Dynamics and friction at incommensurate contacting surfaces.

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ABSTRACT

We study the mechanisms for dissipation of mechanical energy during the sliding of two bodies against each other, namely the origin of friction at an atomic scale. We consider the most likely case of incommensurate contacting lattices. For this purpose, we study the dynamics of an infinite incommensurate chain onto a periodic lattice, modeled by the Frenkel Kontorova Hamiltonian with initial kinetic energy. By means of numerical and analytical results we have shown that transfer of translational energy from the center of mass to internal vibrations (heat) occurs via a novel kind of dissipative parametric resonances involving several resonant phonons. We review these results focusing on the computational aspects related to incommensurate structures.

Here we show that the above mechanism leads to thermal equilibrium via a dynamical transition which is characterized by a redistribution of the phonon modes from a floating to a pinned state, analogous to the Aubry transition of the static model.

Keywords: Atomistic friction, phonons, incommensurate systems.

1 Introduction

The possibility of measuring friction at the atomic level provided by lateral force microscope [1] and quartz crystal microbalance [2] has stimulated an intense theoretical research on this topic in recent years [3]. The goal of these investigations is to describe the onset and behavior of friction and to establish the mechanisms giving rise to energy dissipation during the sliding of a body onto a crystalline surface. Most studies have been carried out for one-dimensional models of non-linear lattices [4–10] and in particular for the Frenkel-Kontorova (FK) model where the surface layer is modeled by a harmonic chain and the substrate is replaced by a rigid periodic modulation potential. The FK model is particularly suitable to study the most likely case of an incommensurate lattice parameter of the contacting surfaces. The ground state properties of this model have been thoroughly studied [11]. At a critical value of the coupling to the external potential the ground state of the system displays a structural transition (Aubry transition) from a floating to a pinned configuration. Below this threshold, the ground state of the static system corresponds to a situation where the chain can be displaced on the substrate without energy costs. Therefore, one might expect a frictionless regime also in a dynamic situation. For this case, Shinjo and Hirano [4] have predicted that for incommensurate values of the chain lattice parameter to the period of the modulation, a *superlubric* regime should exist where the chain would slide indefinitely without dynamic friction but with a recurrent exchange of kinetic energy between center of mass and internal vibrations. This work was followed by an STM study [12] showing a drop of the friction force to values below experimental resolution (3nN) in going from commensurate to incommensurate contacts for a Si tip sliding on the W(001) surface. In a previous paper [14] we have addressed the question whether the experimentally observed superlubricity could be due to the blocking of the phonon channels caused by an incommensurate contact of the two sliding surfaces. We have shown that the conclusions of Ref. [4] are highly oversimplified and that resonances with the basic frequencies related to the modulation period lead to a complex hierarchy of couplings to the internal modes of the chain during the motion. The essential mechanism for the transfer of kinetic energy from the center of mass to the internal vibrations is the parametric resonant excitations of phonons mediated by ordinary resonances with phonons related to the modulating potential. The rise time of the parametric resonances can become as long as to yield an apparent frictionless behavior at large time scales but will always eventually cause an effective damping and lead to the decay of the center of mass (CM) velocity. Therefore, the experimental results of Ref. [12] should be related to the static rather than dynamic friction in accordance with the extremely slow sliding velocity. Here we show that, as a consequence of the resonant excitation of phonon modes during the sliding, the system goes through a dynamical transition which is related to the appearance of Umklapp terms [13] and, in analogy to the Aubry transition, can be described as a transition from an incommensurate to a pinned state.

