

Molecular dynamics simulation of synchronization in driven particles

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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 mediated by temperature fluctuations,² the vibrations of singing wine glasses interacting through sound waves,³ and metronomes vibrating through a supporting platform⁴ 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 muscle⁸ 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. 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 and superconducting vortices in the presence of periodic pinning arrays. 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) simulation of area $A = L \times L$, where $L = 46.\bar{6} a_0$ where a_0 is a dimensionless unit of length. The particle 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

$$U(y) = U_0 \cos(2\pi y/\lambda), \quad (1)$$

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 white and the minima colored gray.

The confining force on the particle is given by

$$\vec{F}_\ell(\vec{r}) = -\vec{\nabla}U(\vec{r}). \quad (2)$$

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 .

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

$$\vec{F}_d(t) = [F_{dc} + F_{ac} \sin(\omega t)]\hat{y}, \quad (3)$$

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

$$\eta\vec{v} = \vec{F}_\ell(\vec{r}) + \vec{F}_d(t). \quad (4)$$

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

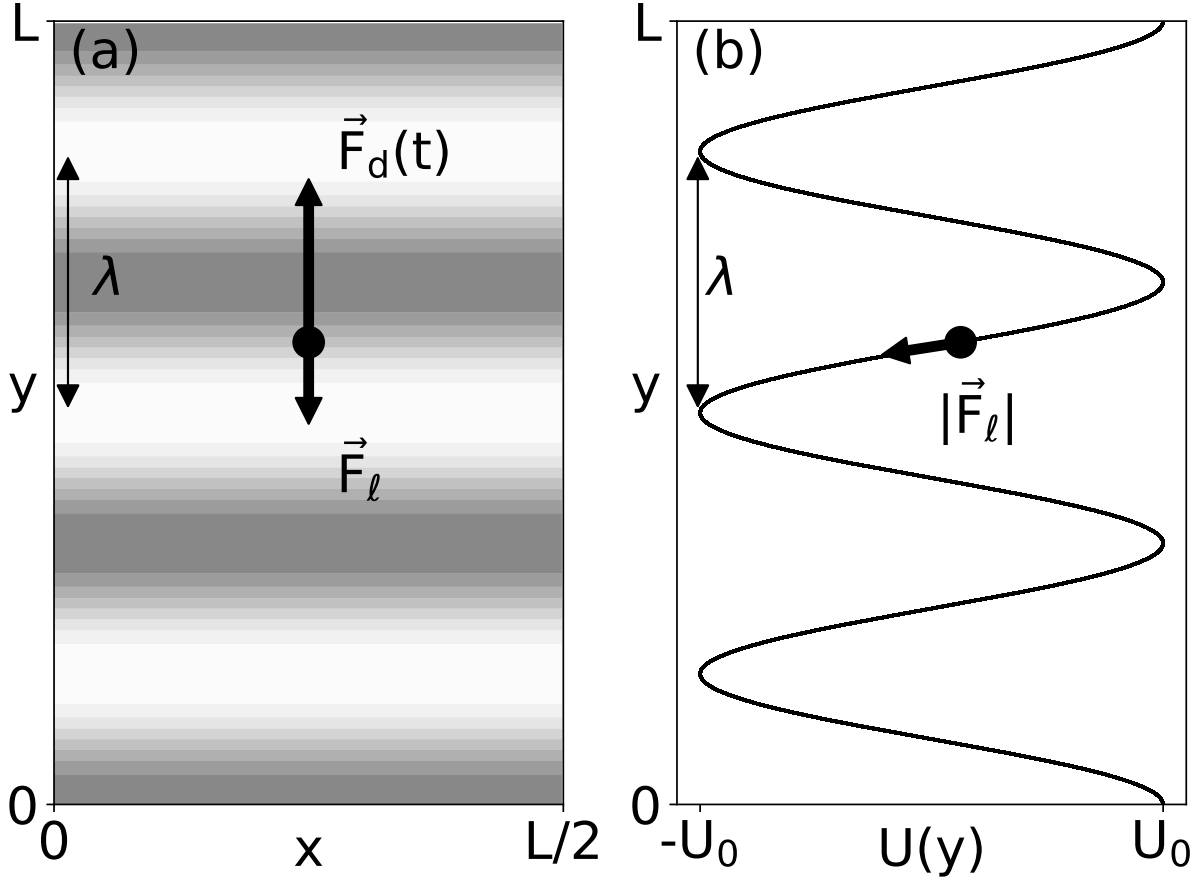


FIG. 1. Schematic of the simulation of a single particle driven across a washboard potential energy landscape. (a) View of the x - y plane. The time-dependent applied driving force \vec{F}_d is parallel to the y -axis. The landscape is shown with maxima in the potential energy marked in white and minima marked in gray. A particle is subject to competing forces of the landscape and applied driving force. (b) The potential energy function along the y -axis $U(y)$. The particle in (a) is shown at the same y -position. The slope of $U(y)$ is the magnitude of force \vec{F}_ℓ .

