Phonon analysis of the dynamic to static friction crossover in a 1D model

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Abstract

In this work we analyze a 1D model for the simulation of dynamic friction at the atomic scale. The model consists of a point mass (slider) that moves over and interacts weakly with a linear chain of masses interconnected by springs. The interaction results in an energy transfer from the slider to the chain, in which phonon waves are induced. Therefore the slider experiences a friction force. Previous work observed the existence of dissipation peaks at certain values of the slider speed. In the present work, our main purpose is to understand this behavior. We focus on the low-speed regime, analyzing the phonon excitations induced in the chain by the slider. Through a Fourier analysis of the excited phonon modes, we provide an explanation of the dissipation peaks and we find a relation predicting which phonons get excited at which slider speed.

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1 Introduction

Frictional motion affects a huge variety of phenomena which span vast ranges of scales, and its practical and technological importance is enormous. It is no surprise, then, that we find the study of friction among the most ancient problems addressed by physics. Nevertheless, the field as a whole failed to attract adequate interest by the scientific community until the last few decades, and many fundamental aspects of friction dynamics are still understood only partly. In particular, nanofriction (the study of friction at the atomic scale) lacks a theoretical model capable of providing quantitative explanations of all its features.

Among the so-called “minimalistic” models of nanofriction, the most successful and influential is the Prandtl-Tomlinson (PT) model \[1\]. The PT model assumes that a point mass \(m\) is dragged over a one-dimensional sinusoidal potential representing the interaction between the slider and the crystalline substrate. The mass is pulled by a spring of effective elastic constant \(K\), extending between the mass and a support, that is driven with a velocity \(v\) constant relatively to the substrate. Therefore the total potential experienced by the point mass can be written as:

\[
U(x, t) = U_0 \cos \left( \frac{2\pi}{a} x \right) + \frac{K}{2} (x - vt)^2,
\]

where \(U_0\) is the amplitude and \(a\) is the periodicity of the sinusoidal potential. The PT model describes naturally the transition between stick-slip regimes at soft spring (small \(K\)) to smooth sliding for hard spring (large \(K\)). All dissipation is described by a viscous-like force \(-\gamma \dot{x}\), where \(\gamma\) is a damping coefficient. This model has a weakness: it makes no attempt to describe realistically the energy dissipation in the substrate, but achieves it through an “ad hoc” viscous term.

In the present work, we analyze a different model that takes into account the elasticity of the substrate: when a cursor passes by and interacts with an elastically deformable crystal, phonons are generated and propagate from the point of the interaction. In this way the cursor mechanical energy is converted into crystal vibrational energy and thus dissipated. This mechanism virtually allows us to dispose of the viscous dissipation.

The model we examine was introduced and characterized in a previous work by G. Giusti \[2\], who studied the dependence of the kinetic friction force on the cursor velocity and observed that it exhibits resonant peaks at certain values of the cursor velocity. The main purpose of this work is to extend the zero-temperature investigation:

- to study the transition between dynamic and static friction, and
- to understand the resonant behavior observed by Giusti.
Earlier work also investigated the velocity dependence of the kinetic friction force in different models [3, 4].

Section 2 introduces our model. Section 3 discusses a method for the evaluation of static friction. Section 4 studies kinetic friction as a function of the cursor velocity and focuses on the low speed regime, where the dynamic-static friction transition occurs. Section 5 analyzes the phonon waves induced in the crystal and, through a connection of the slider speed with their phase velocities, a relation is provided that predicts the excited phonon modes when the cursor is moving at a given constant velocity. This study of the phonon phase velocities accounts for the dissipation peaks observed by Giusti.

2 The model

We briefly review our model, the same introduced by Giusti [2] and represented in Fig. 1. We simulate the classical dynamics of a system consisting of a linear chain of \( N \) pointlike atoms plus a “cursor” or “slider”. The atoms, of mass \( m \) and positions \( x_j \), are regularly spaced with spacing constant \( a \) and are connected by springs to two nearest neighbors. The cursor slides over a guide at a fixed distance \( d \) from the chain. The simulation is done inside a supercell with periodic boundary conditions \( x + Na = x \). The slider is a pointlike particle with horizontal position \( x_{SL} \) and mass \( m_{SL} \), larger than the mass \( m \) of the atoms of the chain. The slider-chain interaction is described by a sum of Lennard-Jones two-body terms. If \( R_j = \sqrt{d^2 + (x_{SL} - x_j)^2} \) is the distance between the slider and the \( j \)-th particle in its nearest periodic replica, the slider-chain interaction is expressed by

\[
V_{SL-C} = \sum_{j=1}^{N} V_{LJ}(R_j),
\]
where

\[ V_{LJ} = \begin{cases} V_{LJ}^{Th}(R_j) - V_{LJ}^{Th}(R_{cutoff}) & \text{if } R_j \leq R_{cutoff} \\ 0 & \text{otherwise} \end{cases} \]  

is a truncated version of the usual Lennard-Jones potential:

\[ V_{LJ}^{Th} = \epsilon \left[ \left( \frac{\sigma}{R_j} \right)^{12} - 2 \left( \frac{\sigma}{R_j} \right)^6 \right]. \]  

