Simulations of the Velocity Dependence of the Friction Force

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Abstract

The motion of an elastic body over a rough surface is simulated in one dimension using Newtonian dynamics. We drive the body by prescribing a constant velocity. We extract the friction force from the work done by the applied force in order to maintain the motion of the body. A positive amount of work is needed because energy is converted into the internal elastic degrees of freedom of the body. The velocity dependence of the friction force is studied as function of the roughness of the surface and the elastic properties of the mobile body. We pay special attention to the low velocity limit. It is shown that the friction force goes to a finite value as the velocity goes to zero when the substrate is sufficiently rough to induce elastic instabilities. For smooth substrates, where elastic instabilities are absent, the friction force goes to zero when the velocity goes to zero.

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1 Introduction

The present paper represents an attempt to understand how the velocity dependence of the friction force is related to the roughness of the substrate and to the elastic properties of the sliding material.
The role friction plays in our everyday lives, and many technological applications, is immense and yet there still does not exist a successful quantitative theory that explains this phenomena. The variation of the frictional force with the sliding velocity is interesting in a practical engineering sense where the aim is to control or eliminate friction, but it is also of relevance to workers in a number of other fields. Experimentally, dynamic friction is important in the study of stick-slip motion [1], for example. Theoretically, friction is relevant, for instance, to models of earthquake faults [2, 3, 4] and railway wheel squeal [5]. In such problems a specific form of the velocity dependence of the friction force is postulated on phenomenological grounds. The friction law may be nonlocal and nonlinear [3, 5], local and nonlinear [2, 3, 5] or simply local and linear [8].

Cieplak, Smith and Robbins [9] called the linear relationship \( f_{fr}(v) \propto v \) between velocity \( v \) and the friction force \( f_{fr} \) for viscous friction in their beautiful study of the microscopic origin of the friction force. If \( \lim_{v \to 0} f_{fr} \neq 0 \) they refer to the behaviour as static friction. They found a change from viscous to static friction as the corrugation of the substrate potential is increased. We believe that this change in velocity dependence is related to the onset of elastic instabilities similar to those described in Ref. [10, 11, 12, 13, 14]. When the local curvature of the substrate potential becomes sufficiently large the static force balance equation for the individual atoms supports multiple solutions. The abrupt jump from one of these solutions to the other leads to a finite dissipation even in the limit \( v \to 0 \). Cieplak et al. discuss at the end of their paper Ref. [9] the reason why static friction is more often encountered than static friction. We suggest that the reason might be that a slight roughness at the interfaces will produce elastic instabilities and therefore a finite friction force in the limit of vanishing velocity.

Shinjo and Hirano have observed friction in a Frenkel-Kontorova type of model with added kinetic energy terms [15]. The friction force they observe in the limit of low velocity is non-zero when the coupling in the system is greater than a critical value, this being the Aubry transition point [16]. Shinjo and Hirano also found a vanishing friction force in the limit of high velocity. Their findings imply that elastic instabilities are important for the existence of a finite static friction force. This is in agreement with the work presented in the present paper. Sokoloff has also made the point that local jumping motion is essential for the occurrence of a dynamical threshold force in a microscopic model of idealized surfaces [17]. He suggests that this is probably also applicable to macroscopic surfaces if we think of these surfaces as consisting of two elastic media which interact more strongly at some points on their surfaces than others. Our macroscopic model shows behaviour which is consistent with this idea.

Sokoloff has performed simulations which give clear evidence for a transition from friction free motion to a dissipative regime as function of system size [18].
The transition can be understood in terms of Chirikov’s overlap criterion\cite{18, 19}. This criterion states that the frequency of the driving force (for instance the washboard frequency of the substrate potential) must overlap with one of the eigenfrequencies of the elastic modes in order for energy to be dissipated into the phonon system. Since the spacing between the eigenfrequencies decreases with increasing system size the overlap criterion is likely to be fulfilled as the size of the system is increased. This is what Sokoloff has demonstrated in fact happens. The elastic instability induced friction mentioned above can be seen as an alternative mechanism for inducing dissipation. Chirikov-Sokoloff resonance mechanism is of dynamical origin, whereas the elastic instability mechanism originates in the possible multivalued character of the static force balance.