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

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

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)

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

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 a variety of hopping patterns in the particle motion. The relative values of F_{ac} , F_{dc} and A_p control the rate and distance a particle moves forward and backward in the landscape. If $F_d(t) > A_p$, 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 $F_d(t)$, but is modulated by the landscape period. We explore changes in the frequency and different values of F_{ac} in Problem 2. Here we vary F_{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	$\tau = \eta a_0/F_0$	$\tau \sim 3\text{ s}$
velocity	$v_0 = a_0/\tau$	$v \sim 5\mu m/s$
substrate period	$\lambda = 2.3 a_0$	$\lambda = 3.5\mu m$
substrate amplitude	$A_p = 0.1 F_0$	$U_0 = 25k_B T \sim 1\text{ J}$
temperature	$T_0 = 0$	$T \sim 290\text{ K}$

In Fig. 2(a) we plot $F_d(t)$ as a function of time with the constants $F_{dc} = 0.07$, $F_{ac} = 0.07$ and $f = 0.01$ cycles per time unit τ . The temporal period of the driving force is $T = 1/f =$

100τ . 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 $F_d(t)$. If $F_d(t)$ is large, the particle moves across the substrate minima, shown in gray with the contour plot. The slope of y/λ equals zero twice during a driving period, indicating zero forward motion due to a coincidence of the negative driving force and motion over the landscape maxima.

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

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

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_{dc} . In Fig. 3 we sweep F_{dc} with $F_{ac} = 0.07$ 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_{dc} the average velocity $\langle v_y \rangle$ is zero. Because A_p is large compared to the extrema of $F_d(t)$, the particle oscillates back and forth in a single minima with no net velocity, an example of a 0:0 mode. At higher F_{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 $0.05 < F_{dc} < 0.08$, $n = 2$ for $0.08 < F_{dc} < 0.11$, $n = 3$ for $0.12 < F_{dc} < 0.13$, $n = 4$ for $0.14 < F_{dc} < 0.155$, and $n = 5$ for $0.155 < F_{dc} < 0.16$. Higher modes are not visible. The step width is nonlinear and depends on the strength of F_{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

