Friction at the Nanoscale[†,‡]

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Dissipation mechanisms at the nanoscale are influenced by finite size effects that may significantly affect the frictional response of sliding objects. In particular, locking of temporal and spatial dynamics may introduce several distinct modes of motion leading to friction selection. Here, we discuss such nonlinear mechanisms leading to stick−slip dynamics at the atomic scale.

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 regime, new forms of energy flow through the mesoscopic system and dissipation to the underlying substrate can dominate the frictional properties of mesoscopic particle arrays. In addition to the conventional dissipation mechanisms due to phononic[2,3] and electronic[2,4] friction, nonlinear systems can be significantly affected by the dynamical properties of the strongly coupled array as a whole. In general, nonlinear systems driven far from equilibrium can exhibit a variety of complex spatial and temporal behaviors. In particular, fluctuations of the individual elements about the center of mass motion can exhibit a variety of coherent modes of motion, each corresponding to a different frictional response.

In this paper, we address the specific question of how dissipation in such small driven nonlinear particle arrays depends on the form of spatiotemporal dynamics of the particles. We will describe the manner in which energy is transferred between the center of mass motion and its spatiotemporal fluctuations, and, consequently, how the degree of phase synchronization in the array affects its velocity of motion. As our arrays are highly nonlinear, we expect that several spatiotemporal modes of motion are possible for a fixed set of control parameters each associated with its own particular frictional properties. We will find that for certain types of dynamics we can derive an approximate relation between the average velocity of the chain and its spatial and temporal fluctuations.

It has recently been shown[5−7] that simple phenomenological models of friction, which are typically low dimensional compared to the large number of degrees of freedom available in the array, give reasonable agreement with the experimental results on nanoscale friction.[8,9] A possible explanation for this agreement is the following observation: a nonlinear dynamical system can exhibit a variety of modes of motion including chaotic behavior; if the dynamics is synchronized, however, as is the case for kinks or solitons, a reduced description, keeping only a few macroscopic variables, can capture the main features of the dynamics of the driven array. Therefore, in this situation the most valuable information lies in identifying this reduced description.

Here, we demonstrate the efficiency of this approach. We derive a relatively simple set of equations which correctly capture the dynamics of a nonlinear one-dimensional array of particles sliding on a periodic surface. The equations are structure dependent, in the sense that the parameters in the equation depend on the particular mode of motion, and the resulting friction depends on the degree of phase synchronization of the array. Analysis of this reduced set of equations of motion also suggests that the average velocity in the array (or associated friction coefficient) undergoes a set of abrupt transitions as the coupling coefficient or number of particles in the array is varied. Each transition corresponds to a new dynamical state with a different mode of locking temporal and spatial dynamics. This is a generic phenomenon observed in the dynamics of driven nonlinear arrays[10,11] and, for example, also appears in the dynamics of parallel arrays of Josephson junctions.[12,13]

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[14]

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

where x_j is the coordinate of the *j'th* particle, m 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 pairwise potential $V(x_i - x_j)$.

Equation 1 provides a general framework for modeling friction. However, the details and the complexity of the resulting coupled equations vary in different studies.[15−22] Here, we will specifically consider the case where the substrate potential has a simple periodic form, there is a zero misfit length between the array and the substrate, the same force f is applied to each particle and the particle coupling is linear. The coupling with the substrate is, however, strongly nonlinear. For this case, using the dimensionless phase variable $\phi = 2\pi x/a$, the equation of motion reduces to the dynamic Frenkel−Kontorova model,

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

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which has been extensively studied (for example, see ref 23 and references therein). Our motivation is to understand how the spatiotemporal fluctuations in the array affect the motion of the center of mass. A critical parameter in eq 2 is κ, the ratio between the interparticle to substrate particle potential.

