Friction Selection in Nonlinear Particle Arrays

H. G. E. Hentschel,[1] F. Family,[1] and Y. Braiman[2]
[1]*Department of Physics, Emory University, Atlanta, Georgia 30322*
[2]*Center for Engineering Science Advanced Research, Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831*
(Received 3 November 1998)

When a discrete nonlinear array is driven across a periodic surface spatially coherent modes of motion can coexist associated with different average velocities due to resonant parametric forcing of the particle fluctuations by the center of mass motion. Depending on the coupling strength κ and size of the array N, jumps in the minimum friction (maximum velocity) exhibited by the array occur at $\kappa_m(N) \sim (N/m)^2$ as new modes stabilize and are selected by the dynamics. The existence of such coherent modes allows both an effective low dimensional description of the dynamics to exist and the possibility for control of friction close to these instabilities.

PACS numbers: 46.55.+d, 05.40.–a, 81.40.Pq

New developments in nanoscale technology [1] make it important to understand the motion of driven nonlinear particle arrays and clusters on periodic and disordered substrates. In this mesoscale regime, in addition to conventional single particle phononic and electronic dissipation mechanisms [2], the friction of a nonlinear system can be significantly affected by the dynamical properties of the array as a whole.

In this Letter, we address this specific question of how friction in small driven nonlinear particle arrays depends on the form of spatiotemporal fluctuations of individual particles in the array about their center of motion. We study how the energy is transferred between the center of mass motion and these fluctuations, and, consequently, how the degree of phase synchronization in the array affects its velocity. Since the arrays are highly nonlinear, we expect that several spatiotemporal modes of motion are possible for a fixed set of control parameters each with its own associated frictional properties. We find that the maximum average center of mass velocity (or the minimal friction coefficient) undergoes a set of transitions as the array coupling or the number of particles in the array N are varied. These results suggest that close to these instabilities which occur in arrays of well-defined quantized sizes there exists the strong possibility that small perturbations may be used to switch the array dynamics and thus control friction [3].

The basic equations for the driven dynamics of a one-dimensional particle array of N identical particles moving on a surface are given by a set of coupled nonlinear equations of the form [2]

$$\mu \ddot{x}_j + \gamma \dot{x}_j = -\partial U/\partial x_j - \partial V/\partial x_j + f_j + \eta(t), \tag{1}$$

where x_j is the coordinate of the jth particle, μ is its mass, γ is the linear friction coefficient representing all single particle energy exchange with the substrate, f_j is the applied external force, and $\eta(t)$ is the Gaussian noise. The particles are subjected to a periodic potential $U(x_j + a) = U(x_j)$ and interact with each other via a pair-wise potential $V(x_i - x_j)$ which typically has an equilibrium separation b which may be incommensurate with a.

This set of equations provides a generic framework for the modeling of dry friction in nonconfined systems though the level of detail in the particle-substrate and particle-particle interactions and the dimensionality of the model varies in different studies from 1D models [4], through generalizations to 2D models [5] to full sets of molecular dynamics simulations [6].

Numerically we study the case where the substrate potential has a simple periodic form, the interparticle interaction is via Morse potential, and the same force f is applied to each particle. We are interested in the regime where the nonlinearities are important, specifically where the time average of the substrate force $\overline{-\partial U/\partial x}$ is significant compared to the driving, and the average velocity of the chain $v_{av} \ll f/\gamma$ is much smaller than the single particle limit. Using the dimensionless phase variable $\phi = 2\pi x/a$, where a is the lattice periodicity, Eq. (1) reduces to

$$\ddot{\phi}_n + \gamma \dot{\phi}_n + \sin(\phi_n) = f + (\kappa/\beta)[F(\beta(\phi_{n+1} - \phi_n - p_0)) - F(\beta(\phi_n - \phi_{n-1} - p_0))], \tag{2}$$

where $F(x) = \exp(-x) - \exp(-2x)$, κ is the dimensionless coupling constant (the ratio of the strength of interparticle interaction to the strength of the periodic potential), β is the nonlinearity parameter (β^{-1} is the range over which the nearest-neighbor coupling is effectively linear), $p_0 = (b - a)/a$ is the misfit length, and we consider periodic boundary conditions. For very small values of $\beta \to 0$, Eq. (2) reduces to the Frenkel-Kontorova model

$$\ddot{\phi}_n + \gamma \dot{\phi}_n + \sin(\phi_n) = f + \kappa(\phi_{n+1} - 2\phi_n + \phi_{n-1}). \tag{3}$$

 0031-9007/99/83(1)/104(4)$15.00 © 1999 The American Physical Society

The dissipative dynamics of the Frenkel-Kontorova model has been extensively studied [7]. This model provides a reasonable understanding of the mechanisms in dry friction, in particular when the interatomic potential is of the same order or larger than the substrate potential (the case of intermediate or strong coupling κ).

