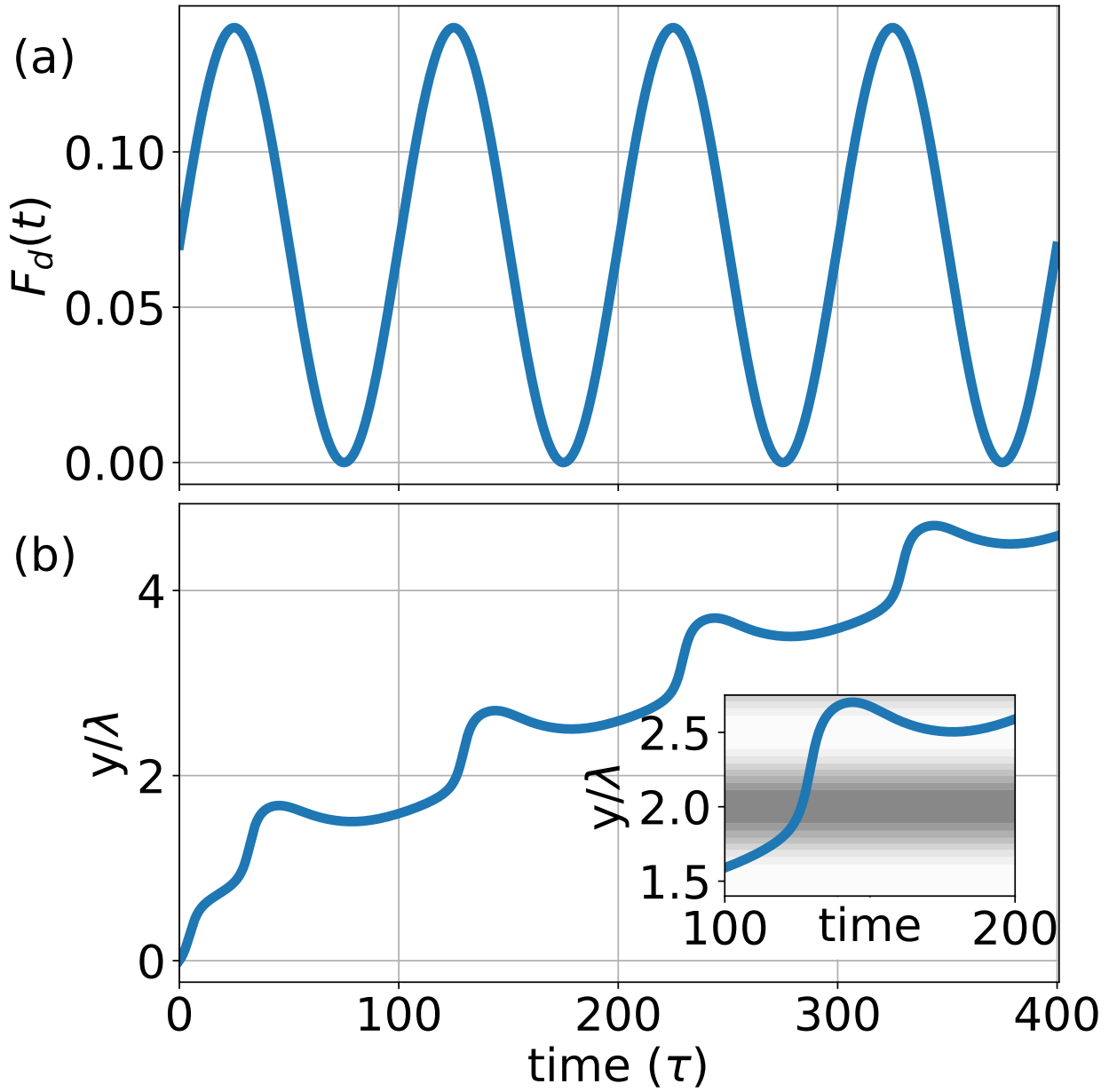

FIG. 2. (a) The applied driving force $F_{\rm d}(t)$ with parameters $F_{\rm dc} = 0.07$, $F_{\rm ac} = 0.07$ and $f = 0.01$. (b) The y-position of the driven particle normalized by the period of the substrate λ. The substrate strength is $A_p = 0.1$. The inset shows the y-position through the second period $100\tau < t < 200\tau$ along with the contour plot depicting the landscape potential described in Fig. 1(a).

increases monotonically above the depinning threshold F_c such that

$$\langle v_y \rangle \propto (F_{\rm dc} - F_c)^{-\beta}. \tag{7}$$

where the power β varies with the system type and can be used to identify universality

class.[16] The critical force F_c is equal to the maximum substrate force A_p.

