Nonlinear friction of a damped dimer sliding on a periodic substrate

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The nonlinear sliding friction of a dimer over a substrate is studied within a one-dimensional model, consisting of a vibrating dimer (two masses connected by a spring), internally damped, sliding over a sinusoidal potential. Molecular dynamics simulations show that the friction force has an approximate $v^{-3}$ dependence if the velocity is sufficiently large, and that there is a striking periodic variation of the proportionality coefficient with the ratio of the length of the dimer to the substrate wavelength. The nonlinear velocity dependence was predicted earlier for a Langevin model of an adsorbed layer in the presence of strong external force. We study it here in detail in the transient regime and without external force. We obtain the dependence on key parameters (internal dissipation, dimer mass, substrate corrugation, and length ratio), and examine the validity of the friction law. A semi-analytical expression is suggested which confirms the numerical observations in the high-velocity regime.

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I. INTRODUCTION

In the last two decades much progress has been made in the fundamental understanding of the origin of friction.\textsuperscript{1} The significance of this progress is particularly clear if we compare it with what had been done in the centuries after the friction laws were stated by Amonton and Coulomb, and elaborated upon by Leonardo da Vinci.\textsuperscript{2} Microscopic experiments on friction,\textsuperscript{3} and subsequent theory and simulation were started only in the last 15 years.\textsuperscript{4–7} Of the work that remains to be done to achieve a coherent picture of this complex phenomenon, an important aspect concerns nonlinear sliding friction. In his seminal paper,\textsuperscript{8} Persson presented numerical findings of the sliding friction of a dimer from that observed in an extended adsorbate. To answer the first two of these questions, we present here results for a sliding dimer over a periodic substrate potential. The nonlinear part of the friction, and at the same time to improve the signal-to-noise ratio, we perform simulations at zero temperature and without external dissipation: friction acts, in our model, only on the internal motion. We focus on the time behavior of this dimer in the absence of external forces. We compare our results with the prediction of Persson for the adsorbate with external force, and look for similarities and differences. We also suggest an analytical explanation supporting our results.

II. MODEL

A single particle moving in a periodic potential provided by the substrate would not exhibit friction as its energy would be repeatedly transformed from potential to kinetic, with no overall depletion. Some studies have addressed the effective friction of such a particle in the presence of noise. Such noise can be externally imposed\textsuperscript{10,11} or produced effectively by the motion of a harmonic chain of atoms (rather than a fixed potential) as representing the substrate.\textsuperscript{12} We consider the system in the absence of noise. In the sliding object, let a second particle be attached to the first. A part of its sliding energy can be converted into internal vibrational energy. It is trivial to see that the equations

\begin{equation}
\begin{align*}
m\ddot{x}_1 &= +k(x_2 - x_1 - a) + \frac{2\pi u_0}{b}\sin\left(\frac{2\pi x_1}{b}\right), \\
m\ddot{x}_2 &= -k(x_2 - x_1 - a) + \frac{2\pi u_0}{b}\sin\left(\frac{2\pi x_2}{b}\right),
\end{align*}
\end{equation}

where $x_{1,2}$ are the coordinates of the two particles of equal mass $m$, and $k$, $a$, $b$, $u_0$ are, respectively, the spring constant, equilibrium length of the dimer, wavelength of the substrate...
potential and half the amplitude of the potential, which lead to coupled equations for the center of mass coordinate $x_+$ and the internal coordinate $x_-$. The latter are defined as half the sum and difference of $x_1, x_2$, respectively. It is the presence (and additionally, the nonlinearity) of the substrate potential that is responsible for the coupling between the otherwise independent coordinates $x_+$ and $x_-$. Analytic solutions of the coupled equations do not appear possible. The dynamics can be very complex depending on the initial energy, and numerical procedures become necessary.

The “normal” behavior of the dimer includes oscillations within potential barriers for low initial energy, and ballistic motion for high initial energy but with a velocity periodically modulated by the substrate potential. As the initial energy is increased, this oscillation becomes smaller compared to the dc component. For an intermediate narrow range of initial energies, the evolution is unpredictable and exhibits chaos. As an illustration of some of this behavior, we show in Fig. 1 the center of mass evolution for two different initial velocities, below and above the upper chaos threshold, respectively. The behavior in the intermediate region shows three characteristics as a result of the interchange of energy between translational and vibrational modes: forward movement, backward movement, and temporar...
NONLINEAR FRICTION OF A DAMPED DIMER... PHYSICAL REVIEW B 70, 195415 (2004)

FIG. 3. Evidence for our proposed power law ($\alpha=3$). Shown is the relation between the apparent stopping time $t_s$ and the initial velocity $v_0$, for $a/b=2$ and different sets of $\gamma$, and $k$. Velocity and the stopping time are given in units of $\sqrt{u_0/m}$ and $b\sqrt{m/u_0}$, respectively; $\gamma$ is in units of $u_0/m$, and $k$ in units of $u_0/b^2$. The lines are a linear regression of the log-log relation given consistently by an exponent $\approx 4$, thus $\alpha \approx 3$.

\[ t_s = \frac{v_0^{\alpha+1}}{(\alpha + 1) \eta}. \] (5)

We plot in Fig. 3 the velocity dependence of the numerically obtained apparent stopping time and interpret it in terms of Eq. (5). The plot provides clear evidence that the exponent in expression (5) is $\alpha \approx 3$, with less that 2% error.

