# Onset of Sliding Friction in Incommensurate Systems

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We study the dynamics of an incommensurate chain sliding on a periodic lattice, modeled by the Frenkel-Kontorova Hamiltonian with initial kinetic energy, without damping and driving terms. We show that the onset of friction is due to a novel type of dissipative parametric resonances, involving several resonant phonons which are driven by the (dissipationless) coupling of the center of mass motion to the phonons with the wave vector related to the modulating potential. We establish quantitative estimates for their existence in finite systems and point out the analogy with the induction phenomenon in Fermi-Ulam-Pasta lattices.

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The possibility of measuring friction at the atomic level provided by the lateral force microscopes [1] and quartz crystal microbalance [2] has stimulated intense research on this topic [3]. Phonon excitations are the dominant cause of friction in many cases [4]. Most studies are carried out for one-dimensional nonlinear lattices [5–12] and in particular for the Frenkel-Kontorova (FK) model [13], where the surface layer is modeled by a harmonic chain and the substrate is replaced by a rigid periodic modulation potential. The majority [6–12] examines the steady state of the dynamical FK model in the presence of dissipation, representing the coupling of phonons to other, undescribed degrees of freedom.

We study the dynamics of an undriven incommensurate FK chain. Our aim is to ascertain if the experimentally observed superlubricity [14] can be due to the blocking of the phonon channels caused by an incommensurate contact of the sliding surface. Therefore we do not include any explicit damping of the phonon modes, since we wish to find out if they can be excited at all by the motion of the center of mass (c.m.). In an earlier study, Shinjo *et al.* [5] found a superlubric regime for this model. We will show that their finding is oversimplified by either too short simulation times or too small system sizes. The inherent nonlinear coupling of the c.m. to the phonons leads to an irreversible decay of the c.m. velocity, albeit with very long time scales in some windows. The dissipative mechanism is driven by the coupling of the c.m. to the modes with modulation wave vector, $q$, or its harmonics, $\omega_{nq}$, and consists of novel types of parametric resonances with much wider windows of instabilities than those derived from the standard Mathieu equation. The importance of resonances at $\omega_{nq}$ has already been pointed out [6,8,10], with the suggestion [10] that they could be absent in finite systems due to the discrete phonon spectrum. However, it has not been realized that they act as a *driving* term for the onset of dissipation via subsequent complex parametric excitations which we will describe, establishing quantitative estimates for their existence in finite systems. A related mechanism has recently been identified in the resonant energy transfer in the induction phenomenon in Fermi-Ulam-Pasta (FPU) lattices [15].

We start with the FK Hamiltonian

$$\mathcal{H} = \sum_{n=1}^{N} \left[ \frac{p_n^2}{2} + \frac{1}{2} (u_{n+1} - u_n - l)^2 + \frac{\lambda}{2\pi} \sin\left(\frac{2\pi u_n}{m}\right) \right], \tag{1}$$

where $u_n$ are the lattice positions and $l$ is the equilibrium spacing for $\lambda = 0$, $\lambda$ being the coupling strength scaled to the elastic spring constant. The stiffness of the system is inversely proportional to $\lambda$ [8]. We take an incommensurable ratio of $l$ to the period $m$ of the periodic potential, namely, $m = 1$, $l = (1 + \sqrt{5})/2$. We consider chains of $N$ atoms with periodic boundary conditions $u_{N+1} = Nl + u_1$. Hence, in the numerical implementation, we have to choose commensurate approximations for $l$ so that $l \times N = M \times 1$ with $N$ and $M$ integer; i.e., we express $l$ as the ratio of consecutive Fibonacci numbers. The ground state of this model displays the so-called Aubry transition [16] from a modulated to a pinned configuration above a critical value $\lambda_c = 0.14$. Here we just note that in the limit of weak coupling ($\lambda \ll \lambda_c$), deviations from equidistant spacing $l$ in the ground state are modulated with the substrate modulation wave vector $q = 2\pi l/m$ [17] as being due to the frozen-in phonon $\omega_q$. Higher harmonics $nq$ have amplitudes which scale with $\lambda^n$.