In Eq. (3) \( V_{LJ} \) is defined with a cutoff distance \( R_{cutoff} \) so that the potential has a finite range (this is necessary when one adopts periodic boundary conditions). We use \( R_{cutoff} = 15a \), like Giusti did. The chain particles interact with the nearest neighbors by means of a harmonic potential:

\[ V(x_j) = \frac{1}{2} K \sum_{j=1}^{N-1} (x_{j+1} - x_j - a)^2, \]

where \( K \) is the elastic constant of the springs and \( a \) is the equilibrium lattice spacing. The particles of the chain are also affected by a weak viscous force, so that the phonon waves that propagate in the crystal get dampened and eventually fade while they move away from the point where they were generated, namely the vicinity of the slider. The viscous force that acts on the \( j \)-th atom of the chain is

\[ F_{\text{diss},j} = -\gamma \dot{x}_j, \]

where \( \gamma \) is the damping coefficient. Thanks to this term the oscillations generated by the slider are confined in a region smaller than the supercell, thus preventing the waves from coming back to the slider position. In practice, this damping term simulates the effect of energy dissipation at great distance.

Ignoring for the moment the damping of Eq. (6), a sinusoidal wave propagating in the chain follows this dispersion relation [5] between its angular frequency \( \omega \) and its 1D wave vector \( k \):

\[ \omega = 2 \sqrt{\frac{K}{m}} \left| \sin \left( \frac{k a}{2} \right) \right|. \]

In the long wavelength limit, \( |k| \ll a^{-1} \), we can expand the term \( \sin \left( \frac{k a}{2} \right) \) and rewrite Eq. (7) as

\[ \omega \simeq a \sqrt{\frac{K}{m} |k|}. \]

From this last equation, we obtain the speed of sound:

\[ v_s = \omega / |k| = a \sqrt{\frac{K}{m}}. \]
<table>
<thead>
<tr>
<th>Physical quantity</th>
<th>Natural units</th>
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<tbody>
<tr>
<td>length</td>
<td>$a$</td>
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<td>mass</td>
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<td>spring constant</td>
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<td>$a(K/m)^{\frac{1}{2}}$    \equiv v_s</td>
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<tr>
<td>force</td>
<td>$Ka$</td>
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<tr>
<td>damping coefficient</td>
<td>$(Km)^{\frac{1}{2}}$</td>
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Table 1: Natural units for several physical quantities in our system.

The units listed in Table 1 for the mechanical quantities in the present model are expressed naturally in terms of the quantities $a$, $m$, and $K$ characterizing the linear chain. The natural unit for speed is the speed of sound $v_s$; so if the slider velocity $v_{SL}$ is greater than 1 in these natural units, it means that the slider is moving at a supersonic speed; conversely, if $v_{SL}$ is less than 1, the slider speed is subsonic.

In our simulations, unless otherwise specified, we adopt the same standard set of parameters used in Giusti’s work:

- the chain has $N = 500$ atoms;
- $\epsilon = 5 \cdot 10^{-4} Ka^2$;
- $\sigma = 0.5 a$;
- $\gamma = 0.1 (Km)^{\frac{1}{2}}$;
- distance between the slider and the chain, $d = 0.475 a$.

### 3 Evaluation of the static friction force

To evaluate the static friction force $F_{static}$, initially we adopt the following procedure. First we run a simulation in which the slider starts with a small initial velocity, that is allowed to freely change as a consequence of the slider-chain interaction. The motion of the slider during this first calculation is shown in Fig. 2. Eventually, the slider stops at an equilibrium position between two atoms of the chain, corresponding to a minimum of the slider-chain potential. There are two inequivalent minima at which the slider can stop, depending on its initial position.
Figure 2: The solid line reports the slider motion as it stops at a minimum of type I; the dashed line reports the slider motion as it stops at a minimum of type II. The two dotted lines display the position of two nearby atoms of the chain.

and velocity, and Fig. 2 illustrates both cases; with reference to this figure, we call the two equilibrium positions minimum of type I and type II. For each of these two cases, we obtain a different estimation of the static friction force with the method we are about to explain. We call the two results $F_{\text{static}}^I$ and $F_{\text{static}}^{II}$. At the end of this section, we will show that in a way $F_{\text{static}}^I$ is the “true” static friction. We first examine the case in which the slider stops at a minimum of type I.

We run a second simulation during which the slider, starting from the equilibrium condition reached at the end of the first calculation, is pulled by a spring of elastic constant $K_{\text{ext}}$ extending from the slider to a support, which moves at a constant velocity $v_{\text{ext}}$. Figure 3 reports the positions of the slider and support, and the spring length, as a function of time. At the beginning, the spring elongates while the slider remains stuck between the two atoms; meanwhile, as a result of the force between the slider and the atoms, the chain slowly accelerates in the same direction of the motion of the support. If $v_{\text{ext}}$ is large enough, there comes a time in which the spring becomes long enough for the elastic force to exceed the static friction $F_{\text{static}}^I$, and the slider suddenly abandons its initial position between these two atoms, oscillates around the support dissipating the elastic energy accumulated in the driving spring, and then eventually stops at
Figure 3: (a): Motion of the slider (solid line) as it is pulled by a spring having elastic constant $K_{ext} = 10^{-3} K$ and extending from it to a support (dashed line) that is moving at a constant velocity $v_{ext} = 3 \cdot 10^{-5} a(K/m)^{1/2}$; the dotted lines show the positions of successive atoms of the chain. (b): Spring length as a function of time. It is clearly seen that it reaches a maximum value before the slider slips forward, suddenly overtaking one of the atoms.

a new equilibrium position between two new atoms. This is the case of Fig. 3 simulated with $v_{ext} = 3 \cdot 10^{-5} a(K/m)^{1/2}$ and $K_{ext} = 10^{-3} K$. Conversely, if $v_{ext}$ is less than a certain critical value $v_{crit}$, the chain’s velocity gets asymptotically close to $v_{ext}$, so that the support and the chain move together at about the same velocity and the spring never gets long enough for the elastic force to exceed the static friction.