In the limit $\kappa \ll 1$, where the substrate potential dominates the interparticle interactions, we find that the family of wave-propagating solutions[10] defined by

$$x_j(t) = x(t - j\tau) + x(t + j\tau) \tag{3}$$

where τ is a characteristic time scale, may adequately characterize the emerging dynamics. We find that for a given set of values of the external force f and the linear friction coefficient γ, there is a critical value of the coupling constant κ_c, below which the linear wave (defined by eq 2) will not propagate across the array. Here we will focus on the behavior of the chain in the close vicinity of this critical coupling as $\kappa \rightarrow \kappa_c$. At $\kappa = \kappa_c$, the motion is localized; at each moment effectively only one oscillator moves, driven by the force applied from its neighbors. This force can be to a high degree of accuracy approximated as a constant by assuming $x_{j+1} = y + 2\pi$ and $x_{j-1} = y$, where $y = \sin^{-1} f$, is the stable fixed point of the single uncoupled oscillator. Thus, an approximate one-oscillator equation can be derived

$$\ddot{x} + \gamma\dot{x} + \sin x = f + \kappa(y + 2\pi + y - 2x) \tag{4}$$

Equation 4 represents the lowest order in a sequence of n-cluster approximations in which N coupled oscillators are treated exactly in the presence of a force generated by the remaining quiescent oscillators assumed to take the values $x_{right} = y + 2\pi$ and $x_{left} = y$ representing a linear wave propagating through the array from right to left.

The minimal value of the average velocity $v_0 = \langle\dot{x}\rangle$ is given by $v_0 = 2\pi/T_N$, where T_N is the period of oscillation for the complete set of N oscillators in the array. For free-end boundary conditions, $T_N = 2N\tau$, while for periodic boundary conditions we similarly have $T_N = N\tau$. Therefore, writing in general $T_N = nN\tau$ (n is an integer), the minimal velocity is given by $v_0 = 2\pi/nN\tau$.

We approximate the characteristic time τ for the excitation to be passed between oscillators (a property of the array) by $\tau = T$, where T is the time each oscillator moves separately. Therefore, τ and consequently the velocity can be calculated using eq 4 together with the matching initial conditions,

$$x(0) = sin^{-1} f = y \tag{5a}$$

$$\dot{x}(0) = 0 \tag{5b}$$

To find T, we integrate eq 4. To a good approximation, as $\kappa \rightarrow \kappa_c$ this time period is given by the expression 10:

$$T \approx \gamma \sqrt{\frac{\pi}{\pi - \cos^{-1} f}}(\kappa - \kappa_c)^{-1/2} \tag{6}$$

This leads to the following expression for the minimal velocity of the chain:

$$v_0 = \frac{2\pi}{nN\gamma}\sqrt{\frac{\pi - \cos^{-1} f}{\pi}}(\kappa - \kappa_c)^{1/2} \tag{7}$$

and, to leading order the average velocity scales as $(\kappa - \kappa_c)^{1/2}$. The nonlinear friction coefficient defined as $\eta = (f/v_0 - \gamma)/\gamma$ in consequence diverges as $\eta \propto (\kappa - \kappa_c)^{-1/2}$ and is given by the expression

$$\eta = \frac{nNf}{2\pi}\sqrt{\frac{\pi}{\pi - \cos^{-1} f}}(\kappa - \kappa_c)^{-1/2} - 1 \tag{8}$$

where the critical value of the coupling $\kappa_c(f,\gamma)$ is a function of the forcing f and linear friction γ and an upper bound is given by the high linear friction limit

$$\kappa_c(f,\gamma) \leq \kappa_c(f,\infty) \approx \frac{(1 - f)}{2(\pi - \cos^{-1} f)} + \frac{(1 - f)^2}{4(\pi - \cos^{-1} f)^3} + ... \tag{9}$$

where the right-hand side of eq 9 is valid as $f \rightarrow 1$.

Equation 8 indicates that the friction coefficient of an array can get much larger than the friction coefficient of a single uncoupled oscillator, even though the same constant force is applied to each oscillator in the array. In fact, as $\kappa \rightarrow k_c$, the friction coefficient is proportional to the size of the chain $\eta \propto N$, while the motion of the center of mass tends to zero due to large fluctuations of the particles in the array about the center of mass.