We define the c.m. position and velocity as $Q = \frac{1}{N} \sum_n u_n$, $P = \frac{1}{N} \sum_n p_n$. By writing $u_n = nl + x_n + Q$, the equations of motion for the deviations from a rigid displacement $x_n$ read

$$\ddot{x}_n = x_{n+1} + x_{n-1} - 2x_n + \lambda \cos(qn + 2\pi x_n + 2\pi Q). \tag{2}$$

We integrate by a Runge-Kutta algorithm the $N$ equation (2) with initial momenta $p_n = P_0$ and $x_n(t = 0)$ corresponding to the ground state. For a given velocity $P$, particles pass over the maxima of the potential with frequency $\Omega = 2\pi P$, the so-called washboard frequency

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[8,10]. In Fig. 1 we show the time evolution of the c.m. momentum for $\lambda \sim \lambda_c/3$ and several values of $P_0$. According to the phase diagram of Ref. [5], a superlubric behavior should be observed for this value of $\lambda$ and $P_0 \geq 0.1$. We find instead a nontrivial time evolution with oscillations of varying period and amplitude and, remarkably, a very fast decay of the c.m. velocity for $P_0 \sim \omega_q/(2\pi)$ despite the absence of a damping term in Eq. (2). A similar, but much slower, decay is found for $nP_0 \sim \omega_{nq}/(2\pi)$. In the study of the driven underdamped FK [8] it is shown that, at these superharmonic resonances, the differential mobility is extremely low. Here, we work out an analytical description in terms of the phonon spectrum which explains this complex time evolution and identifies the dissipative mechanism which is triggered by these resonances. In the limit of weak coupling $\lambda$, it is convenient to define Fourier transformed coordinates $x_k = \frac{1}{N}\sum_n e^{-ikn}x_n$, with $k = 2\pi n/N$. The equations of motion become:

$$\ddot{x}_k = -\omega_k^2 x_k + \frac{\lambda}{2N}\sum_n e^{-ikn}[e^{iqn}e^{i2\pi Q}e^{i2\pi x_n} + \text{c.c.}], \tag{3a}$$

$$\ddot{Q} = \frac{\lambda}{2N}\sum_n [e^{i2\pi Q}e^{iqn}e^{i2\pi x_n} + \text{c.c.}], \tag{3b}$$

with $\omega_k = 2|\sin(k/2)|$. We expand Eq. (3a) in $x_n$ as:

$$\begin{aligned}\ddot{x}_k = &-\omega_k^2 x_k + \frac{\lambda}{2}\sum_{m=0}^{\infty}\frac{(i2\pi)^m}{m!} \\ &\times \sum_{k_1\ldots k_m}[e^{i2\pi Q}x_{k_1}\cdots x_{k_m}\delta_{k_1+\cdots+k_m,-q+k} \\ &+ (-1)^m e^{-i2\pi Q}x_{k_1}\cdots x_{k_m}\delta_{k_1+\cdots+k_m,q+k}].\end{aligned} \tag{4}$$

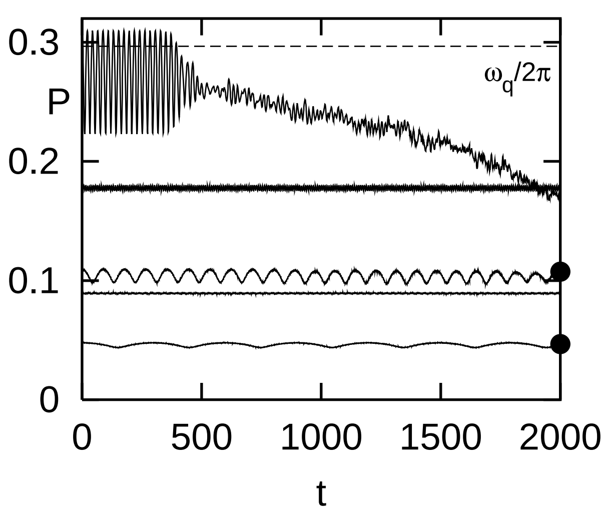


FIG. 1. Time dependence of the c.m. velocity for several values of $P_0$ for $N = 144$, $\lambda = 0.05 \sim \frac{\lambda_c}{3}$. The dashed line corresponds to $P_0 = \frac{\omega_q}{2\pi} = 0.2966$. Close to higher resonances (solid dots) a similar oscillatory behavior is observed, accompanied by a slower decay which is not apparent on the time scale of the figure.

Since in the ground state the only modes present in order $\lambda$ are $x_q = x_{-q} = \lambda/2\omega_q^2$, the c.m. is coupled only to these modes up to second order in $\lambda$:

$$\ddot{Q} = i\lambda\pi(e^{i2\pi Q}x_{-q} - e^{-i2\pi Q}x_q), \tag{5a}$$

$$\ddot{x}_{\pm q} = -\omega_q^2 x_{\pm q} + \frac{\lambda}{2}e^{\pm i2\pi Q}. \tag{5b}$$

In Fig. 2 we compare the behavior of $P(t) = \dot{Q}(t)$, obtained by solving the minimal set of Eqs. (5a) and (5b) with the appropriate initial conditions $Q(t = 0) = 0$, $P(t = 0) = P_0$, $x_q(t = 0) = \lambda/(2\omega_q^2)$, and $\dot{x}_q(t = 0) = 0$ with the one obtained from the full system of Eq. (2). Equations (5a) and (5b) reproduce very well the initial behavior of the c.m. velocity which displays oscillations of frequency $\Delta$ around the value $\Omega/2\pi$ but do not predict the decay occurring at later times because, as we show next, this is due to coupling to other modes. To this aim, we analyze the relation between the initial c.m. velocity $P_0$ and $\Omega/2\pi$, respectively, $\Delta_\pm$.