A wealth of experimental work has led to the qualitative aspects of friction being well defined (for a review see \cite{11, 20, 21, 22}). Recently, interest has concentrated on a microscopic description and understanding of the origins the friction force \cite{11, 15, 23, 24}. Experimental techniques such as atomic force microscopy (AFM) \cite{25, 26} and friction force microscopy (FFM) \cite{27} allow the processes of friction to be studied in three dimensions and \textit{ab initio} molecular dynamics simulations have been used to study atomic scale mechanisms of energy dissipation \cite{4}. Work by Sokoloff \cite{8} has found the velocity dependence of the friction force in a model where the internal degrees of freedom of the moving system are subject to linear damping described by a damping coefficient $\gamma$. The obtained velocity dependence of the friction force remains unchanged in the limit of $\gamma \to 0$.

We have previously studied the limit $v \to 0$. In this limit we were able to show that in order to calculate the restoring static friction force perturbatively one must expand at least to third order in the random substrate potential \cite{14}. This is consistent with the observation that a finite static friction force is produced by the existence of non-linear elastic (or plastic) instabilities \cite{12}. We have studied the effect as well as the statistical properties of these instabilities \cite{13, 28}. In these studies we assumed that the time evolution was controled by a set of over-damped dynamical equations. We did not study the mechanisms behind the damping. In the present paper we attempt to treat the damping in a more realistic maner. We study an elastic system consisting of a large number of internal degrees of freedom (light particles) which do not interect with the external potential. These degrees of freedom act the heat bath which is able to absorb the energy released during the instabilities.

In the simplest phenomenological description one assumes some specific functional form for velocity dependence of the friction force. There are two main classes of behaviour. These are namely velocity strengthening, where the friction increases with velocity, and velocity weakening, where the opposite occurs, often
in a nonlinear fashion. A simple example of a velocity strengthening friction function is the traditional proportionality assumption $f_f = -\eta v$. However, often one observes velocity weakening of the friction force. Velocity weakening and strengthening behaviour have been observed in experiments with cast iron \cite{20} and recently with rubber against glass \cite{29} and serpentinite \cite{30}. One will expect strengthening to cross over to weakening for large velocities when the interaction time between the individual extremal point of the two sliding surfaces goes to zero. This is, indeed, what we observe in our simulations.

2 One Dimensional Model

The specific model we consider is similar to the Burridge-Knopoff spring-block model\cite{31}. This model has been studied recently by several authors\cite{2, 3, 4}. Our study differs from these investigations in the following important way. The work in Ref. \cite{2, 3, 4} assume a specific form for the velocity dependent friction force acting on the individual blocks. In the present study we use purely Newtonian dynamics and study the velocity dependence of the effective friction force produced by dissipation of kinetic energy of the blocks into internal energy of a mechanical heat bath attached to the blocks.

We have the relative motion of two macroscopic bodies in mind. We imagine the two interfaces to be rough on an atomic scale and focus on the interaction of the asperities reaching out from the two surfaces. See insert to Fig. 1. For simplicity we model the lower material by a static potential. The elastic deformations induced in the sliding upper material are captured by the following somewhat oversimplified Hamiltonian. We focus our attention at only two asperities which we represent by two heavy particles of mass $M$ and position $q_i$ (See Fig. 1). I.e. the asperities are modeled as stiff bodies. They interact with a substrate potential $U(q_i)$. The induced elastic deformation is represented by the elastic distortion of the bar of eigenfrequency $\Omega$ coupling the two particles together. The heat bath constituted by the phonons in the bulk of the material is represented by an elastic chain of $N$ light particles of mass $m$ and position $x_n$ coupled to the two heavy particles. The overall stiffness of the material is modelled by the spring of stiffness $K = M\Omega^2$. The Hamiltonian of the system is given by

\begin{equation}
H = \frac{1}{2}M\dot{q}_1^2 + \frac{1}{2}M\dot{q}_2^2 + \frac{1}{2}M\Omega^2(q_1 - q_2 - L)^2 + \frac{1}{2}m\omega^2(q_1 - x_1 - a)^2 + \frac{1}{2}m\omega^2(x_N - q_2 - a)^2 + U(q_1) + U(q_2) - q_1 F - q_2 F
\end{equation}
\[ + \sum_{n=1}^{N} \left[ \frac{1}{2} m_i^2 + \frac{1}{2} m \omega^2 (x_n - x_{n+1} - a)^2 \right] \]