How does the coefficient $\eta$ of this sliding friction depend on the topology and dynamics of the system? To answer this question, we vary the parameters $a$, $b$, $u_0$, $k$, $m$, and $\gamma$, and the initial velocity $v_0$ over wide regions. In fact it is only necessary to do this for the relevant dimensionless quantities $a/b$, $k b^2/u_0$, and $\gamma b\sqrt{m/u_0}$, and the initial dimensionless velocity $v_0/\sqrt{m/u_0}$. The striking results are in Fig. 4. In addition to confirming that the coefficient of proportionality $\eta$ is directly proportional to $\gamma^3$, and also proportional to $(u_0/m)^2$, but independent of $k$, we find an important result. The coefficient $\eta$ has a periodic dependence on $a/b$ fitted excellently by a simple sinusoid. All these results may be combined into the following phenomenological friction law we propose:

\[ \frac{dv}{dt} = -\gamma \left( \frac{U_0}{2m} \right)^2 \sin \left( \frac{\pi a}{b} \right) v^3. \] (6)

FIG. 4. Periodic dependence of the friction coefficient $\eta$ on the ratio of the dimer length to substrate wavelength. Plotted is $\eta$ in units of $\gamma U_0(m)^2$ vs $a/b$.

Agreement of the predictions of our law with numerical simulations is remarkably good provided the initial velocity is large enough and the times are not too close to the stopping time. We will elaborate on its limitations below.

IV. ANALYTICAL CALCULATION

The internal coordinate $x_\pm$ has the natural frequency $\omega_0 = \sqrt{2k/m}$. When scaled and translated through $\xi = \left( x_\pm / a/2 - 1 \right)$, the internal coordinate obeys [see Eq. (2)] the damped driven oscillator equation

\[ \frac{d^2 \xi}{dt^2} + \gamma \frac{d\xi}{dt} + \omega_0^2 \xi = \left( \frac{4mU_0}{amb} \right) \sin \left( \frac{\pi a}{b} \right) \left( 1 + \xi \right) \times \cos \left( \frac{2\pi x_\pm(t)}{b} \right). \] (7)

The complexity of this equation relative to that for a harmonic oscillator driven linearly through a sinusoidally varying forcing term arises from two factors that appear on the right hand side: the $\xi$ dependence of the sin term and the generally nonsinusoidal $t$ dependence of the cos term. In Fig. 5 we have shown the behavior of the internal coordinate in a typical case. We see there that the internal coordinate has a small amplitude of oscillation supporting the $x \ll a/2$ assumption; $x$ is in units of $b$, time is in units of $b\sqrt{m/u_0}$, and parameters are the same as in Fig. 2.

\[ \cos \left( \frac{2\pi x_\pm(t)}{b} \right) = \cos \left( \frac{2\pi}{b} \int_0^t v(s)ds \right) = \sum_i B_i \cos(\omega_i t), \] (8)

where the complex $t$ dependence of the center of mass velocity has been resolved into Fourier components of frequencies $\omega_i$ and coefficients $B_i$. With the notation $A_j = (2/a) \times (2\pi m b) \sin(\pi a/b) B_j$, we therefore study the linear damped oscillator

\[ \frac{d^2 \xi}{dt^2} + \gamma \frac{d\xi}{dt} + \omega_0^2 \xi = \sum_i A_i \cos(\omega_i t) \] (9)

whose behavior is known from textbooks. The coordinate $\xi$ may be decomposed into components $\xi_i$, each of which satisfies, after transients have died down...
\[ \xi(t) = \frac{A_i}{\sqrt{(\omega_i^2 - \omega_j^2)^2 + \omega_j^2 \gamma^2}} \cos(\omega_j t - \delta_i), \]  

where the lag factor \( \delta_i \) equals \( \tan^{-1}(\omega_i \gamma/(\omega_i^2 - \omega_j^2)) \) for each Fourier component. Dissipation of energy from the center of mass motion into the internal coordinates occurs at the rate \( R \) given by 

\[ R = \frac{m \gamma}{2} \sum_i \frac{A_i^2 \omega_i^2}{(\omega_i^2 - \omega_j^2)^2 + \omega_j^2 \gamma^2} = \frac{m \gamma}{2mb} \sin^2\left(\frac{\pi a}{b}\right) \sum_i \frac{B_i^2 \omega_i^2}{(\omega_i^2 - \omega_j^2)^2 + \omega_j^2 \gamma^2}. \]  