The addition of an ac drive leads to the formation of modes. A mode is a periodic pattern of hops with a constant average particle velocity, $\langle v_y \rangle$ over a range of driving forces $F_{\rm dc}$. In Fig. 3 we sweep $F_{\rm dc}$ with $F_{\rm ac} = 0.07$ and $f = 0.01$. Each step represents a different pattern of hops between substrate minima performed by the particle due to the landscape confinement. At low $F_{\rm dc}$ the average velocity $\langle v_y \rangle$ is zero. Because A_p is large compared to the extrema of $F_{\rm d}(t)$, the particle oscillates back and forth in a single minima with no net velocity, an example of a 0:0 mode. At higher $F_{\rm dc}$ the particle velocity $\langle v_y \rangle$ increases in steps of uniform height, $\langle v_y \rangle = n\lambda f$, where n is an integer. We observe a mode of $n = 1$ for the range $0.05 < F_{\rm dc} < 0.08$, $n = 2$ for $0.08 < F_{\rm dc} < 0.11$, $n = 3$ for $0.12 < F_{\rm dc} < 0.13$, $n = 4$ for $0.14 < F_{\rm dc} < 0.155$, and $n = 5$ for $0.155 < F_{\rm dc} < 0.16$. Higher modes are not visible. The step width is nonlinear and depends on the strength of $F_{\rm ac}$ for this landscape potential.[13,30] These steps, known as Shapiro steps, can have a variety of interesting patterns such as a devil's staircase related to chaotic dynamics.[19]

To study synchronization patterns, it is useful to compare mode-locked quantities in a two-dimensional phase plot. For a driven pendulum confined to a single potential well, an appropriate phase space is the particle velocity v_y versus the position y. For a particle driven through multiple identical wells we define phase variables to account for the net increase in the position. The phase position is

$$\phi(t) = 2\pi[y(t) - \langle v_y \rangle t]/\lambda, \tag{8}$$

centered about the average particle displacement $\langle v_y \rangle t$ and normalized by the substrate period λ.[12] The phase velocity is

$$\dot{\phi}(t) = 2\pi[v_y(t) - \langle v_y \rangle]/\lambda. \tag{9}$$

For zero landscape force, the phase velocity is zero when $F_{\rm d}(t) = F_{\rm dc}$. [DM rewrite following sentence] If the system is strictly mode-locked, the particle velocity recurs at a particular spatial location, and a closed loop appears in phase space. A 1:1 mode appears as a circle or oval. Nodes appear for higher modes, sometimes forming figure-eights or other recognizable patterns. A system that is nearly phase locked will appear as an almost closed loop. Such quasiperiodic systems are not fully synchronized so the position-velocity relation shifts in time as in Fig. 4.