To study the influence of spatiotemporal fluctuations on dry friction we therefore first separate the center of mass motion of the array from the spatiotemporal fluctuations which dissipate only energy. This proposed analysis of the motion allows a low dimensional reduced description of the dynamics in which only a few key variables capture its main features. For such coherent states it is possible to justify the use of phenomenological models [8], and it becomes possible to extract both the form of the equations of motion for the key state variables describing the dynamics, and make an analysis of the parameter range for which they form an effective description.

We define the spatial average $\langle X\rangle(t) = 1/N \sum_n X_n(t)$, and the temporal average $\overline{X_n} = 1/T \int_t^{t+T} X_n(t)\,dt$ for any array variable of interest $X_n(t)$. Then we split the dynamics into a center of mass contribution and a spatiotemporal fluctuation by

$$\phi_n(t) = \phi(t) + \psi_n(t)\,, \tag{4}$$

where $\langle\psi_n(t)\rangle = 0$ by construction. In terms of these variables we can equate the average energy input into the array to the average dissipation to the substrate due to the average center of mass motion, its temporal fluctuations, and the spatial fluctuations as

$$f\overline{\dot\phi} = \gamma[(\overline{\dot\phi})^2 + \overline{\delta\dot\phi^2} + \overline{\langle\dot\psi_n^2\rangle}]\,. \tag{5}$$

The center of mass motion obeys

$$\ddot\phi + \gamma\dot\phi + \sin(\phi)\langle\cos(\psi_n)\rangle + \cos(\phi)\langle\sin(\psi_n)\rangle = f\,, \tag{6}$$

while the spatiotemporal fluctuations ψ_n obey

$$\ddot\psi_n + \gamma\dot\psi_n + \sin(\phi)[\cos(\psi_n) - \langle\cos(\psi_n)\rangle] + \cos(\phi)[\sin(\psi_n) - \langle\sin(\psi_n)\rangle] = \kappa(\psi_{n+1} - 2\psi_n + \psi_{n-1})\,. \tag{7}$$

The power spectrum of the spatiotemporal fluctuations (see Fig. 1) indicates that the $\overline{\dot\phi}/2$ parametric excitation is a significant mechanism in the dynamics of the array, where $\overline{\dot\phi}$ is the average velocity of the center of mass motion. There is a qualitative similarity to the Suhl instability [9] for ferromagnetic resonance, which is a high microwave power phenomenon. The analog of the microwave field is $\partial U/\partial x$, and spin waves rather than lattice vibrations are excited. Assuming therefore that the main mechanism for the transfer of energy from the center of mass motion to the spatiotemporal fluctuations in the array is due to this subharmonic $\overline{\dot\phi}/2$ parametric resonance, we can neglect $\sin(\phi)[\cos(\psi_n) - \langle\cos(\psi_n)\rangle] \approx 0$ as it has no resonant contributions. We also make the quasilinear approximation $[\sin(\psi_n) - \langle\sin(\psi_n)\rangle] \approx C\psi_n$, where we choose $C = \sqrt{\langle\sin^2(\psi_n)\rangle - \overline{\langle\sin(\psi_n)\rangle}^2]/\overline{\langle\psi_n^2\rangle}} \approx \sqrt{1/[1 + 2\overline{\langle\psi_n^2\rangle}]}$ self-consistently so that the spatiotemporal average of the first two moments of the fluctuations are correct (the final approximation is a parametrized fit between $C \approx 1$ valid for small fluctuations and $C \approx \sqrt{1/[2\overline{\langle\psi_n^2\rangle}]}$ valid for large fluctuations). This self-consistent approximation made to yield a set of analytically tractable equations, can be justified both by their agreement with numerical results and by the fact that to order $\overline{\langle\psi_n^2\rangle}$ the fluctuations are correctly preserved. Thus Eq. (7) reduces to