If we make a simulation using a $v_{ext}$ greater than the (hitherto unknown) critical value $v_{crit}$, the length of the spring reaches a maximum value before the slider abandons his equilibrium position. If we multiply this maximum length by the elastic constant of the spring $K_{ext}$, we obtain the maximum elastic force experienced by the slider, which is a overestimation of the static friction. We repeat this calculation for different values of $v_{ext}$, with an elastic constant $K_{ext} = 10^{-3} K$. We start from $v_{ext} = 10^{-4} a(K/m)^{1/2}$ and reduce its value each time, obtaining better and better estimations of $F_{static}$. The results are plotted in Fig. 4. Before running these simulations, we did not know $v_{crit}$, so we continued to lower
Figure 4: Estimated static friction $F_{I \text{static}}^I$ for different values of the support velocity $v_{\text{ext}}$. These estimations were obtained evaluating the maximum elastic force experienced by the slider just before it overtakes one atom of the chain. Therefore, they are systematic overestimations. The dotted line shows our best guess for $F_{I \text{static}}^I$, see Eq. (10).

$v_{\text{ext}}$ until we produced a simulation in which, after a time of $10^6 \ (m/K)^{1/2}$, the slider had not yet abandoned his position between the two starting atoms. This occurs for $v_{\text{ext}} = 2.38 \cdot 10^{-5} \ a(K/m)^{1/2}$. Conversely, the lowest $v_{\text{ext}}$ which produces stick-slip, and therefore yields an estimation of $F_{I \text{static}}^I$, is $v_{\text{ext}} = 2.39 \cdot 10^{-5} \ a(K/m)^{1/2}$. Therefore, our best guess for the static friction is the one we get from this last simulation, which is:

$$F_{I \text{static}}^I \simeq 1.1931 \cdot 10^{-3} \ Ka. \quad (10)$$

This result allows us to obtain a corresponding estimation of $v_{\text{crit}}^I$, because it is related to $F_{I \text{static}}^I$ by a simple relation that we now derive. Consider a small-speed simulation where the chain, the slider and the pulling support are all moving together at the same velocity $v_{\text{ext}} \leq v_{\text{crit}}^I$. This means in particular that the total force acting on the chain is zero. Then the force $F_{SL-\text{chain}}$ between the slider and the chain must be equal to the total damping force that acts on the chain, which is $N \gamma v_{\text{ext}}$. So we obtain

$$F_{SL-\text{chain}} = N \gamma v_{\text{ext}}. \quad (11)$$

The maximum value of $v_{\text{ext}}$ for which this situation can occur is $v_{\text{crit}}^I$, that corresponds to the maximum possible value of $F_{SL-\text{chain}}$, that is $F_{I \text{static}}^I$. Then, as a
special case of Eq. (11), we get
\[
F_{\text{static}}^I = N \gamma v_{\text{crit}}^I, \tag{12}
\]
from which, taking \( N = 500, \gamma = 0.1 (Km)^{\frac{1}{2}} \) and \( F_{\text{static}}^I \) as in Eq. (10), we obtain
\[
v_{\text{crit}}^I = \frac{F_{\text{static}}^I}{N \gamma} \simeq 2.3862 \cdot 10^{-5} a(K/m)^{\frac{1}{2}}, \tag{13}
\]
which agrees with simulations.

Until now, we focused only on the case in which the slider starting position is a minimum of type I (see Fig. [2]). Performing the same procedure with the slider starting from a minimum of type II, we obtain a static friction force
\[
F_{\text{static}}^{II} \simeq 6.845 \cdot 10^{-4} K a \approx 0.57 F_{\text{static}}^I \quad \text{and a critical velocity} \quad v_{\text{crit}}^{II} \simeq 1.369 \cdot 10^{-5} a(K/m)^{\frac{1}{2}}.
\]

The crucial observation is that \( F_{\text{static}}^{II} < F_{\text{static}}^I \). For this reason, we say that the “true” static friction is \( F_{\text{static}}^I \). Indeed, consider a slider stuck in a minimum of type II and apply to it a constant force greater than \( F_{\text{static}}^{II} \) but less than \( F_{\text{static}}^I \). It will leave the minimum of type II only to stop and remain stuck at a minimum of type I: no steady sliding begins. Conversely, if the constant force applied on the slider is greater than \( F_{\text{static}}^I \), it will overtake all minima of the potential it will run into, and start to slide relatively to the chain. For this reason, from now on we will call \( F_{\text{static}}^I \) and \( v_{\text{crit}}^I \) simply \( F_{\text{static}} \) and \( v_{\text{crit}} \).

4 Dynamic friction force dependence on \( v_{SL} \)

Starting from the methods and results of G. Giusti [2], we studied further the dependence of the kinetic friction force on the slider velocity. First, we briefly review the method that Giusti used to study this dependence; then we introduce the method adopted in the present work, by means of which Fig. [3] is realized.