Take, as an ansatz for the c.m. motion,

$$Q(t) = \frac{\Omega}{2\pi}t + \alpha_+\sin(\Delta_+ t) + \alpha_-\sin(\Delta_- t). \tag{6}$$

By inserting the ansatz (6) into the coupled set of Eqs. (5a) and (5b) keeping only terms linear in $\alpha_\pm$, we find that both $\Delta_\pm$'s are roots of

$$\Delta^2 = \lambda^2\pi^2[2Z(0) - Z(\Delta) - Z(-\Delta)], \tag{7}$$

with $Z(\Delta)$ being the impedance

$$Z(\Delta) = \frac{1}{\omega_q^2 - (\Omega + \Delta)^2}. \tag{8}$$

In general, Eq. (7) has (besides the trivial solution $\Delta = 0$) indeed two solutions, related to the sum and difference of the two basic frequencies in the system, $\omega_q$ and $\Omega$:

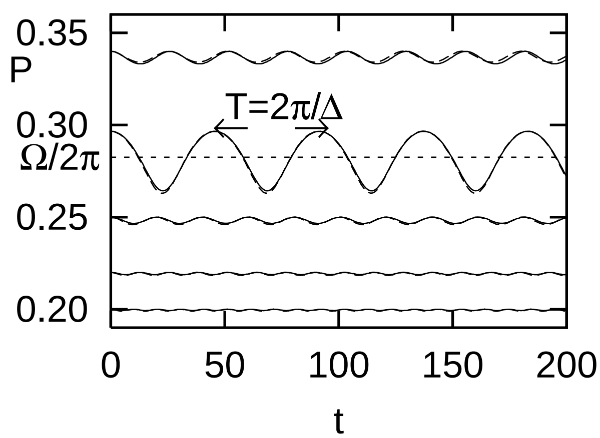


FIG. 2. Simulation of the full FK system according to Eq. (2) (solid lines) and numerical solution of Eqs. (5a) and (5b) (dashed lines) for $N = 144$, $\lambda = 0.015$, and several values of $P_0$ at about $P_0 = 0.29$. The differences between the two approaches are negligible. The average value of the c.m. velocity $\Omega/2\pi$ (horizontal dashed line) and the period of the oscillation for $P_0 = 0.29$ are also shown.

$$\Delta_\pm \cong \left| \omega_q \pm \Omega + \frac{\lambda^2\pi^2}{2\omega_q(\Omega \pm \omega_q)^2} + \dots \right| . \quad (9)$$

Close to resonance, $\Omega \sim \omega_q$, the amplitude $\alpha_-$ dominates (see below) and the c.m. oscillates with a single frequency $\Delta = \Delta_-$ (see Fig. 2). Very close to resonance (more precisely $\omega_q < \Omega < \omega_q + (2\lambda^2\pi^2/\omega_q)^{1/3}$), the root $\Delta_-$ becomes imaginary, signaling an instability. In fact, the system turns out to be bistable, as can be seen in Fig. 3 by the jump in $\Omega(P_0)$ as $P_0$ passes through $\omega_q/(2\pi)$.

Analytically, the relation between $\Omega$ and $P_0$, and the amplitudes $\alpha_\pm$, is determined by matching the ansatz (6) with the initial condition:

$$\alpha_\pm = \frac{\lambda^2\pi\Omega}{2\omega_q^2}\frac{1}{(\omega_q \pm \Omega)^3}, \quad (10)$$

$$P_0 = \frac{\Omega}{2\pi} + \frac{\lambda^2\pi\Omega}{2\omega_q^2}\left[\frac{1}{(\Omega+\omega_q)^2} + \frac{1}{(\Omega-\omega_q)^2}\right] + \dots . \quad (11)$$

The fact that Eq. (11) has multiple solutions for $\Omega$ when $P_0 \sim \omega_q/2\pi$ is in accordance with the jump seen in Fig. 3. However, Eq. (11), is derived by keeping only linear terms in $\alpha_-$ and cannot describe in detail the instability around $\omega_q$ where $\alpha_-$ diverges.