This description leads to a deeper understanding of the mechanism of the stick−slip motion in friction. If $f_{min} < f < 1$ (f_{min} is the minimal value of the force to obtain nonzero average velocity solution), two distinct solutions are possible, depending on the initial conditions. The first is the fixed point, defined by $\sin x = f$. This solution corresponds to the static solution, $v_{av} = 0$, when all the particles in the chain are inside their potential wells. The second solution is the limit cycle, corresponding to a running solution $v_{av} > 0$ with the particles hopping over the potential maxima. For $\kappa \rightarrow \kappa_c$, this dynamic phase can further be understood in terms of a mechanism involving a single slipping oscillator and $N - 1$ oscillators in a stick phase.

We now consider the situation where the coupling constant κ is not small.[11] This corresponds to the case where the contribution from the substrate potential is equal to or less than the contribution from the interparticle interaction. In this case, the dynamics of the array may reveal the structure of the propagating spatial modes, each depending on the initial conditions and the parameters of the system.

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

$$\phi_n(t) = \phi(t) + \psi_n(t) \tag{10}$$

where $\langle\psi(t)\rangle = 0$ 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

$$f\bar{\dot{\phi}} = \gamma[\bar{\dot{\phi}} + \overline{\delta\dot{\phi}^2} + \overline{\langle\dot{\psi}_n^2\rangle}] \tag{11}$$

Exact coupled equations of motion for the center of mass dynamics and the fluctuations can be derived. The center of mass motion obeys

$$\ddot{\phi} + \gamma\dot{\phi} + \sin\phi\,\langle\cos\psi_n\rangle + \cos\phi\,\langle\sin\psi_n\rangle = f \tag{12}$$

Assuming the fluctuations to be small, eq 12 reduces to $\ddot{\phi} + \gamma\dot{\phi} + \sin\phi\,[1 - \langle\psi_n^2\rangle/2] = f$. This equation has a propagating solution where the center of mass of the array moves with velocity ω. While the spatiotemporal fluctuations ψ_n obey

$$\ddot{\psi}_n + \gamma\dot{\psi}_n + \sin\phi\,[\cos\psi_n - \langle\cos\psi_n\rangle] + \cos\phi\,[\sin\psi_n - \langle\sin\psi_n\rangle] = \kappa(\psi_{n+1} - 2\psi_n + \psi_{n-1}) \quad (13)$$

We assume 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 a subharmonic $\omega/2$ parametric resonance.[11]

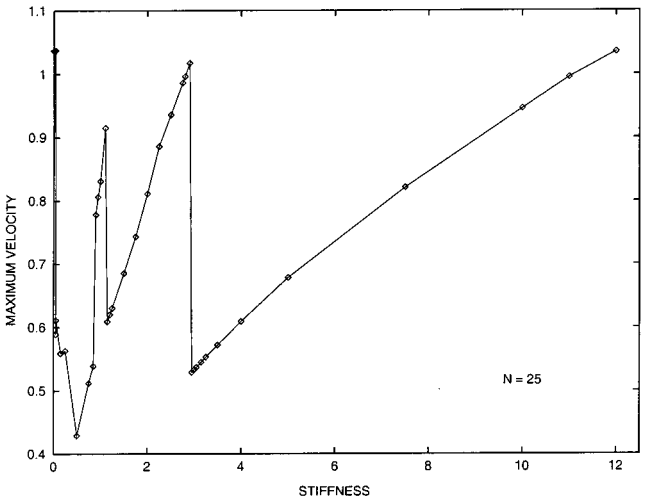
Then the term $\sin(\phi)[\cos(\psi_n) - \langle\cos(\psi_n)\rangle] \approx 0$ as there are no resonant contributions present. We also make the self-consistent approximation $[\sin(\psi_n) - \langle\sin(\psi_n)\rangle] \approx C\psi_n$ (this assumption is well supported by our numerical results) by replacing the nonlinear term with a quasilinear term. We also choose C so that the spatiotemporal average of the first two moments of both terms would be identical:

$$C = \sqrt{[\overline{\langle\sin^2\psi_n\rangle} - \overline{\langle\sin\psi_n\rangle}^2]/\overline{\langle\psi_n^2\rangle}} \approx \sqrt{1/[1 + 2\overline{\langle\psi_n^2\rangle}]}$$