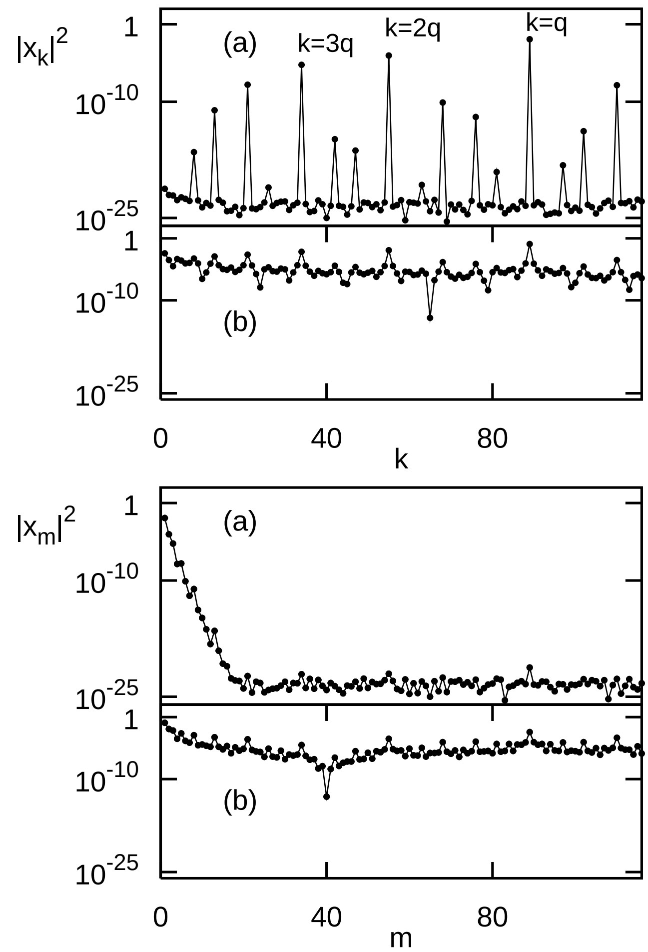

Figure 1: Top) Phonon amplitudes of the static FK model with N=233. a) $\lambda = 0.05 < \lambda_c$, b) $\lambda = 0.16 > \lambda_c$. Bottom) Phonon amplitudes of the static FK model plotted against multiples m of the wavevector q, a) and b) as in top panel.

2 The model

The dynamical FK model

$$\begin{aligned}\mathcal{H} &= K + V \qquad (1)\\ &= \sum_{i=1}^{N} \frac{p_i^2}{2} + \\ &\quad \sum_{i=1}^{N} \left[\frac{1}{2}\left(u_{n+1} - u_n - l\right)^2 + \frac{\lambda}{2\pi}\sin\left(2\pi u_n/b\right)\right]\end{aligned}$$

describes a harmonic chain of N atoms interacting with a periodic modulating potential. The ratio between l and the period of the potential b is taken to be incommensurate. We scale u so that $b = 1$ and l is taken to approximate the golden mean $\tau = (\sqrt(5) - 1)/2$ as $l = F_i/F_{i+1} = M/N$ where F_i are Fibonacci numbers [14]. The boundary condition $u_{N+1} = Nl + u_1$ is

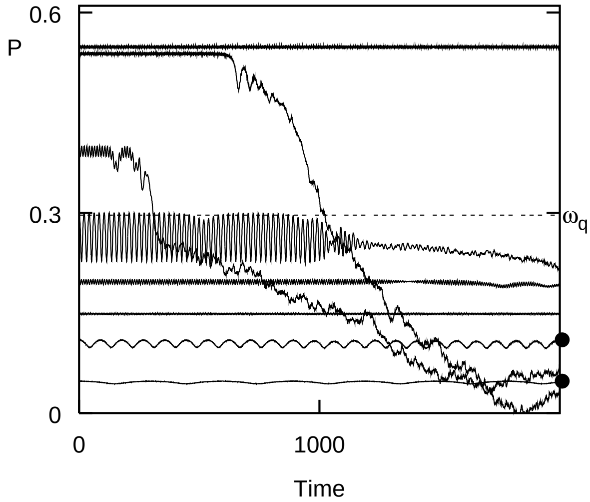

Figure 2: Temporal behavior of the CM velocity P for N =233, $\lambda = 0.05$. Each solid line corresponds to a different initial value P_0. The main resonance ω_q is indicated by a dashed line. The solid dots correspond to higher resonances.

imposed.

We define the CM position and velocity as $Q = \frac{1}{N}\sum_n u_n$, $P = \frac{1}{N}\sum_n p_n$. By writing $u_n = nl + x_n + Q$ we can integrate the equations of motion for x_n. As initial conditions we take the momenta $p_n(t = 0) = P_0$ and the coordinates $x_n(t = 0)$ corresponding to the ground state. The chosen boundary condition implies periodic boundary conditions for x_n.

In the limit of weak coupling λ it is convenient to go from real to reciprocal space by defining Fourier transformed coordinates $x_k = \frac{1}{N}\sum_n e^{-i2\pi kn/N} x_n$ which represent the phonon modes of the system. The dispersion for the linear chain with $\lambda = 0$ is $\omega_k = 2|\sin(\pi k/N)|$. In the limit of weak coupling, deviations from equidistant spacing l in the ground state ($K = 0$) are modulated by the substrate modulation wavevector $q = 2\pi l = 2\pi M/N$ as due to the frozen-in phonon ω_q. Higher harmonics mq have amplitudes which scale with λ^m. This is shown in Fig. 1 where we plot the phonon amplitudes as a function of the usual wavevector label k as well as reordered in units of the modulation wavevector q via the relation $k = mM\mathrm{mod}(N)$. For both cases, we consider two values of λ, below and above λ_c, which for our model has the value $\lambda_c \simeq 0.154$. It is evident that a description in terms of harmonics of the modulation wavevector is more appropriate to describe the incommensurate phase below λ_c. The expected exponential decay with λ^m is found numerically up to a high order where the finite numerical precision starts playing a role. Above the Aubry transition, the effect of the modulation is lost as seen from the rather featureless distribution of phonon amplitudes. In the next section we will show that a similar behavior is found also in the dynamical model with