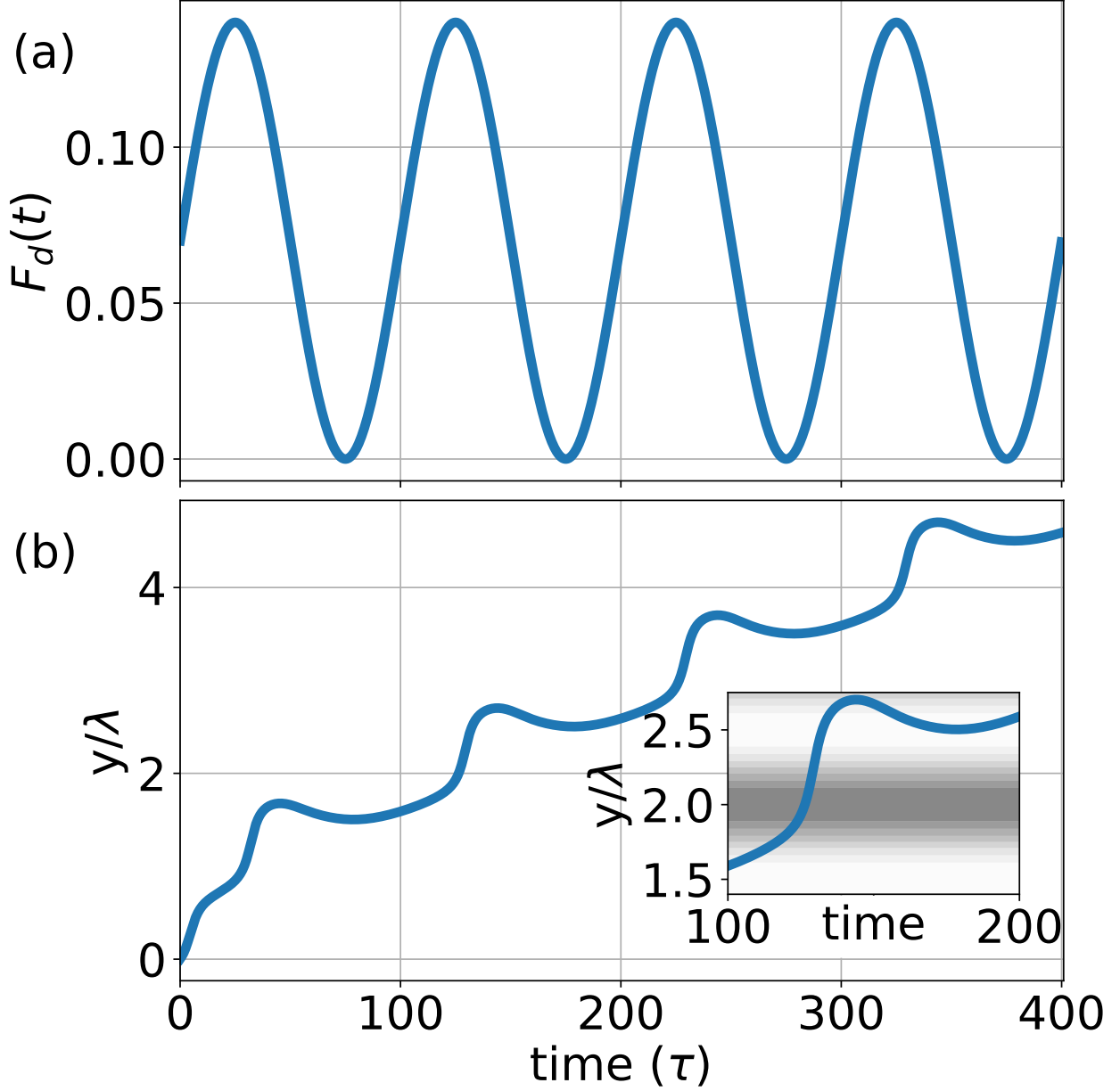


FIG. 2. (a) The applied driving force $F_d(t)$ with parameters $F_{dc} = 0.07$, $F_{ac} = 0.07$ and $f = 0.01$. (b) The y -position of the driven particle normalized by the period of the substrate λ . The substrate strength is $A_p = 0.1$. The inset shows the y -position through the second period $100\tau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