After a first calculation at constant \( v_{SL} \), done in order to eliminate any initial transient, Giusti ran a second simulation in which, starting from the condition reached at the end of the first simulation, the slider was allowed to change his velocity as a consequence of the slider-chain interaction. From the slider average slowing rate during this second simulation, Giusti extracted the kinetic friction force with the following method: time was divided into regular intervals of 5000 time units, a very long time compared to the period of the fluctuations of \( v_{SL} \); then a linear regression was performed over each interval; the slope of the line fitting \( v_{SL} \) as a function of time represents the slider average acceleration; the average dynamic friction force \( F_d \) experienced by the slider was obtained by multiplying the acceleration by \( (-m_{SL}) \). Associating this value of \( F_d \) to the average value of \( v_{SL} \) in the same interval, Giusti obtained the dependence \( F_d(v_{SL}) \).
Figure 5: Dynamic friction force as a function of the speed of the slider. The horizontal dotted line shows the static friction threshold. The vertical dashed line is the speed of sound.

We come now to describe the method used in the present work. We run a single calculation with $v_{SL}$ constant, and discard the initial part in which the transients are still present. We record the total force experienced by the slider as a function of time. This force has fluctuations due to the slider running up against the consecutive atoms of the chain. Thus the period of these fluctuations is $a/v_{SL}$. We average this force over an integer number of these periods, and interpret the result as the friction force $F_d$ corresponding to the velocity $v_{SL}$. Obviously, a different simulation must be done for every value of $v_{SL}$ of interest.

A word of caution, though, about the meaning of $v_{SL}$. Once all the transients have been eliminated, the chain center of mass has acquired a velocity $v_{CM}$ that has a nonzero average, due to the balancing of the forces generated by the slider and the dissipation terms of Eq. (6), as discussed in Sec. 3. Thus, while the slider is moving, the chain as a whole is moving too. So the slider speed relative to the chain is lower than the imposed $v_{SL,abs}$ precisely by $\langle v_{CM} \rangle$. From now on, we will denote by $v_{SL,abs}$ the velocity we imposed on the slider, and by $v_{SL}$ the average relative velocity:

$$v_{SL} = v_{SL,abs} - \langle v_{CM} \rangle,$$

(14)

where $\langle v_{CM} \rangle$ is the average value of the velocity of the chain center of mass. This is also the meaning of $v_{SL}$ in all the plots. For high $v_{SL,abs}$ we find that $v_{CM} \ll$
so that \( v_{SL} \simeq v_{SL, abs} \), but for \( v_{SL, abs} \lesssim 10^{-4} a(K/m)^{1/2} \) the difference between \( v_{SL} \) and \( v_{SL, abs} \) starts to be significant. The effects of this fact are discussed later.

Keeping \( v_{SL, abs} \) constant is equivalent to assuming \( m_{SL} \) to be infinite, which could lead to different values of \( F_d \) compared to taking e.g. \( m_{SL} = 10 m \), as in Giusti’s simulations. To check this approximation, we investigate a possible dependence of \( F_d \) on \( m_{SL} \): we run simulations using Giusti’s method, with \( m_{SL} \) spanning a range from 5 \( m \) to 50 \( m \). No significant variation in \( F_d \) is observed for \( v_{SL} = 0.05 a(K/m)^{1/2} \), and this result supports our assumption that running at constant speed, i.e. taking \( m_{SL} = \infty \), should not be too bad, as long as we remain far from the static friction limit. As a further check, we use our method to calculate the dependence \( F_d(v_{SL}) \) over the same range of \( v_{SL} \) studied by Giusti and find no significant difference between our results and Giusti’s ones.

Nevertheless, for a finite-mass slider there always comes a time when its motion stops under the effect of the friction force, and, just before the slider stops, the effects of friction on the slider’s velocity cannot be neglected, see Fig. 2. So our results in the low-speed limit are valid only for a slider of very high mass, whose motion is still far from stopping.

Figure 5 shows the resulting dependence \( F_d(v_{SL}) \) obtained with our method. The vertical dashed line indicates the speed of sound \( v_s = a(K/m)^{1/2} \). The horizontal dotted line shows the value of the static friction force \( F_{static} \approx 1.1931 \cdot 10^{-3} Ka \), evaluated as discussed in Sec. 3.

As Giusti already observed, several peaks of \( F_d \) are clearly visible for \( v_{SL} \gtrsim 10^{-1} a(K/m)^{1/2} \). That regime of speeds is discussed in Sec. 5. We focus our attention first on the low-speed regime.

### 4.1 Transition dynamic-static friction

The dependence \( F_d(v_{SL}) \) in the low-speed regime is explored in greater detail in Fig. 6. Focusing the solid curve, reporting the results obtained with \( N = 500 \) particles and \( \gamma = 0.1 (Km)^{1/2} \), starting from \( v_{SL} = 10^{-4} a(K/m)^{1/2} \) and moving toward lower speeds, we see that the slope of the curve \( F_d(v_{SL}) \) initially increases and then decreases, approaching zero while \( F_d \) gets closer and closer to \( F_{static} \). This is the region where \( v_{CM} \) becomes comparable with \( v_{SL, abs} \). Note that if we run the simulation with a chain of 5000 atoms rather than 500 (dashed line in Fig. 6), we do not find this behavior in this speed region. For the 5000-atoms chain the same behavior may occur at lower speed, because at the same \( v_{SL, abs} \), \( v_{CM} \) is lower for a larger chain (the total viscous friction is larger for the chain of 5000 atoms than for the chain of 500 atoms) and becomes comparable with
Figure 6: Dynamic friction as a function of the speed of the slider in the low-speed regime. The solid line is the dependence $F_d(v_{SL})$ computed for a chain of $N = 500$ atoms and a damping coefficient $\gamma = 0.1 \, (Km)^{1/2}$ (same parameters as Fig. 5). The dashed line is the same dependence calculated with $N = 5000$ and $\gamma = 0.1 \, (Km)^{1/2}$. The dot-dashed line has $N = 5000$ and $\gamma = 0.01 \, (Km)^{1/2}$. The dot-dashed-dashed line has $N = 100000$ and $\gamma = 0.0005 \, (Km)^{1/2}$. The horizontal dotted line marks the static friction threshold. The dot-dot-dashed line is the best fit of the “physical” power-law $A/v_{SL}$ zone, with $A \simeq 2.73 \cdot 10^{-7} a^2 K^{1/2} m^{-1/2}$.