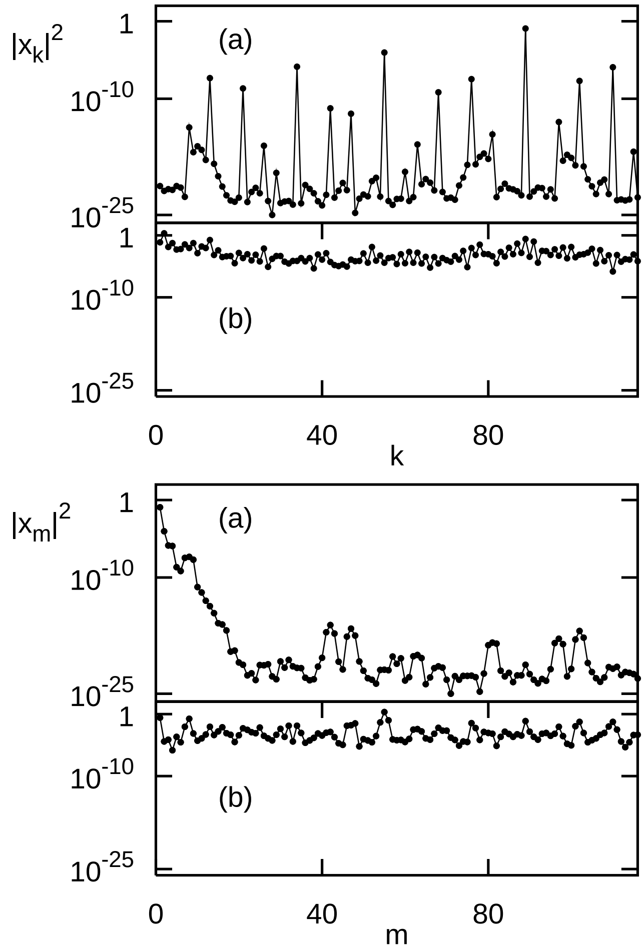

Figure 3: Top) Phonon amplitudes of the dynamical FK model for the case of Fig.2 for $P_0 = 0.29$. a) $t = 300$ b) $t = 1000$. Bottom) Phonon amplitudes of the dynamical FK model plotted against multiples m of the wavevector q, a) and b) as in top panel. Notice the similarity with Fig.1

kinetic energy as a function of time, also for $\lambda < \lambda_c$.

3 Short time behavior, onset of friction

In Fig. 2 we show the temporal behavior of the CM velocity for several initial values P_0. One can see that several regimes exist, with decay of the CM velocity over very different time scales. This is related to the resonant coupling to particular modes of the chain with wavevector related to the modulation periodicity q. In Ref. [14,16] we have developed an analytical framework which allows us to understand how harmonic resonances at ω_{mq} act as a *driving* term for the onset of dissipation via subsequent complex parametric excitations. Here we show that this mechanism leads to a dynamical transition in the system.

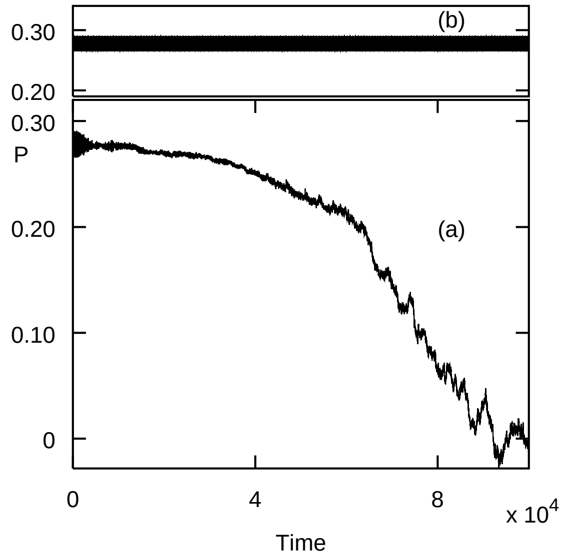

Figure 4: Temporal behavior of P for $\lambda = 0.015$ and $P_0 = 0.29$ for two values of N. a) $N = 144$, b) $N = 21$. In the last case, no decay occurs due to the discreteness of the spectrum, which prevents modes from becoming unstable, see text.