Therefore, we finally need to analyze

$$\ddot{\psi}_n + \gamma\dot{\psi}_n + C\cos\phi\,\psi_n = \kappa(\psi_{n+1} - 2\psi_n + \psi_{n-1}) \quad (14)$$

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



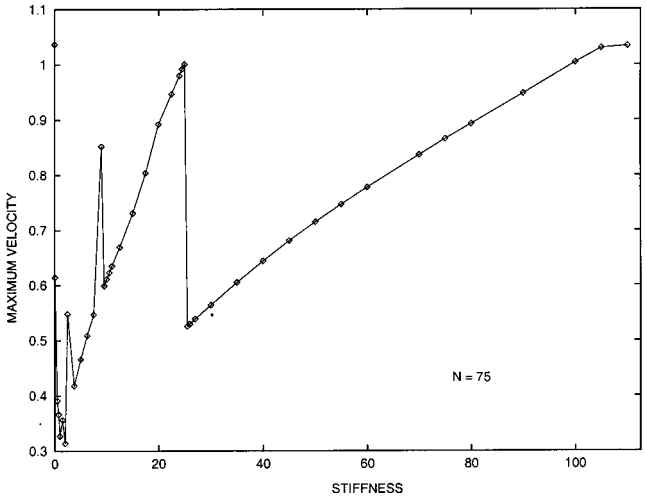


Figure 1. Maximal average velocity V_{max} as a function of the coupling k for (a) $N = 25$ particle array and (b) $N = 75$ particle array. Note the dynamical scaling with system size N provided the array coupling κ is properly scaled.

$$\ddot{\psi}_m + \gamma\dot{\psi}_m + [\Omega_m^2 + C\cos\phi]\psi_m = 0 \quad (15)$$

where $\Omega_m = 2\sqrt{\kappa}\,\sin(\pi m/N)$.

We now parametrize the center of mass motion as $\phi(t) = \phi_0 + wt + B\sin(\omega t)$ and a solution for the mth mode of the form $\psi_m(t) = b_m \sin(\omega t/2 + \beta_m)$. The expression[11] for the center of mass velocity in the mode m is then

$$v_m = (f/\gamma)/[(1 + B^2/2) + b_m^2/8] \quad (16)$$

The friction coefficient $\eta_m \equiv (f/v_m - \gamma)/\gamma$ is $\eta \approx B^2/2 + b_m^2/8$. This result clearly indicates that the average velocity of the center of mass decreases with the increase in spatial fluctuations.

In Figure 1, 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 a mode number m). We also indicate that the maximum velocity at a given mode of motion m decreases as a function of the coupling strength κ. This behavior can be explained if we assume that the degree of phase synchronization diminishes when the coupling strength between the particles in a chain decreases.

We have considered the dynamics of small atomic chains with $10 < N < 100$ particles. Our numerical observations and theoretical analysis suggest that size effects might significantly alter frictional response of the sliding nanosystem. These resonance phenomena may disappear for larger arrays because of the density of states available for the fluctuations. At the mesoscale, however, chains of particles, clusters, and indeed more complex atomic architectures driven across surfaces can be expected to exhibit a variety of coherent modes of motion as well. Some indirect preliminary evidence that phase synchronization can affect friction in a mesoscopic system might be attributed to the most recent findings indicating that small amounts of noise or/and spatial quenched disorder can significantly reduce friction coefficient.[24−26]

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