$v_{SL,abs}$ for lower values of $v_{SL,abs}$ itself.

We want to understand the phenomena occurring when $v_{CM}$ is comparable with $v_{SL,abs}$, thus we take a closer look at what happens to the 500-atoms chain in the range $v_{SL} \lesssim 10^{-4} a(K/m)^{1/2}$. Fig. 7 shows the ratio $v_{SL}/v_{SL,abs}$ as a function of $v_{SL,abs}$. It is apparent that for comparably large $v_{SL,abs}$ we have $v_{SL} \simeq v_{SL,abs}$, and that as $v_{SL,abs}$ approaches the critical value $v_{crit}$, $v_{SL}$ decreases to zero. If we run a simulation with $v_{SL,abs} \leq v_{crit}$, we find $v_{SL} = 0$, i.e. $v_{CM} \equiv v_{SL,abs}$. So $v_{crit}$ is the value of $v_{SL,abs}$ below which the slider drags the chain along with it and its value is $v_{crit} \simeq 2.3862 \cdot 10^{-5} a(K/m)^{1/2}$, evaluated as discussed in Sec. 3.

Consider now the relative motion of the slider and the chain. We select two different velocities of the slider. Figure 8 reports the position of the slider (solid line) and of the two nearest atoms (dotted lines) for $v_{SL,abs} = 10^{-4} a(K/m)^{1/2}$. In the displayed time interval we see the slider passing by two atoms. Here $v_{SL,abs} \simeq 4.2 v_{crit}$, significantly above the region of Fig. 6 where the slope of
Figure 7: The average velocity of the slider $v_{SL}$ relative to the chain center of mass divided by $v_{SL,abs}$, the slider absolute velocity, as a function of $v_{SL,abs}$. These data are relative to the chain of $N = 500$ atoms. This ratio approaches 1 in the high-$v_{SL,abs}$ limit, as the horizontal dashed line shows, and approaches 0 for $v_{SL,abs} \to v_{crit}$. The arrow identifies the point where $v_{SL} = 2.4 \cdot 10^{-5} a(K/m)^{1/2}$ and $v_{SL}/v_{SL,abs} \simeq 0.15$.

$F_d(v_{SL})$ starts to increase. In this simulation we have $\langle v_{CM} \rangle \simeq 3.64 \cdot 10^{-6} a(K/m)^{1/2}$ and $v_{SL} \simeq 9.64 \cdot 10^{-5} a(K/m)^{1/2} \simeq 0.96 v_{SL,abs}$. The two panels of Fig. 8 are very similar, because $\langle v_{CM} \rangle$ is small relatively to $v_{SL,abs}$. A similar behavior is observed for higher $v_{SL,abs}$.

Figure 8 illustrates a very different situation. For this simulation, we take a much smaller $v_{SL,abs} = 2.4 \cdot 10^{-5} a(K/m)^{1/2}$, namely $v_{SL,abs} = 1.006 v_{crit}$. In this simulation we obtain $\langle v_{CM} \rangle \simeq 2.03 \cdot 10^{-5} a(K/m)^{1/2}$ and $v_{SL} \simeq 3.70 \cdot 10^{-6} a(K/m)^{1/2} \simeq 0.15 v_{SL,abs}$, identified by the arrow in Fig. 7. As Fig. 9 shows, for most of the time the slider and the chain atoms move at nearly the same velocity, with the slider standing almost still between two consecutive atoms, but creeping slowly forward. Eventually, the slider reaches and overtakes an inflection point of the interaction potential, and then overtakes an atom in a short time. After the overtaking, the slider enters the next minimum of the slider-chain interaction and becomes again almost steady relatively to the chain. This behavior is very similar to stick-slip and occurs only when $v_{CM}$ is comparable to $v_{SL,abs}$. 
4.2 **The scaling region** \( (10^{-4} v_s \lesssim v_{SL} \lesssim 10^{-1} v_s) \)

We focus again on Fig. 8 on the solid curve reporting the results obtained with \( N = 500 \) particles and \( \gamma = 0.1 (Km)^{\frac{1}{2}} \). Starting from \( v_{SL} = 10^{-1} a(K/m)^{\frac{1}{2}} \) and moving toward lower speeds, we encounter a region in which the curve \( F_d(v_{SL}) \) behaves approximately as a straight line in this log-log plot; moving further to the left, close to \( v_{SL} \approx 10^{-2} a(K/m)^{\frac{1}{2}} \) we observe a transition to another broad rectilinear-looking region, but with a different slope. The two scaling regions represent two different power laws.