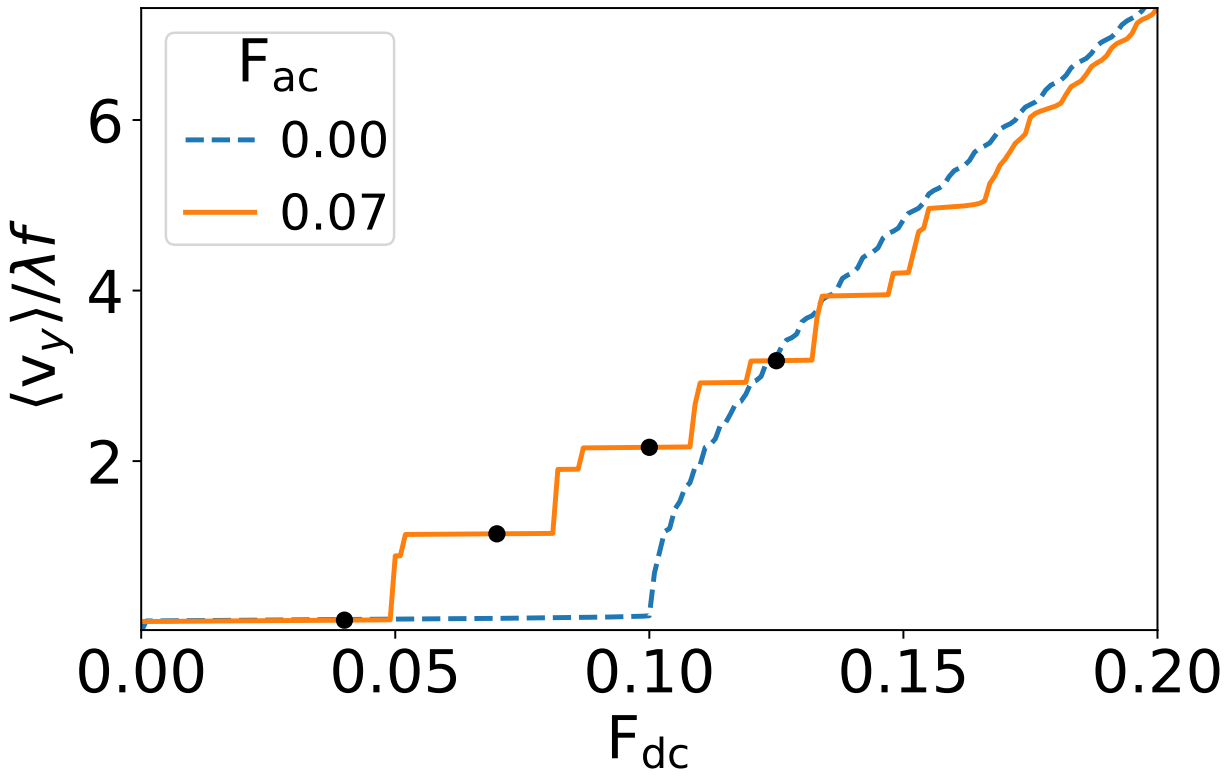

FIG. 3. Average particle velocity $\langle v_y \rangle$ as a function of $F_{\rm dc}$. We let $F_{\rm ac} = 0.0$ (blue dashed) and $F_{\rm ac} = 0.07$ (orange) with $f = 0.01$ as in Fig. 2. The value of $F_{\rm dc}$ for the first four steps correspond with the fixed value of $F_{\rm dc}$ in each of the phase plots in Fig. 4(a-d). [DM - clarified? xx don't understand meaning of indicating a system plotted in Fig. 4 xx]

In Fig. 4 we plot $\dot{\phi}(t)$ versus $\phi(t)$ for increasing $F_{\rm dc}$, with the remaining parameters fixed as in Fig. 2. For $F_{\rm dc} = 0.04$ the phase plot in Fig. 4(a) with is an asymmetric curve. A tail appears due to the initial transient motion of the particle. The particle is confined to a single substrate minima, and has no net velocity. The asymmetry is caused by bias induced by $F_{\rm dc}$. In Fig. 4(b) with $F_{\rm dc} = 0.07$ the phase loop is a symmetric triangular shape, indicating a 1:1 match between the particle motion and velocity consistent with Fig. 2(a). As $F_{\rm dc}$ is increased, nodes form in the phase diagram, which occur due to repeated values of $\dot{\phi}$ over multiple phase positions. In Fig. 4(c) with $F_{\rm dc} = 0.1$ two nodes form. The particle moves a distance 2λ during one time period. For $F_{\rm dc} = 0.125$ as in Fig. 4(d), three nodes form as the particle moves across 3λ.