Where \( L = (N + 1)a \) and \( \omega \) is the eigenfrequency of the springs connected to the light particles. We do not include any friction term in the dynamical equation of the model. The dynamics of the model are directly given by Newton’s equation \( md^2x/dt^2 = -\delta H/\delta x \) where \( x = q_1, q_2, x_1, \ldots, x_N \) and calculated numerically using the leapfrog algorithm. The potential \( U \) representing the rough surface is produced by randomly positioning Gaussian pinning centres with density \( n_p \) along the x-axis. Each individual pinning well \( U_p \) has the form

\[ U_p(r) = -A_p \exp(-(r/R_p)^2). \]  

We drive the model by prescribing a centre of mass velocity, \( v_{com} \) which is then kept constant during the simulation. This is obtained by adjusting the applied force \( F \) in each time step such that the total force on the system \( F_{tot} = 2F - \partial U/\partial q_1 - \partial U/\partial q_2 \) is always kept equal to zero. The friction force is identified as the time average of the force \( F \). The average is taken over a time window during which the rate of change of the internal kinetic energy of the heat bath is constant. This time interval begins after a short transient period after which the kinetic energy of the bath increases linearly with time. We make sure to stop the measurement before the process becomes non-stationary due to heating of the heat-bath degrees of freedom.

We used the following set of units. The mass \( M = 1 \), the length \( L = 1 \), and time \( 1/\Omega = 1 \). A series of constant velocity simulations were carried out using a range of values for the pin amplitude \( A_p \), small spring constant \( m \omega^2 \) and pin range \( R_p \). All simulations were done with a light particle mass \( m = 0.1 \), number of small particle \( N = 999 \), and a density of pinning wells \( n_p = 1000 \). The time step of the discrete numerical integration of the equation of motion were \( \Delta = 0.001 \). All results reported were found after averaging over a number of realizations of the background potential.

\section{Simulation Results}

We are particularly interested in the effect of elastic instabilities. Let us briefly discuss the nature of these instabilities. Consider a particle of position \( x \) elastically coupled by a spring of stiffness \( k \) to a moving coordinate \( X(t) = Vt \), where \( V \) is a constant velocity. I.e. the elastic energy of the particle is \( E_{el} = \frac{1}{2} k (x - Vt)^2 \). Let the particle move through a pinning well of the form given in Eq. 2. It is
easy to show (See the third paper of Ref. [12]) that the force balance equation
for the particle in the limit $V \to 0$ will have multiple solutions (See Fig. 2) when

$$k < \frac{4}{\epsilon^{3/2} R_p^2} A_p.$$  \hspace{1cm} (3)

The particle undergoes discontinuous jumps (in the limit where $X(t)$ moves forward quasistatically) when the solution of the stability equation becomes multi-valued. The two heavy particles of our model will influence each other during the instabilities. The condition for instabilities in Eq. 3 is therefore only approximately applicable to our model.

We present in Fig. 3 simulations of the velocity dependence of the friction force for parameters around the threshold value given in Eq. 3. Fig. 3a presents a set of data for different values of the range of the individual wells and Fig. 3b show the behaviour for different amplitudes of the pinning wells.

One observe in Fig. 3a a crossover in the behaviour at low velocities for $R_p$ about equal to the threshold value $R_p^* = (4A_p/\epsilon^{3/2}k)^{1/2}$. Similarly in Fig. 3b a change in the behaviour occur for $A_p$ around $A_p^* = \frac{\epsilon^{3/2}}{4} k R_p^2$. In the case where Eq. 3 predicts the absence of elastic instabilities in the limit $v \to 0$ one see that the the friction force is an increasing function of the velocity for small velocities. The intercept with the y-axis vanishes gradaully as the instabilities cease to exist. This behaviour can clearly be identified despite the difficulties of producing high quality statistics in the limit of vanishing velocity. (Remember that due to the randomness in the position of the pining centres the local curvature can be stronger than the maximum curvature of a single well.)

That a non-zero value of $\lim_{v \to 0} f_{fr}(v)$ is linked to the existence of elastic instabilities is more clearly demonstrated in Fig. 4. In Fig. 4a we show the time dependence of the kinetic energy of the bath as one of the heavy particles moves through a single potential well. Fig. 4b shows how the change in the energy of the bath depends on the velocity of the system. It is unfortunately difficult to simulate the very low velocity limit with high accuracy. However, one sees that $\Delta E_{kin}$ (the change in the energy of the bath) can be extrapolated to zero as $v \to 0$ when $A_p < A_p^*$.