The data we just discussed are computed using a damping coefficient \( \gamma = 0.1 (Km)^{\frac{1}{2}} \) and a chain of \( N = 500 \) atoms. In order to see if the transition between the two power-law zones is affected by \( \gamma \), we repeated the calculation with \( \gamma = 0.01 (Km)^{\frac{1}{2}} \). A low \( \gamma \) creates a problem, though: with a low damping, the oscillations induced in the chain by the interaction with the slider can travel almost undisturbed across the chain and return to the slider position. Here they interfere with the generation of other oscillations, producing a reduction of friction named “thermolubricity” [2]. To prevent these returning waves, we use a longer chain, with \( N = 5000 \) atoms, so that the oscillations are completely
Figure 9: The position of the slider (solid) and of the chain particles (dotted) as a function of time, for the simulation with $v_{SL,abs} = 2.4 \cdot 10^{-5} a(K/m)^{1/2}$. (a): Positions in the lab frame of reference. (b): Positions in a frame of reference that is moving with constant velocity, equal to the average velocity of the chain center of mass $\langle v_{CM} \rangle \simeq 2.03 \cdot 10^{-5} a(K/m)^{1/2}$.

dampened before they can come back to the slider’s position. The resulting data are represented by the dot-dashed line in Fig. 6. We see that the transition between the two power-laws now has moved to a lower $v_{SL}$, close to $10^{-3} a(K/m)^{1/2}$. Since the viscous dissipation term is unphysical and was introduced with the sole purpose of preventing the oscillations from coming back to the slider’s position, the lower $\gamma$ is, the closer our model is to the real physical situation, of atoms moving conservatively in vacuum. We conclude that the real physical behavior is the one observed for $\gamma = 0.01 (Km)^{1/2}$ and $v_{SL} \gtrsim 10^{-3} a(K/m)^{1/2}$ (and also for $\gamma = 0.1 (Km)^{1/2}$ and $v_{SL} \gtrsim 10^{-2} a(K/m)^{1/2}$). From the comparison of the $\gamma = 0.1 (Km)^{1/2}$ and $\gamma = 0.01 (Km)^{1/2}$ curves, we conclude that the transition to a different power law for lower $v_{SL}$ is due to the damping force becoming dominant in the low-speed limit. Therefore the behavior of the model in the dynamic-static friction transition discussed in Sec. 4.1 does not represent a real physical behavior, because in that regime the non-physical damping force term is dominant.

The friction-speed curve in the physically significant power-law zone is well fitted by a function of the form $F_d(v_{SL}) = A/v_{SL}$, with $A \simeq 2.73 \cdot 10^{-7} a^2 K^{3/2} m^{-1/2}$ (this fit is the dot-dot-dashed line in Fig. 6). A further calculation with $\gamma =$
Figure 10: (a): Snapshot of the velocities of the chain particles while the slider moves at $v_{SL} = 0.1 a(K/m)^{1/2}$; the black dashed line shows the current position of the slider. (b): Squared modulus of the Fourier transform of the velocities, as defined in Eq. (15).

0.0005 $(Km)^{1/2}$ and $N = 100000$ (dot-dashed-dashed line in Fig. 6) confirms this inverse proportionality $F_d(v_{SL}) = A/v_{SL}$ which extends down to even lower speeds $v_{SL} \simeq 5 \cdot 10^{-4} a(K/m)^{1/2}$. Eventually, at smaller speed even this calculation shows deviation from the power law as $F_d$ approaches $F_{static}$. Even longer simulations with even smaller gamma and larger chain size would be needed to clarify if this behavior is really representative of the transition from dynamic to static friction.

5 Phonon excitations

We proceed to analyze the phonon excitations induced in the chain by the interaction with the slider for varying $v_{SL,abs}$ and, accordingly, $v_{SL}$. We now explain the protocol for this analysis.

We run a simulation with the desired $v_{SL,abs}$. After the end of the transients, we take a snapshot of the velocities $v_j$ of the chain atoms at a given time $t$, like the one in Fig. 10a. Figure 10b shows the squared modulus of the spatial Fourier
transform of these instantaneous velocities. The Fourier transform is defined by

\[ \tilde{v}(k, t) = \sum_{j=1}^{N} e^{ikaj} v_j(t) \]  

with \( k = \frac{\pi}{a} \left( \frac{2n}{N} - 1 \right) \) and \( n = 1, \ldots, N \),

where \( i \) is the imaginary unit and \( k \) spans the first Brillouin zone \((-\pi/a, \pi/a] \).

A simple observation about the graph of \(|\tilde{v}|^2(k)| in Fig. 10b: it is clearly an even function of \( k \), because \( \tilde{v} \) is the Fourier transform of a real sequence \( v_j \); therefore \( \tilde{v}(-k) = \tilde{v}^*(k) \), where \(|\tilde{v}(-k)| = |\tilde{v}^*(k)| = |\tilde{v}(k)|\). Due to this symmetry in the following figures reporting Fourier transforms we will focus on the positive half \([0, \pi/a] \) of the Brillouin zone.