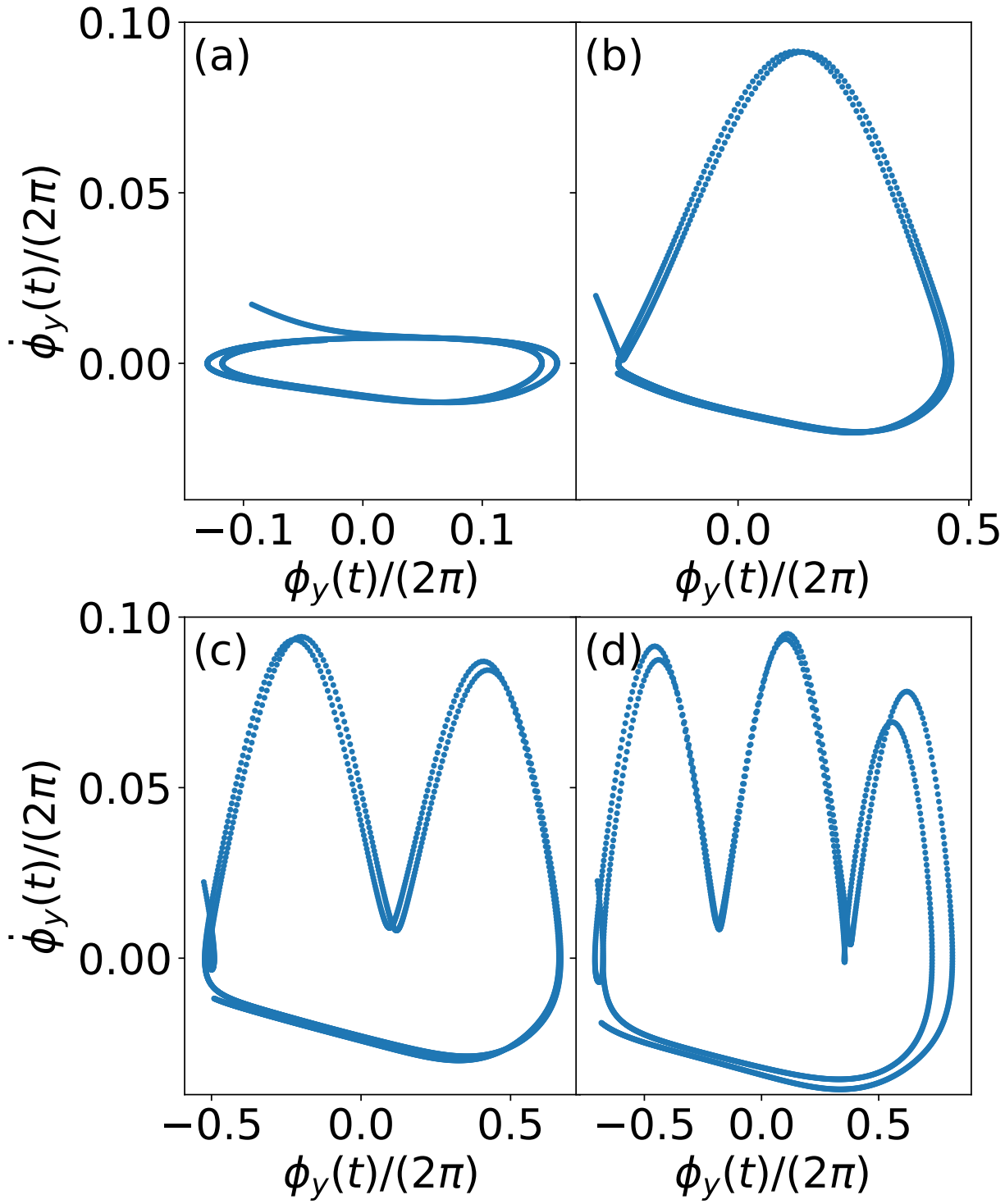

FIG. 4. Phase plot of $\dot{\phi(t)}/(2\pi)$ versus $\phi(t)/(2\pi)$. The particle is driven with $F_{\rm dc}$ equal to (a) 0.04, (b) 0.07, (c) 0.1, and (d) 0.125. These values are denoted as black circles in Fig. 3. The other parameters are $F_{\rm ac} = 0.07$, $f = 0.01$, and $A_p = 0.1$ as in Fig. 2.