We will now restrict our analysis to situations and time domains in which we can replace the \( i \) sum by a single term involving an average frequency \( \omega_a \), which may be weakly dependent on time. We then have 

\[ \cos\left(\frac{2 \pi}{b} \int_0^t v(s)ds\right) = \cos(\omega_a t), \]

\( \omega_a \) being related to the center of mass velocity \( v(t) \) through \( \omega_a = 2 \pi \nu(t)/b \) (the “washboard” frequency). Consider now the case that the washboard frequency \( \omega_a \) is much larger than the natural frequency \( \omega_0 \) and the damping rate \( \gamma \). We can then write

\[ R = \frac{m \gamma}{2mb} \sin^2\left(\frac{\pi a}{b}\right) \left(\frac{1}{\omega_a}\right)^2. \]  

Equating the rate at which the internal mode gains energy to that at which the center of mass loses it, viz., \(-2m \nu (d\nu/dt)\), we get the equation for the center of mass velocity

\[ \frac{dv}{dt} = -\frac{\gamma}{2m} \frac{v_0^2}{\sin^2\left(\frac{\pi a}{b}\right)} \left(\frac{1}{v}\right). \]

This is precisely the result (6) we proposed above on the basis of an empirical inspection of our numerical results.

The analytical argument we have presented is valid under three assumptions. The first is that the amplitude of the internal dimer coordinate always remains small relative to the equilibrium value of the length of the dimer (\( \xi \ll 1 \)). The second is that the characteristic rate of variation of the center of mass velocity, viz., \((1/\nu)(d\nu/dt)\), is smaller than both the natural frequency of the internal coordinate, \( \omega_0 \), and the dissipation rate, \( \gamma \). The third assumption is that the washboard frequency \( \omega_a \) which is proportional to the center of mass velocity \( v \) is itself larger than the other characteristic frequencies, viz., \( \omega_0 \) and \( \gamma \). Of these three assumptions, the last is easiest to realize practically or understand physically. It is valid provided we take the initial velocity to be sufficiently large and the time considered not too close to the stopping time. The specific values of the initial velocity required for this validity are determined by the specific given values of the system parameters \( \omega_0 \) and \( \gamma \). In order to study the applicability of the assumptions, we present Fig. 6, where we compare the behavior of the dimer velocity according to expression (4) and with two numerical simulations made with two different values of the spring constant \( k \) separated by a factor of 500. At the time scale of the plot, it is hard to see the difference between the analytical prediction and the simulation with the smaller of the two \( k \), while for the larger \( k \) the discrepancies between simulation and analytical results are quite evident.

The origin of the periodic dependence of the friction coefficient on the ratio of the equilibrium dimer separation to the substrate wavelength, evident from Fig. 4 and from Eq. (13), should be clear from our analytic argument given at the beginning of the present section. Physically, the importance of this commensurability of dimer and substrate lengths can be understood as follows. When \( a \) equals integral multiples of \( b \), the two masses constituting the dimer feel exactly the same substrate force when in equilibrium. The overall effect of this in-phase situation is that the internal motion is never excited, and friction disappears. Analytically, this is also clear from the sine term in Eq. (13), which vanishes identically for this case. On the other hand, when \( a \) equals semi-integral multiples of \( b \), the two masses tend to be precisely out of phase (counterphase), which is the most effective situation to excite the internal motion, and gives rise to maximum friction. Analytically, this is represented by the sine term being equal to 1.

V. CONCLUSIONS

Our general aim in the present paper has been the investigation of some puzzling features of atomic friction. Specifically, we have pursued the dynamics of a model addressing the sliding friction of a dimer. The model is simple: a linear damped oscillator sliding in a sinusoidal periodic potential. Yet, except for the limitation that it is restricted to a single spatial dimension, it has the necessary and sufficient ingredients to be an acceptable model for a real dimer or molecule settled in a controlled microscopic sliding experiment. For example, a molecule sliding along channels of a crystalline well-oriented substrate might exhibit the described behavior, provided that the temperature is so low that all external
If both dynamics were present simultaneously, we expect that both kinds of sliding friction would appear: normal viscous friction derivable from substrate phonons, and the nonlinear friction because of the internal damped dimer motion that we have analyzed. Such work is under way.

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4 M. Cieplak, E. S. Smith, and M. O. Robbins, Science 265, 1209 (1994).