The peaks of the Fourier transform highlight the phonons most excited by the interaction with the slider. For a given \( v_{SL} \), though, there is not a uniquely defined configuration of peaks, because during a simulation the velocity pattern, and therefore its Fourier transform, evolves in time. However, as shown in Fig. 11, \(|\tilde{v}(k, t)|^2 \) is periodic in time with period \( T = a/v_{SL} \), thus

\[ |\tilde{v}(k, t + T)|^2 = |\tilde{v}(k, t)|^2, \quad \text{with} \ T = \frac{a}{v_{SL}}. \]  

To obtain a time-independent description of the typical excited phonon spectrum at a given \( v_{SL} \), we evaluate the average squared modulus of the Fourier transform over a period \( T \): we take \( M \) instants of time, equally spaced within the period, and compute \( \tilde{v} \) for each of them; then we calculate the average Fourier transform as follows:

\[ \langle |\tilde{v}|^2 \rangle(k) = \frac{1}{M} \sum_{m=1}^{M} | \tilde{v} \left( k, m \cdot \frac{T}{M} \right) |^2. \]  

We use \( M = 50 \). A check with \( M = 100 \) for \( v_{SL} = 0.1 a(K/m)^{1/2} \) shows no significant difference.

Figure 12 illustrates a few of the resulting average spectra \( \langle |\tilde{v}|^2 \rangle(k) \), for different velocities \( v_{SL} \). We see that for supersonic velocities of the slider the Fourier transform is quite flat, with no sharp peak: almost all the phonons are excited with comparable intensities, except those closest to \( k = 0 \). If \( v_{SL} \) is less than the speed of sound \( v_s \), but greater than about 0.2 \( v_s \), the spectrum is dominated by a single peak. When \( v_{SL} \) is less than about 0.2 \( v_s \), multiple peaks having different intensities appear, and, as \( v_{SL} \) decreases, their number increases progressively. As \( v_{SL} \) further decreases, the positions of all peaks approach \( k = 0 \), where they gradually merge into a single sharp peak.
Figure 11: The squared modulus of the Fourier transform of the velocities, at six subsequent times. Here the slider velocity is $v_{SL} = 0.1 a(K/m)^{\frac{1}{2}}$, and $T = a/v_{SL} = 10 (m/K)^{\frac{1}{2}}$. Comparing the plots for $t = 0$ and $t = T$, it is clearly seen that after one period $T$ the function $|\tilde{v}(k)|^2$ is identical. As discussed in the text $|\tilde{v}(k,t)|^2$ is indeed periodic in time with period $T$. 
Figures 13 and 14 display the positions and heights of the observed peaks of $\langle |\hat{v}|^2 \rangle (k)$ as functions of $v_{SL}$. These data are obtained by fitting the functions $\langle |\hat{v}|^2 \rangle (k)$ with sums of up to 7 Lorentzian curves. Figures 13 and 14 track the positions and heights of the Lorentzian curves resulting from the fits. For $v_{SL}$ greater than the speed of sound, as shown in the upper panel of Fig. 12, the smooth spectrum shows no sharp peaks. Even in this regime, we fit the spectrum with the sum of four Lorentzian curves. These four Lorentzian profiles do their best to interpolate that continuum spectrum. Not surprisingly, the Lorentzian centers, shown in Fig. 13, follow a rather erratic variation with $v_{SL}$. We are satisfied with this outcome, as in this region these Lorentzian centers should not be interpreted as the position of any sharp peaks.

Below the speed of sound we see that, as $v_{SL}$ decreases, new peaks appear with $k$ close to $\pi/a$ and then they move down toward $k = 0$. We already observed these properties in Fig. 12 but now we note another interesting feature: new peaks always appear in pairs.

Figures 15 and 16 compare peaks positions with the dependence of the dynamic friction $F_d$ on $v_{SL}$. We already observed in Sec. 4 that several peaks arise as $v_{SL}$ is lowered. In concrete, at certain values of $v_{SL}$ the dissipation increases suddenly. Remarkably, Fig. 16 shows that the starting of these dissipation peaks matches the appearance of new peaks of $\langle |\hat{v}|^2 \rangle$. The important conclusion of this coincidence is the following: dissipation increases suddenly for certain values of $v_{SL}$ because new phonons start to get excited.

### 5.1 Phonon phase velocities

To understand why certain phonons get excited at certain speeds and not at others, we compare the $k$’s of the observed peak phonons with the wave vectors of the phonons whose phase velocities $\omega/k$ match $v_{SL}$. First, we detail how we calculate the angular wavenumbers $k$ of the phonons that have a phase velocity equal to a given $v$. Then we compare the results with the $k$’s of the observed excited phonons at $v_{SL} = v$.

We search for all values of $k$ such that the phase velocity matches a given speed $v$:

$$\frac{\omega(k)}{|k|} = v,$$

where the dependence $\omega(k)$ is given by the dispersion relation in Eq. (7). Then Eq. (18) becomes

$$2\sqrt{\frac{K}{m}} \left| \sin \left( \frac{ka}{2} \right) \right| = v|k|,$$
from which, defining the dimensionless quantities $V = v/(a\sqrt{K/m})$ and $x = \frac{1}{2}ka$, we obtain the 1-parameter equation

$$|\sin(x)| = V|x|.$$  \hspace{1cm} (20)

The values of $x$ that solve Eq. (20) provide the values of $k$ that solve Eq. (19).

The solutions of this transcendent equation are obtained graphically in Fig. 17(a) over the full extended zone scheme. We then bring all the found values of $k$ inside the first Brillouin zone, Fig. 17(b). We proceed now to compare them to the positions of the peaks of $\langle |\hat{v}|^2 \rangle(k)$, Fig. 17(c). In Fig. 17 this procedure is followed for $v_{SL} = 0.12 a(K/m)^{\frac{1}{2}}$, showing that the solutions of Eq. (19) perfectly match the positions of all observed peaks obtained for $v_{SL} = v$.