$$\ddot\psi_n + \gamma\dot\psi_n + C\cos(\phi)\psi_n = \kappa(\psi_{n+1} - 2\psi_n + \psi_{n-1})\,, \tag{8}$$

and because these equations are quasilinear we make the Fourier decomposition $\psi_n(t) = \sum_m \psi_m(t)e^{i2\pi mn/N}$ to find equations of motion for the modes ψ_m

$$\ddot\psi_m + \gamma\dot\psi_m + [\Omega_m^2 + C\cos(\phi_m)]\psi_m = 0\,, \tag{9}$$

where $\Omega_m = 2\sqrt{\kappa}\sin(\pi m/N)$. Assuming that the fluctuations from the center of mass of motion are small, Eq. (6) for the center of mass motion also reduces to

$$\ddot\phi_m + \gamma\dot\phi_m + \sin(\phi_m)[1 - \psi_m^2/2] = f\,, \tag{10}$$

where in deriving Eq. (10) we assumed that the spatiotemporal dynamics consists of only one coherent mode. We now show that such mode selection indeed occurs and therefore a reduced description of the dynamics given by Eqs. (9) and (10) is possible.

In the absence of coupling Eq. (10) has a propagating solution where the center of mass of the array moves with

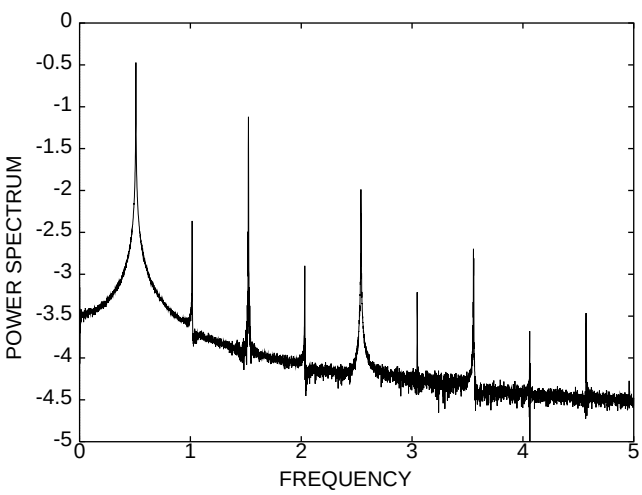

FIG. 1. The logarithm of the power spectrum $S(\omega)$ versus the scaled frequency $\omega/\overline{\dot\phi}$ of the spatiotemporal fluctuations $\psi_6(t)$ for the particle No. 6 in the $N = 25$ particle array (the power spectrum of the other particles show qualitatively very similar behavior). The other parameters are $f = 0.9$, $\gamma = 0.7$, $p_0 \approx 0.2$, $\beta \approx 0.01$, and $\kappa = 2.9$. Note the strong parametric resonance at $\omega = \overline{\dot\phi}/2$ (the highest peak).

a velocity $\omega_0 = \overline{\dot{\phi}_0}$. Let us assume that in the presence of coupling the propagating solution remains with a perturbed center of mass velocity $\omega_m = \overline{\dot{\phi}_m}$. We can therefore neglect higher harmonics and parametrize the center of mass motion as $\phi_m(t) \approx \omega_m t + B_m \sin(\omega_m t)$. In consequence we can rewrite Eq. (9) as

$$\ddot{\psi}_m + \gamma\dot{\psi}_m + [\Omega_m^2 - CJ_1(B_m) + C[J_0(B_m) + J_2(B_m)]\cos(\omega_m t)]\psi_m = 0, \qquad (11)$$

where $J_n(x)$ are Bessel functions of order n. Equation (11) clearly shows resonant parametric forcing when $\sqrt{[\Omega_m^2 - CJ_1(B_m)]} = \omega_m/2$.