4 Discussion

The above observed behaviour of the friction force can qualitatively be understood in terms of the following simple model. Consider a single particle of position $x$. 
Let the particle of mass \( m \) be coupled harmonically, through a spring of stiffness \( m\omega_0 \), to a frame which is moving with velocity \( v \). Assume furthermore that the particle is in contact with a heat bath which enables a damping proportional to the velocity of the particle to take place. The interaction with a rough substrate potential is represented by the force \( F \). In the frame moving with velocity \( v \) the equation of motion is

\[
\frac{d^2x}{dt^2} = -m\omega_0 x - \gamma \frac{dx}{dt} + f(x(t)).
\] (4)

We can solve this equation immediately if we replace the position dependent force \( f(x(t)) \) by a time dependent force \( F(t) \). We shall chose the following mean field-like form \( F(t) = f(vt) \). This is a reasonable approximation for smooth over-damped motion. The time averaged work-per-time involved in the motion is given by

\[
\dot{W} = \lim_{T \to \infty} \frac{1}{T} \int_{T/2}^{T/2} F(t) \frac{dx}{dt}(t).
\] (5)

The work is readily expressed in terms of the Fourier transform of the Green’s function

\[
\chi(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \chi(t) = \left[m(\omega_0^2 - \omega^2) - i\gamma\omega \right]^{-1}
\] (6)
of Eq. 4. One obtains

\[
\dot{W} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \langle F(\omega)F(-\omega) \rangle (-i\omega) \chi(\omega).
\] (7)

We introduced the Fourier transform of the force auto-correlation function

\[
\langle F(\omega)F(-\omega) \rangle = \int_{-\infty}^{\infty} dt e^{i\omega t} \langle F(t)F(t + t_0) \rangle t_0.
\] (8)

The time dependence of \( F(t) \) is taken to be given by a linear super-position of the individual forces exerted by the randomly superpositioned pinning wells. A pinning well positioned at \( x_i \) is encountered at time \( t = x_i/v \). We have

\[
F(t) = \sum_{i=-\infty}^{\infty} f_p(t - t_i).
\] (9)

The auto-correlation of \( F(t) \) is according to Campbell’s theorem given by

\[
\langle F(t)F(t + t_0) \rangle t_0 = n_p v \int_{-\infty}^{\infty} dt_0 f_p(t_0) f(t_0 + t)
\] (10)

We will consider two types of time evolution of \( f_p(t) \). Firstly, in the absence of instabilities \( f_p(t) \) will be a smooth function of \( t \). We chose to represent \( f_p(t) \) by the continuous function

\[
f_p^c(t) \equiv -\frac{2A_p v}{R_p^2} t e^{-\left(\frac{t}{\Delta}\right)^2}.
\] (11)
We have introduced the time scale \( \Delta = R_p/v \). The second type of time dependence involves to rapid changes in \( f_p(t) \) encountered when an elastic instability takes place. See Fig. 2b. We will represent these abrupt jumps in \( f_p(t) \) by the following function

\[
f_p(t) = f_p^c(t) - \alpha \frac{t}{\Delta} \Theta(\Delta - t)
\]  

(12)

The force correlator is easily calculated in both cases. When no instabilities exist one finds

\[
\langle F^c(\omega)F^c(-\omega) \rangle = {\pi n_p (A_p R_p)^2 \over v^3} \omega^2 e^{1 \over 2} (\Delta \omega)^2.
\]  

(13)

When elastic instabilities take place the correlator is slightly more complicated

\[
\langle F(\omega)F(-\omega) \rangle = \langle F^c(\omega)F^c(-\omega) \rangle + 8 A_p n_p \alpha {\sin(\Delta \omega) \over \omega^2} \int_{-\infty}^{\infty} dz \sin(\Delta \omega z) e^{-z^2/2} 
+ {n_p R_p \alpha^2 \over \Delta} \left[ {1 \Delta^2 \over \omega^2} (\cos(2\Delta \omega) + 1) 
- {2 \over \omega^4} (\cos(2\Delta \omega) - 1) - {4 \Delta \over \omega^3} \sin(2\Delta \omega) \right].
\]  

(14)

It is now easy to calculate the friction force \( f_{fr} = \dot{W}/v \) from Eq. 7. The friction force vanishes in both as an inverse power of \( v \) in the high velocity limit.