IV. CONCLUSION

A single particle driven across a periodic potential landscape synchronizes its motion to environmental and external forces. Our simulations reproduce the experiments and simulations presented in Juniper *et al.*[12,13] of mode locking in driven colloids on a periodic optical landscape. Colloids are relatively easy to manipulate and image in experiments, making ideal proxies for systems such as cold atoms or electron gases.[15] Dynamical mode-locking is observed in technologies such as quantum electronic devices as stepped regions in the relation between current-voltage, where the voltage is the analog of the external driving force and current is the analog of particle velocity. These mode-locked or phase-locked currents (Shapiro steps), due to applied ac voltages in single Josephson junctions[27,28] and coupled arrays of junctions have been observed.[29] Shapiro steps vary in width depending on the strength of the applied ac forces, and are observed in a variety of ac and dc driven systems displaying non-Ohmic behavior in voltage-current curves, including charge density waves, spin density waves and superconducting vortices in landscapes engineered with periodic patterns of pinning sites.[30]

Mode-locking is a useful probe of complex quantum mechanical systems because the motions of individual particles can be inferred only from other measurements. Our results are relevant to synchronization effects in a broad range of experimental systems including optically confined colloids, superconductors with periodic pinning arrays, and the charge and spin of atomic systems.

V. SUGGESTED PROBLEMS

In the following we explore the behavior of our model with suggested problems for interested readers. We discuss the molecular dynamics algorithm and numerical integration techniques in Problem 1. [DM slight rewrite to remove the redundant "we" active voice construction] Changes to the parameters are described in Problem 2. We include analytic solutions to the linear drag equation in Problem 3, the equation of motion in Problem 4. We extend the numerical model to include finite temperature effects in Problem 5.

Problem 1. Write your own MD code To calculate the position of the particle as a function of time we numerically integrate the equation of motion (Eq. 4) using the standard definition

of velocity $\vec{v} = d\vec{r}/dt$ using the Euler method. Eq. 4 provides a direct calculation for the particle velocity from the net force on the particle, as demonstrated in Problem 4.

A working example of this code is available in Ref.[24] If you would like to write your own, the following guide will walk you through our choices. In the code excerpts below, most comments and optional details are removed for clarity. We use the Python programming language for educational purposes. To model additional particles, the authors recommend a more traditional compiled coding language to perform the many operations associated with neighbor lists to compute particle interactions.

(a) **Initialization.** For convenience, we define a Python dictionary to contain the simulation constants that could easily be passed by reference to subroutines. We have left as an exercise to the reader the addition of the remaining parameters of the system.

```
def set_parameters():
    '''set simulation parameters...'''

    #declare the dictionary
    dict={}
    dict['dt'] = 0.1 #timestep in simulation units
    #control the oscillating component of driving force
    dict['F_AC'] = 0.07 #amplitude of force oscillation
    dict['freq'] = 0.01 #frequency of force oscillation
    #left as an exercise to the reader
    #...
    return dict
```

The function is called at the top of the main function followed by a call to a subroutine containing the MD algorithm.

```
if __name__ == "__main__":
    parameters = set_parameters()
```

```
#run the MD simulation
single_particle(parameters)
```

(b) **Time loop.** The Euler method is effective for solving linear ordinary differential equations of the form $dy/dt = f(t, y(t))$ with the initial condition $y(t_0) = y_0$. The solution is calculated algorithmically by stepping in time through n integer steps $t_n = t_0 + n\Delta t$. At each subsequent step the new value for y is calculated as a solution of a map using discrete times $y_{n+1} = y_n + f(t_n, y_n)$. Apply the Euler method to Eq. 4 [DM - resolved xx refer to specific equation by label xx] to determine the analytic expression for the position of a particle y_n at the nth time step.

Add a for loop to step through each integer timestep. With this loop, control the flow of the program and retain information for the particle position and other properties as a function of time. Assume this information will be calculated a subroutine.