A resonant solution to Eq. (11) in the form $\psi_m(t) = b_m \sin(\omega_m t/2 + \beta_m)$ exists where $b_m = \{[J_0(B_m) + J_2(B_m)]Cb_m/2\}\{[\Omega_m^2 - CJ_1(B_m) - (\omega_m/2)^2]^2 + (\gamma\omega_m/2)^2\}^{-1/2}$. Thus either $b_m = 0$, or, as $C = 1/[1 + \sum_{m'} b_{m'}^2]$, there exists for each nonzero mode an equation of the form

$$\{2/[J_0(B_m) + J_2(B_m)]\}^2\{[\Omega_m^2 - CJ_1(B_m) - (\omega_m/2)^2]^2 + (\gamma\omega_m/2)^2\} = 1 \Big/ \left[1 + \sum_{m'} b_{m'}^2\right]. \qquad (12)$$

As the left hand side of this equation takes a mode dependent value while the right hand side is mode independent, these N constraints ensure that mode selection occurs, and only one mode can exist at a time $b_m \neq 0$ and all other $b_{m'} = 0$. There are N such solutions. Each mode is spatially coherent with a different center of mass velocity and different amplitude fluctuations (see Fig. 2).

To study how the dynamics of mode m depends on system size N and coupling κ, we first note that $C = 1/\sqrt{1 + b_m^2}$, and therefore $0 < C < 1$. But $C \approx 2[\sqrt{\{[\Omega_m^2 - (\omega_m/2)^2]^2 + (\gamma\omega_m/2)^2\}} - [\Omega_m^2 - (\omega_m/2)^2]B_m] + O(B_m^2)$. These two equations are only self-consistent in a certain range $\Omega_{\min} < \Omega_m < \Omega_{\max}$. We can calculate approximately the maximal natural frequency for a mode which can exhibit a coherent spatial form as $\Omega_{\max}^2 \approx (\omega_0/2)^2 + B_0/2 + \sqrt{1 - (\gamma\omega_0/2)^2}/2$, where ω_0 and B_0 are the velocity and amplitude of temporal fluctuation of the uncoupled center of mass motion. Similarly the minimal natural frequency supporting a coherent mode is $\Omega_{\min}^2 \approx (\omega_0/2)^2 + B_0/2 - \sqrt{1 - (\gamma\omega_0/2)^2}/2$.

In this range we can solve for the average propagation velocity ω_m and relate it to the degree of spatiotemporal fluctuations in the array by using the balance between forcing and dissipation given by Eq. (5)

$$\omega_m = (f/\gamma)/[(1 + B_m^2/2) + b_m^2/8]. \qquad (13)$$

We are interested in the maximum velocity (minimum friction coefficient) of the array as we change array parameters such as the coupling strength κ, or the number of particles N in the array. In Fig. 3 we show the maximum velocity of the array as a function of the coupling strength κ. We observe quantized jumps in maximum velocity, each corresponding to a transition to a different mode of motion (described by its mode number m). Analysis of these transitions reveals that they are observed if the applied force f is slightly above the critical force to start motion. It is possible to scale the position at which these maximum velocity/minimal friction jumps occur as the coupling strength is varied using the size of the array, as $\kappa_m(N) \sim (N/m)^2$.

Our analytical results explain these quantized jumps in the maximum velocity and the associated system size scaling with N observed in the numerical simulations. As $\Omega_m = 2\sqrt{\kappa}\sin(\pi m/N)$, we see that $\Omega_1 \approx 2\pi\sqrt{\kappa}/N < \Omega_2 < \cdots < \Omega_{N/2} = 2\sqrt{\kappa}$, and therefore a series of dynamical transitions can occur as κ is decreased (for fixed N), or N is increased (for fixed κ). For very large coupling strength or small system size $\Omega_1 > \Omega_{\max}$, there are no coherent modes and a synchronous dynamics is observed. When the coupling is reduced sufficiently so that $\Omega_1 < \Omega_{\max}$ but $\Omega_2 > \Omega_{\max}$ a single coherent mode exists with high center of mass velocity $\omega_1 \approx \omega$. As the coupling is reduced further the spatial fluctuations in mode 1 increase as resonance is approached $\Omega_1 \to \omega/2$ causing ω_1 to decrease in turn. As κ is decreased or the system size N is increased still further, new modes become stable and several possible modes of motion can exist for the array. In general as each new mode becomes stable it will have the highest center of mass velocity because it is furthest from resonance and therefore its fluctuations which only dissipate energy without contributing to the center of mass motion are small. Thus a quantized jump in maximum velocity will occur each time a new mode appears with $\Omega_m = \Omega_{\max}$, or $\kappa_m(N) \approx (\Omega_{\max}N/2\pi m)^2$, in agreement with the observations from numerical simulations of Eq. (2).