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

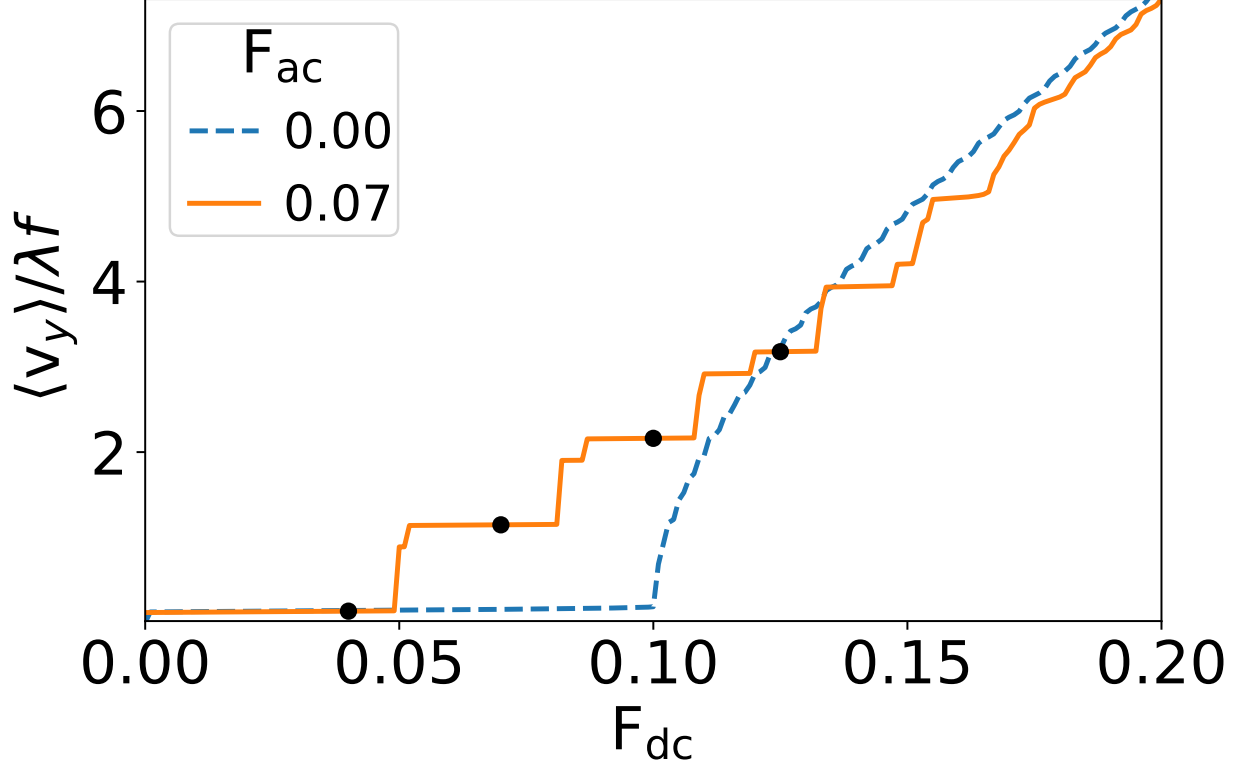


FIG. 3. Average particle velocity $\langle v_y \rangle$ as a function of F_{dc} . We let $F_{ac} = 0.0$ (blue dashed) and $F_{ac} = 0.07$ (orange) with $f = 0.01$ as in Fig. 2. The value of F_{dc} for the first four steps correspond with the panels (a-d) plotted in Fig. 4.

the position. The phase position is

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

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

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

For zero landscape force, the phase velocity is zero when $F_d(t) = F_{dc}$. 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.

In Fig. 4 we plot $\dot{\phi}(t)$ versus $\phi(t)$ for increasing F_{dc} , with the remaining parameters fixed as in Fig. 2. For $F_{dc} = 0.04$ 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_{dc} . In Fig. 4(b) with $F_{dc} = 0.07$ 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_{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 $F_{dc} = 0.1$ two nodes form. The particle moves a distance 2λ during one time period. For $F_{dc} = 0.125$ as in Fig. 4(d), three nodes form as the particle moves across 3λ .

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.