We used the subroutine **single_particle()** calculate the array lengths to hold position, velocity, and time data. The lengths of these arrays will be affected by how much data you choice to save (see comment following sample code). Define a loop to calculate the particle position and velocity through each molecular dynamics time step, calculated in the subroutine **md_step()** which will be described in more detail in (c).

```
def single_particle(parameters,plot="y-position"):
    '''Run MD simulation...'''
    #define empty arrays to hold data as a function of time
    #(left as an exercise to the reader)

    #loop through the integer time steps in the simulation
    for int_time in range(0,maxtime):
        #(left as an exercise to the reader)
        time += dt
```

Comment: A key decision for any MD algorithm is how much information to save during and after the simulation. We define the following constants to manage the

length of arrays containing data. We found in practice that for short simulations times we could save all data.

```
#integer time steps
dict[‘maxtime’]=int(40/dict[’freq’])   #total time steps
dict[‘writemovietime’]=1   #write data to arrays for plotting
```

(c) **Position and force calculations.** In our implementation, we created a subroutine to consider each type of force in the system (external drive, landscape, etc). If the particle moves beyond the limits $0 \leq y < L$, it must be returned using the definition of periodic boundary conditions in Sec. II.

```
def md_step(y, int_time, avg_vy, parameters, ft=0):
  ‘‘‘Calculate net force and integrate eq. of motion...’’’

  #calculate the floating point value for time
  time = int_time * dt

  #reset vy for every timestep since ay = 0
  vy = 0

  #calculate the net force on the particle
  vy = #(left as an exercise to the reader)

  #calculate the new position
  y += #(left as an exercise to the reader)

  #check periodic boundary conditions
  #(left as an exercise to the reader)

  return y, vy, avg_vy
```

The Euler algorithm can be applied to calculate reasonable numerical solutions to nonlinear equations if the time step Δt is kept sufficiently small.[23] In our simulations we use the time step $\Delta t = 0.1$ and find no change in the solution when we decrease the time step to smaller values. In simulations of many interacting particles, a small time step is essential for accurate results. Particle-particle interactions are typically nonlinear, so that the inter-particle force changes significantly over small distances and the simple Euler algorithm is insufficient.

Problem 2. Exploring model parameters

A range of oscillation behaviors can be explored by varying the relative strength of the confining landscape and the external driving force.

(a) Explore the effect of increasing $F_{\rm ac}$ on the hopping pattern. For a single driven particle, the hopping patterns are typically characterized by n_f, the number of forward steps, versus n_b, the number of backward steps in one time period. The total displacement of $(n_f - n_b)\lambda$ is the net hop length. In Fig. 2, the particle moves forward through a minima ($n_f = 1$), and does not move backward through a full minima ($n_b = 0$). To achieve backward hops, the driving parameters must have a ratio of $F_{\rm ac}/F_{\rm dc} > 1$ and a difference $|F_{\rm ac} - F_{\rm dc}| > A_p$. Holding all other parameters fixed, explore how the hopping pattern changes for increasing $F_{\rm ac}$. For example, calculate the patterns of hops for fixed parameters $f = 0.01$, $F_{\rm dc} = 0.07$, and $A_p = 0.1$ and modified parameter $F_{\rm ac} = 0.2, 0.3$ and 0.4.

(b) Explore the effect of increasing the driving frequency on the hopping pattern. In Sec. III the frequency is sufficiently low so that the effect of the applied force is large over a sustained time interval, allowing the particle to hop a substrate maxima. For example fix the parameters $F_{\rm dc} = 0.1$, $F_{\rm ac} = 0.05$, and $A_p = 0.1$ and explore high frequency ($f = 0.1$), intermediate frequency ($f = 0.01$), and low frequency ($f = 0.005$).