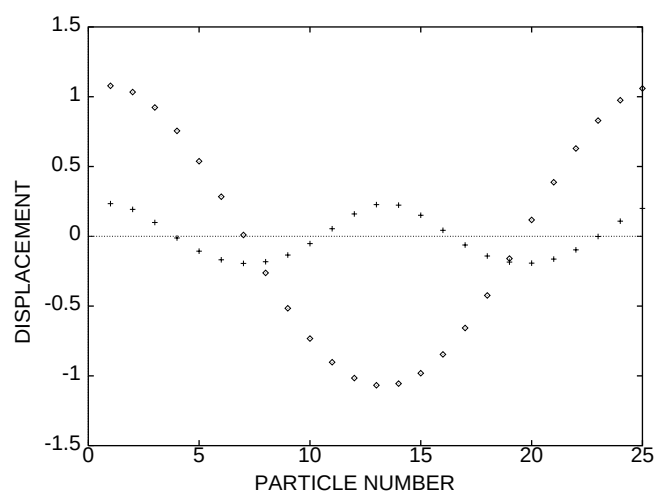

FIG. 2. A snapshot at one instant of time of the spatiotemporal fluctuations $\psi_n(t)$ versus the particle number n. The ◇ symbols represent mode 1 ($\kappa = 10$), while the + symbols represent mode 2 ($\kappa = 2.9$). The other parameters are the same as in the Fig. 1. The strong coherence in the dynamics is evident.

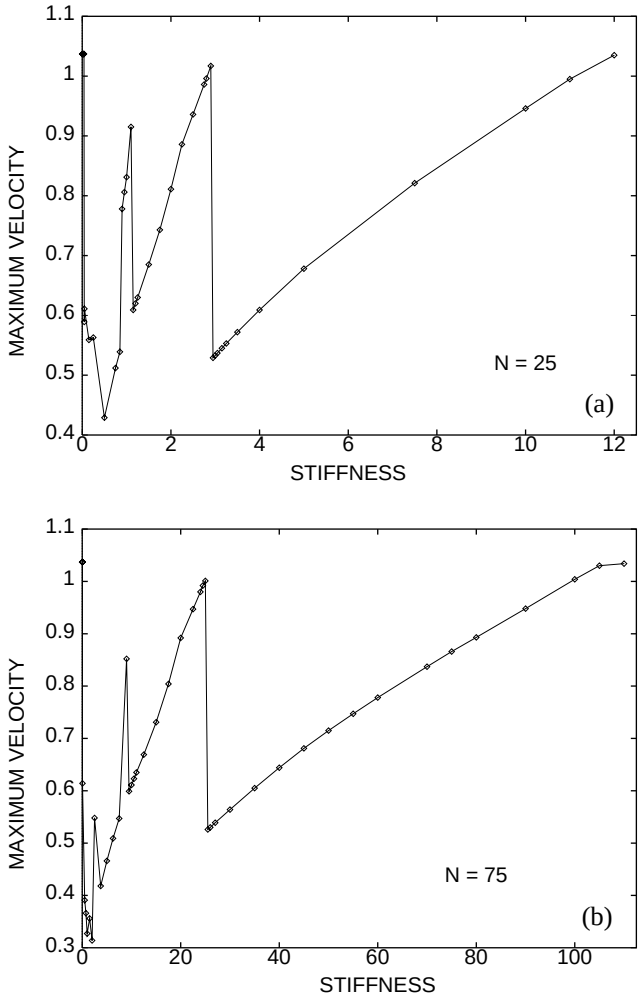

FIG. 3. Maximal average velocity $V_{\max}$ as a function of the coupling κ for (a) $N = 25$ particle array and (b) $N = 75$ particle array. Note the dynamical scaling with system size N provided the array coupling κ is properly scaled. The parameters are the same as in Fig. 1.