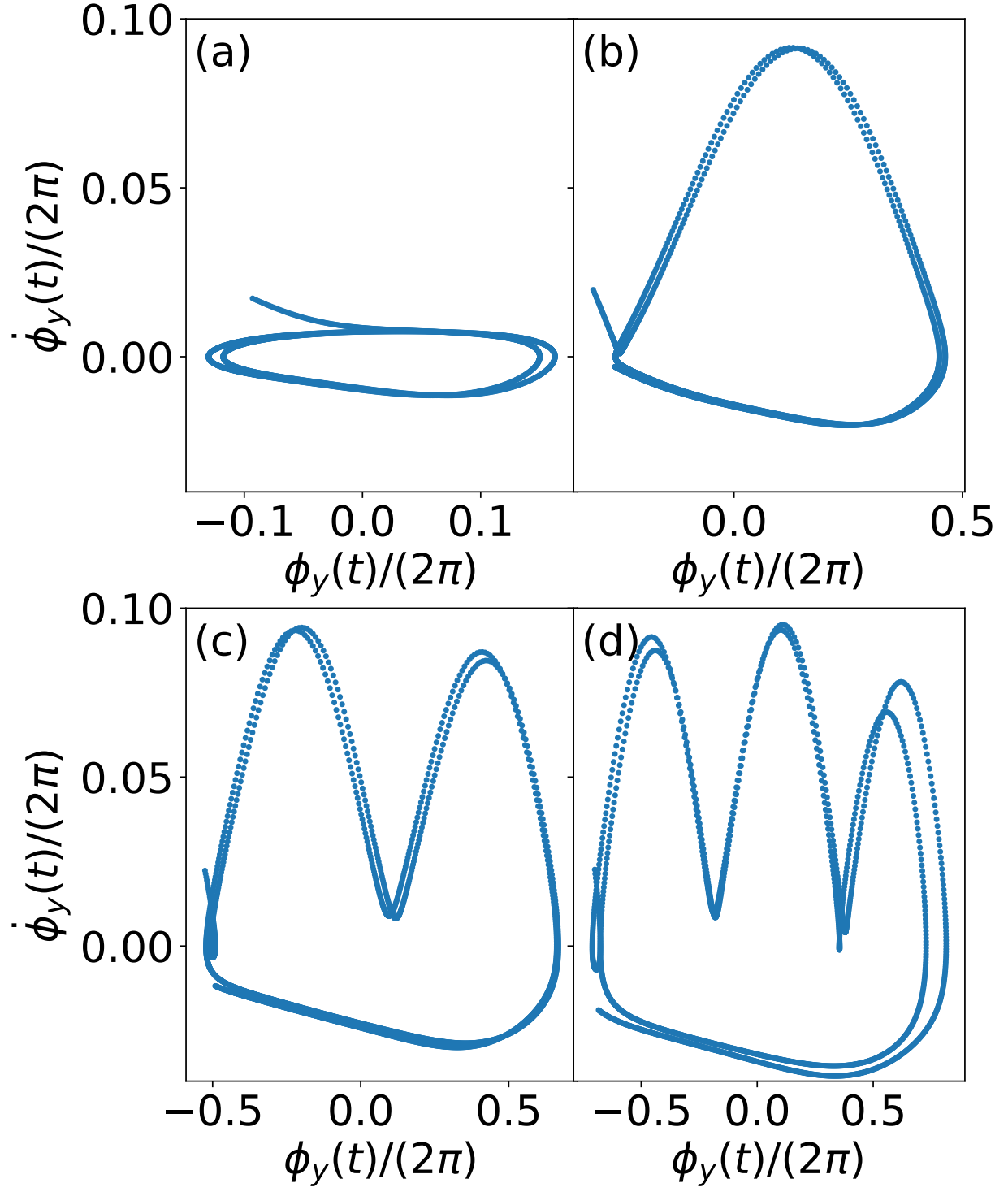


FIG. 4. Phase plot of $\dot{\phi}(t)/(2\pi)$ versus $\phi(t)/(2\pi)$. The particle is driven with F_{dc} equal to (a) 0.04, (b) 0.07, (c) 0.1, and (d) 0.125. These values are denoted as black circles in Fig. 3. The other parameters are $F_{ac} = 0.07$, $f = 0.01$, and $A_p = 0.1$ as in Fig. 2.

V. SUGGESTED PROBLEMS

In the following we explore the behavior of our model with suggested problems for interested readers. We explore changes in the particle motion with parameter changes in Problem 2. We include analytic solutions to the linear drag equation in Problem 3, the equation of motion in Problem 4, and numerical integration techniques in Problem 1. We extend the model with numerical problems to include finite temperature effects in Problem 5.

Problem 1. Write your own MD code

To calculate the position of the particle we numerically integrate the equation of motion using the standard definition of velocity $\vec{v} = d\vec{r}/dt$ using the Euler method. The equation of motion provides a direct calculation for the particle velocity, as demonstrated in Problem 4. 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 to determine the analytic expression for the position of a particle y_n at the n th time step.

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.

A working example of this code is available in Ref.²⁴

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_{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 $F_{ac}/F_{dc} > 1$ and a difference $|F_{ac} - F_{dc}| > A_p$. Holding all other parameters fixed, explore how the hopping pattern changes for increasing F_{ac} . For example, what pattern of hops occurs for fixed parameters $f = 0.01$, $F_{dc} = 0.07$, and $A_p = 0.1$ and modified parameter $F_{ac} = 0.2, 0.3$ 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 $F_{dc} = 0.1$, $F_{ac} = 0.05$, 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_{ac} on the step pattern in Fig. 3. For example sweep the driving force F_{dc} over increments of $\Delta F_{dc} = 0.001$ for a fixed amplitude F_{ac} and frequency $f = 0.01$. Appropriate values for $F_{ac} = 0.1 - 0.4$ will demonstrate a change in the step width in a plot of $\langle v_y \rangle$ vs F_{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 $3\pi D\eta \rightarrow \eta$. Often drag forces are modeled as a polynomial series²⁰

$$\vec{F}_{drag} = -b\vec{v} - cv^2\hat{v} + \dots \quad (10)$$

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.

To first order the viscosity is $\eta \sim 10^{-3}$ Pa-s.²¹ 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, the liquid density $\rho \sim 10^3$ kg/cm³ is a reasonable first order approximation.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

$$m\vec{a} = \sum \vec{F}, \quad (11)$$

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 $m/\gamma \approx 0.5 \mu\text{s}$.
- (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 $F_d(t)$ 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

$$\langle f_T(t) \rangle = \frac{1}{N} \sum_n^N f_{T_n} = 0, \quad (12)$$

where the integer n indicates the number of 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 $k_b T/E_0 \rightarrow T$ 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 $T/A_p = 3.0, 3.5$, and 4.0 . Plot the y – *position* versus time for this particle.

Comment: For a driven particle, we ignore the effects of temperature in these simulations. We note that even for $T/A_p = 4.0$ the hopping rate is much less than the frequency of the applied drive, as can be seen in the time scale in Fig. ??, where the average hopping rate is approximately every 4000τ , a value much larger than the period of the driving force. At sufficiently high temperatures, Brownian motion does affect the formation of mode-locked steps and can be observed in experiments.

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