Figures 18 and 19 compare the positions of the peaks of $\langle |\hat{v}|^2 \rangle(k)$ with the angular wavenumbers of the phonons whose phase velocity equals $v_{SL}$. It is apparent that for $v_{SL} \lesssim 0.9 a(K/m)^{\frac{1}{2}}$ the excited phonons almost perfectly match the phonons whose phase velocities are equal to $v_{SL}$. Therefore Eq. (20) gives us a prediction of the angular wavenumbers of the excited phonons that holds as long as $v_{SL}$ is not too close to the speed of sound $v_s = a(K/m)^{\frac{1}{2}}$, say $v_{SL} \lesssim 0.9 v_s$. Above $v_s$ Eq. (19) has of course no solution and indeed the spectrum displays no sharp peak, see the uppermost panel of Fig. 12.

Now we can use Eq. (20) as a tool to predict the number and wave vectors of the excited phonons when the slider is moving at a given velocity. This leads us to another interesting observation: if we call $P(v_{SL})$ the number of excited phonons at a given $v_{SL}$, we can infer from Eq. (20) that $P$, in the low-$v_{SL}$ regime, is approximately

$$P(v_{SL}) \approx \frac{2}{\pi V_{SL}} = \frac{2a\sqrt{K/m}}{\pi v_{SL}}.$$  \hspace{1cm} (21)

Therefore, for low $v_{SL}$ the number of excited phonons is inversely proportional to $v_{SL}$. Earlier in the present Section we observed that the number of excited phonons is related to the kinetic friction $F_d$, see Fig. 16. Assuming that a comparable power gets dissipated in each one of the phonon modes, Eq. (21) could account for the power law dependence $F_d(v_{SL}) \approx A/v_{SL}$ we observe in the low-speed regime in Sec. 4.2, Fig. 6. This hypothesis, to be confirmed, needs a systematic study of the intensities of the phonon excitations, but we have not yet found a way to predict these intensities, not even in the low-$v_{SL}$ limit.

6 Discussion and Conclusions

Even in the present simple model the transition between dynamic and static friction is elusive, because, as discussed in Sec. 4.2, the unphysical viscous force
of Eq. (6) dominates the low-speed regime. A study of this transition could be done omitting the viscous force, but this would require a chain large enough to prevent the phonon waves to come back to the slider position during the time of the simulation. And the simulation must be long enough for the slider to overtake about 10 chain atoms, so that the initial transient has come to an end. For example, if the slider is moving at a speed $v_{SL} = 10^{-4} v_s$ relative to the chain, to let it overtake 10 atoms we need a simulation whose duration is $(10 a)/v_{SL} = 10^5 (m/K)^{\frac{1}{2}}$. During this time, a phonon wave moving at the speed of sound $v_s$ covers a distance of $v_s \cdot 10^5 (m/K)^{\frac{1}{2}} = 10^5 a$. Thus, to prevent the returning waves, we would need a chain with at least $10^5$ atoms.

Investigation of the present model in the spring-pulling scheme analogous to the Prandtl-Tomlinson model shows that indeed the stick-slip to smooth sliding transition can be investigated, especially for low speed. The nonlinear phenomena occurring at the slip times are also well worth investigating.

The main results of this work are discussed in Sec. 5: the dissipation peaks recorded at certain values of $v_{SL}$ are caused by the excitation of new phonon modes which get excited as $v_{SL}$ decreases. In turn, the phonons excited at a certain slider speed are those whose phase velocity matches $v_{SL}$, and can be predicted by the law expressed in Eq. (20).

In further studies, it would be useful to examine the intensities and widths of the most excited phonon modes, and identify a relation for their prediction. Additionally, a phonon analysis analogous to that discussed in Sec. 5 could and should be performed on the model in a larger number of dimensions, to test in 2D [6] and 3D the analogous of the law in Eq. (20). This is especially important in view of the different density of phonon states of multidimensional crystals compared to 1D. Thermal effects should be studied too.
Figure 12: The average squared modulus of the Fourier transform of the chain velocities, for a few values of $v_{SL}$. 
Figure 13: Positions and heights of the peaks of $\langle |\tilde{v}|^2 \rangle (k)$ as functions of $v_{SL}$.

Figure 14: A zoom of Fig. 13 in the $v_{SL} \leq 0.23 \nu_s$ low-speed region.
Figure 15: A direct comparison of the peaks of $\langle |\tilde{v}|^2 \rangle (k)$, with the dynamic friction $F_d$ over a broad velocity range.

Figure 16: A blow up of the $0.05 \leq v_{SL} \leq 0.23 v_s$ region of Fig. [15]. The dotted vertical lines highlight the relation of the peaks of $F_d$ with the appearance of new excited phonons.
Figure 17: Steps performed to find the phonons whose phase velocity is equal to $v_{SL}$ and compare them to the observed excited phonons when the slider velocity is $v_{SL}$. In this example $v_{SL} = 0.12 a (K/m)^{\frac{1}{2}}$. 
Figure 18: The positions of the observed peaks of $\langle |\tilde{v}|^2 \rangle (k)$ (symbols), compared with the values of $k$ of the phonons whose phase velocity is equal to $v_{SL}$ (solid lines), solutions of Eq. (19).

Figure 19: A blow up of the peak traces as in Fig. 18, enlarging the interval $0 \leq v_{SL} \leq 0.23 v_s$. 
References