As κ is reduced still further so that $\Omega_1 < \omega/2$ modes very close to resonance will always exist and a better ansatz for their spatial fluctuations will be of the form $\psi_m(t) = b_m \sin(\omega_m t/2 + \beta_m) + a_m \sin(\Omega_m t + \alpha_m)$. Under these circumstances the amplitude of the periodic solution of frequency $\omega/2$ will be modulated by a beat frequency of magnitude $\Omega_{\text{beat}} = \Omega_m - \omega/2$. Such predicted beat effects in the dynamics are indeed observed numerically. Finally at low enough values of the coupling or for large enough arrays we will have the condition $\Omega_{N/2} < \Omega_{\min}$. At this point a transition back to synchronous motion occurs. This happens for a coupling strength $\kappa_{\min} = (\Omega_{\min}/2)^2$, which is independent of the system size and is again in agreement with numerical simulations.

In this Letter, we have considered the dynamics of ultrasmall chains with $10 < N < 100$ particles. These resonance phenomena may disappear for larger arrays because of the density of states available for the fluctuations. At the nanoscale, however, chains of particles, clusters, and indeed more complex atomic architectures driven across surfaces can be expected to exhibit a variety of unusual coherent modes of motion and frictional properties, which may have important technological implication if such switching between these dynamical states can be performed in a controlled fashion, for example by using small additional perturbations close to the instabilities, or by making small changes in the material properties of the surface.

We would like to thank Dr. V. Protopopescu for his helpful comments and suggestions on the manuscript. This research was supported by grants from the Office of Naval Research and the National Science Foundation. Additional support was provided by the Engineering Research Program of the DOE Office of Basic Energy Science under Contract No. DE-AC05-96OR22464 with Lockheed Martin Energy Research Corporation.

[1] R. Mabaudian, MRS Bull. **23**, 47 (1998).
[2] B. N. J. Persson, *Sliding Friction* (Springer, New York, 1998).
[3] It has been recently suggested that a feedback control method can stabilize unstable orbits in frictional dynamics [M. G. Rozman, M. Urbakh, and J. Klafter, Phys. Rev. E **57**, 7340 (1998); F. J. Elmer, Phys. Rev. E **57**, R4903 (1998)]. Experimental [M. Heuberger, C. Drummond, and J. Israelachvili, J. Phys. Chem. B **102**, 5038 (1998)], and the full-scale MD simulations [J. Gao, W. D. Luedke, and U. Landman, J. Chem. Phys. B **102**, 5033 (1998)] showed that tiny vibrations applied to the moving surfaces lead to dramatic changes in the sliding properties of the system.
[4] Y. Braiman, F. Family, and H. G. E. Hentschel, Phys. Rev. E **53**, R3005 (1996); Phys. Rev. B **55**, 5491 (1997); M. Weiss and F-J. Elmer, Phys. Rev. B **53**, 7539 (1996); Z. Phys. B **104**, 55 (1997); F-J. Elmer, J. Phys. A **30**, 6057 (1997).
[5] B. N. J. Persson and A. Nitzan, Surf. Sci. **367**, 261 (1996); E. D. Smith, M. O. Robbins, and M. Cieplak, Phys. Rev. B **54**, 8252 (1996); O. M. Braun, T. Dauxois, and M. Peyrard, Phys. Rev. B **56**, 4987 (1997).
[6] B. Brushan, J. Israelachvili, and U. Landman, Nature (London) **374**, 607 (1995); U. Landman, W. D. Luedtke, and J. P. Gao, Langmuir **12**, 4514 (1996).
[7] L. M. Floria and J. J. Mazo, Adv. Phys. **45**, 505 (1996); O. M. Braun, T. Dauxois, M. V. Paliy, and M. Peyrard, Phys. Rev. Lett. **78**, 1295 (1997); Phys. Rev. E **55**, 3598 (1997); M. V. Paliy, O. M. Braun, T. Dauxois, and Bambi Hu, Phys. Rev. E **56**, 4025 (1997).
[8] M. G. Rozman, M. Urbakh, and J. Klafter, Phys. Rev. Lett. **77**, 683 (1996); Phys. Rev. E **54**, 6485 (1996); J. M. Carlson and A. A. Batista, Phys. Rev E **53**, 4153 (1996); B. N. J. Persson, Phys. Rev. B **55**, 8004 (1997).
[9] H. Suhl, J. Phys. Chem. Solids **1**, 209 (1957).