(c) Explore the effect of increasing increasing $F_{\rm ac}$ on the step pattern in Fig. 3. For example sweep the driving force $F_{\rm dc}$ over increments of $\Delta F_{\rm dc} = 0.001$ for a fixed amplitude $F_{\rm ac}$ and frequency $f = 0.01$. Appropriate values for $F_{\rm ac} = 0.1 - 0.4$ will demonstrate a change in the step width in a plot of $\langle v_y \rangle$ vs $F_{\rm dc}$

Problem 3. Drag models and Reynolds numbers

Stokes' law describes the drag force $\vec{F}_{lin} = -3\pi\eta D\vec{v}$ on a sphere moving through a viscous liquid at velocity $\vec{v}$, where η is the dynamic fluid viscosity and D is the particle diameter.[20] In simulations we subsume the constants $3\pi D$ such that $3\pi D\eta \to \eta$. Often drag forces are modeled as a polynomial series[20]

$$\vec{F}_{\text{drag}} = -b\vec{v} - cv^2\hat{v} + \cdots . \tag{10}$$

Truncating the series to the first term is justified by demonstrating the sphere has a low Reynolds number $R = Dv\rho/\eta$, where ρ is the fluid density and v is the particle's speed. If R is small, the quadratic and higher order terms may be ignored.

Use reasonable values for the experimental analog of this system and show that the Reynolds number is small. In addition to the values listed in Table I, to first order the viscosity is $\eta \sim 10^{-3}$ Pa-s.[21] and the liquid density $\rho \sim 10^3$ kg/cm^3.[22]

Problem 4. Equation of motion

Newton's second law states that the acceleration of a particle i is proportional to the sum of the forces on the particle

$$m\vec{a} = \sum \vec{F}, \tag{11}$$

where m is the inertial mass. The addition of a dissipative force to a dynamical equation of colloid motion is typically modeled by a drag force proportional to the particle's velocity in the opposite direction of motion $\vec{F}_{\text{drag}} = -\gamma\vec{v}$, where $\gamma = 3\pi\eta D$ is the drag coefficient described in Problem 3. The ratio of m/γ is known as the momentum relaxation time, and is small for particles with low Reynolds numbers. The mass of a typical colloid particle is 15 picograms, leading to a momentum relaxation time on the order of microseconds.

(a) Given the values listed in Table I, show that the momentum relaxation time is $m/\gamma \approx 0.5\,\mu$s.

(b) If m/γ is small, the particle's acceleration can be ignored entirely. Using Newton's second law for a small momentum relaxation time, show that a particle confined to a landscape exerting force $F_\ell(\vec{r})$ subject to a time dependent drive $F_{\text{d}}(t)$ can be modeled by the equation of motion described in Eq. (4).

Problem 5. Brownian motion

Brownian motion is a phenomena in which visible particles change direction, apparently at random, due to collisions with invisible fluid particles. The rate of collisions depends on the temperature, viscosity and the density of the suspending fluid.[25] An optically trapped colloid executing Brownian motion is a useful probe of microscopic forces.[21]

In molecular dynamics simulations it is common to treat the invisible fluid particles as a continuous fluid to reduce computational expense. Temperature effects can be modeled by applying randomized forces f_T to the visible particles. We use the normal distribution to generate a series of f_{T_n} values for each integer time step n.[26] A normalized random distribution of forces causes fluctuations in motion equally in all directions such that the force f_T averaged over a finite time interval is zero. In one dimension we have

$$\langle f_T(t) \rangle = \frac{1}{N} \sum_{n}^{N} f_{Tn} = 0, \tag{12}$$

where the integer n indicates the number an simulation time steps and $t = N\Delta t$. A particle with sufficient energy $k_b T_{\min}$ may hop over landscape barriers. In our simulations, we let temperature as $k_b T/E_0 \to T$ with constants set to unity to compare directly with force.

For no applied driving force, find the minimum temperature required for a single particle to hop over the maxima in the potential landscape. Assume the particle is confined to move along the y-direction, include Brownian motion in the model. Appropriate temperatures to explore are $3.0 < T/A_p = 7.0$. Plot the $y-$ position versus time for this particle.

For a driven particle, we ignore the effects of temperature in these simulations. We note that even for $T/A_p = 6.0$ the hopping rate is much less than the frequency of the applied drive. At sufficiently high temperatures, Brownian motion does affect the formation of mode-locked steps and can be observed in experiments.

ACKNOWLEDGMENTS

Charles and Cynthia Reichhardt inspired the project and provided the original molecular dynamics code written in the C programming language. We acknowledge funding from the M.J. Murdock Charitable Trust and the Pacific Research Institute for Science and Mathe-

matics.

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