In the low velocity limit one finds in the case of no instabilities

\[
f_{fr}^c \approx {3 \pi \gamma n_p A_p^2 \over 4 \sqrt{2 m^2 R_p^3 \omega_0^4}} v.
\]  

(15)

I.e. the friction force goes to zero linearly with \( v \). The presence of instabilities produces a non-zero value of friction force in the limit \( v = 0 \)

\[
f_{fr}(v = 0) = {n_p \alpha^2 \over m \omega_0^2}.
\]  

(16)

The instabilities also change the coefficient to the term in \( f_{fr}(v) \) linear in \( v \). One note that the zero-velocity limit in Eq. 10 does not depend on the damping coefficient \( \gamma \). This is to be expected since in the limit of quasi-static motion any non-zero value of \( \gamma \) will suffice to extract the energy released during the instabilities. It is important to remember that the coefficient \( \alpha \) describing the jump in the substrate force depends implicitly upon the stiffness of the elastic coupling of the moving particle. The softer the elastic coupling the larger the jumps (See paper 3 of Ref. [12]). This does not change the qualitative significances of Eq. 10.
5 Conclusion

We have studied a one dimensional model of an elastic body moving over a rough surface. We focus our attention on the behaviour of the macroscopic asperities poking out into the rough surface. The body is moved at constant velocity. We find that the velocity dependent friction force always decreases to zero in the limit of large velocity. The value of the friction force as the velocity tends to zero depends on the corrugation of the substrate potential. If the curvature of the potential is large enough to induce elastic instabilities during the quasistatic motion the friction force goes to a non-zero limit. This behaviour was called static friction by Cieplak et al. [9]. For smooth substrate potentials elastic instabilities may be absent and then the friction force goes to zero with vanishing velocity. Cieplak et al. called this velocity dependence for viscous friction.

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Figure Captions

Figure 1.
Schematic diagram of the one dimensional model used in the simulations. We model the relative motion of two macroscopic bodies (inset) and focus on the interaction between two asperities protruding from the upper body and a static potential, which represents the lower body. Elastic deformation is represented by the long elastic bar and a heat bath by an elastic chain of light particles.

Figure 2.
(a) The spatial variation of the force experienced by an harmonic oscillator as it is pulled through a single pinning centre. The slope the dashed lines is the spring constant of the oscillator. When the criterion is met the force balance equation supports multiple solutions and the oscillator will experience jumps in position, represented by the arrows. This gives rise to abrupt jumps in the temporal variation of the force experienced by the oscillator, as shown in (b).

Figure 3.
Simulation results showing the velocity dependence of the friction force for different values of (a) the range \( R_p \) of individual pinning centres; (b) the amplitude \( A_p \). \( R_p* \) and \( A_p* \) are the threshold values for the pin range and amplitude respectively.

Figure 4.
(a) Time dependence of the kinetic energy of the heat bath as one of the heavy particles moves through a single potential well. Values were taken for different values of the pin amplitude \( A_p \). (b) Velocity dependence of the change in the kinetic energy of the heat bath during the motion of one heavy particle through a single potential well. Values were taken for different values of the pin amplitude \( A_p \).
Figure 1. Lindop and Jensen.
Figure 2. Lindop and Jensen.
Figure 3(a). Lindop and Jensen

\[ f_{fr} / 10^{-3} \]

\[ v / 10^{-3} \]

- $R_p = 0.5 \, R_p^*$
- $R_p = 1.0 \, R_p^*$
- $R_p = 2.0 \, R_p^*$
Figure 3(b). Lindop and Jensen

![Graph showing $f_r / 10^{-3}$ vs $v / 10^{-3}$](image)

- $Ap = 0.5 Ap^*$
- $Ap = 1.0 Ap^*$
- $Ap = 2.0 Ap^*$
Figure 4(a). Lindop and Jensen

\[ E_{\text{kin}} / 10^{-6} \]

- \( A_p = 2.0 A_p^* \)
- \( A_p = 1.0 A_p^* \)
- \( A_p = 0.5 A_p^* \)
Figure 4(b). Lindop and Jensen.