In Fig. 3 we show the amplitude of the phonon modes as a function of k and of m in analogy to what we have shown for the ground state in Fig.1. There, we have compared the amplitude of the modes for two values of λ above and below λ_c, whereas in Fig. 3 we show them for a given weak value of λ and two different values of the time, during the dynamics shown in Fig. 2 for $P_0 = 0.29$. One can see a very strong analogy between the Aubry transition of the ground state from a structure well described by the incommensurate modulation to one where the effect of the modulation is washed out. This finding suggests that a dynamical transition is taking place as a function of time also for weak values of the coupling. We are currently studying the nature of this transition [15] and relating it to the appearance of Umklapp terms which destroy the incommensurability of the system. Here we just want to point out that a critical phenomenon is occurring as a result of the onset of friction in the system. In the next Section we show how the system eventually reaches thermal equilibrium.

4 Long time behavior, dynamical transition to thermal equilibrium

In Fig. 4 we show the whole time evolution of the CM velocity, starting with a value close to the main resonance with the mode ω_q.

Before discussing the evolution towards equilibrium a comment on the role of N in numerical simulations of incommensurate systems is in order. For computer simulations, it is important to realize that parametric

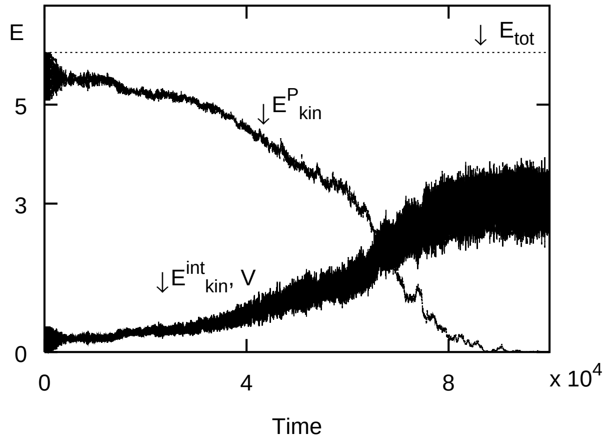

Figure 5: Temporal behavior of kinetic and potential energy terms for the case of Fig.4a. The potential energy V and internal kinetic energy E_{kin}^{int} are not distinguishable in the figure.

resonances give rise to instability energy windows leading to exponential growth of the amplitude of phonons in that energy range. Therefore, if the chain is too small, the discreteness of the spectrum can lead to a situation where no modes fall inside the instability range. We have estimated the conditions for the existence of resonant growth of modes as a function of N and found a threshold value which depend on the values of the parameters. For $N = 144$ the momentum quickly decays whereas for $N = 21$ no decay exist as predicted in [14].

In Fig. 5 all energy terms are examined. Initially the system possesses only the CM kinetic energy E_{kin}^{P} which decays to zero with time, being transferred into potential energy and kinetic energy of the phonons in equal parts. In Fig. 6 we show the behavior of the phonon modes in the initial and final part of the time evolution. Initially, the phonon modes are very far away from equilibrium, their amplitude being dictated by the modulation potential, as already noticed when commenting Fig. 1. At the end of the simulation, where complete energy transfer has occurred from the CM to the internal modes, the modes behave as expected from equipartition as $|x_k|^2 \sim 1/\omega_k^2$.

5 Summary and conclusions

We have identified the mechanism for energy transfer from the CM to internal vibrations during the sliding of a body onto an incommensurable substrate. We have given preliminary results which show that the evolution to thermal equilibrium occurs via a transition from an incommensurately modulated structure to a commensurate one.

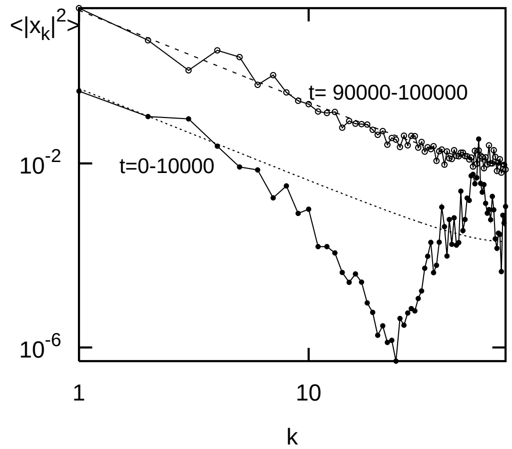

Figure 6: Temporal average of the phonon amplitudes over the indicated time ranges for the case of Fig.4a. The behavior expected from equipartition $|x_k|^2 \sim 1/\omega_k^2$ is given by the broken lines. Notice evolution towards equilibrium.

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