An initial behavior similar to that for $P_0 \simeq \omega_q/2\pi$ is observed in Fig. 1 for $nP_0 \simeq \omega_{nq}/2\pi$. We examine the case $n = 2$. Equation (4) shows that $x_{2q}$ is driven in next order in $\lambda$ by $x_q$:

$$\ddot{x}_{2q} = -\omega_{2q}^2 x_{2q} + i2\lambda\pi e^{i2\pi Q} x_q . \quad (12)$$

At $2\pi Q \simeq \Omega t$, $x_q$ is $\simeq \lambda e^{i\Omega t}$, so that $x_{2q}$ is forced with amplitude $\lambda^2$ and frequency $2\Omega$, yielding resonance for $2\Omega = \omega_{2q}$. Since $x_{2q}$ couples back to $x_q$, we have a set of equations similar to Eqs. (5a) and (5b), but at order $\lambda^2$.

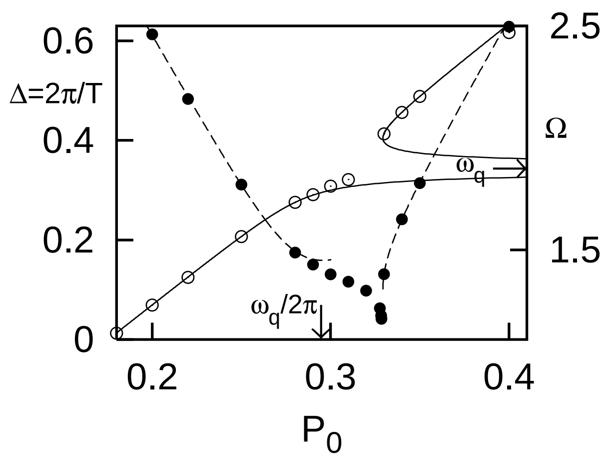


FIG. 3. Closed and open dots, frequencies $\Delta$ (left axis) and $\Omega$ (right axis) versus $P_0$ for simulations for $N = 144$, $\lambda = 0.015$. Dashed and solid lines: solutions of Eqs. (9) and (11), respectively.

We now come to the key issue, namely, the onset of friction causing the decay of the c.m. velocity seen in Fig. 1 at later times, which cannot be explained by the coupling of the c.m. to the main harmonics $nq$. Since $x_q$ is by far the largest mode in the early stage, we consider second order terms involving $x_q$ in Eq. (4):

$$\ddot{x}_k = -[\omega_k^2 + 2\lambda\pi^2(e^{i2\pi Q}x_{-q} + e^{-i2\pi Q}x_q)]x_k . \quad (13)$$

Insertion of the solution obtained above for $x_q$ [Eq. (5b)] and $Q$ [Eq. (6)] yields

$$\ddot{x}_k = -[\omega_k^2 + A + B\cos(\Delta t)]x_k \quad (14)$$

with $A = 2(\lambda\pi)^2/Z(0)$ and $B \sim \alpha_-$. The friction caused by these terms decreases with $\lambda^2$, i.e., with increasing stiffness. Equation (14) is a Mathieu parametric resonance for mode $x_k$. The relevance of parametric resonances has been recently stressed [12]. However, here, due to the coupling of the c.m. to the modulation mode $q$, resonances are not at the washboard frequency $\Omega$ but at $\Delta \sim \Omega - \omega_q$. Hence, we find instability windows around $\omega_k^2 + A = (n\Delta/2)^2$. Since $\Delta$ is small close to resonance, instabilities are expected for acoustic modes with $k$ small. Indeed, as shown in Fig. 4a, we find by solving Eq. (2) that the decay of the c.m. is accompanied by the exponential increase of the modes $k = 2, 3, 4$ and, with a longer rise time, $k = 1$. However, the instability windows resulting from Eq. (14), shown in Fig. 4b, cannot explain the numerical results of Fig. 4a, i.e., the Mathieu formalism cannot explain the observed instability. In Eq. (4), the only linear terms omitted in Eq. (13) are couplings with $x_{k\pm q}$, which are much higher order in $\lambda$. Nevertheless, these terms are crucial since they may cause new instabilities due to the fact that, for small $k$, they are also close to resonance. We have solved the coupled set of equations for mode $x_{\pm k}$ and $x_{k\pm q}$:

$$\ddot{x}_k = -[\omega_k^2 + 2\lambda\pi^2(e^{i2\pi Q}x_{-q} + e^{-i2\pi Q}x_q)]x_k + i\lambda\pi(e^{i2\pi Q}x_{k-q} - e^{-i2\pi Q}x_{k+q}), \quad (15a)$$

$$\ddot{x}_{k\pm q} = -[\omega_{k\pm q}^2 + 2\lambda\pi^2(e^{i2\pi Q}x_{-q} + e^{-i2\pi Q}x_q)]x_{k\pm q} \pm i\lambda\pi e^{\pm i2\pi Q}x_k , \quad (15b)$$

together with Eqs. (5a) and (5b) for continuous $k$. Indeed, we find a wider range of instabilities, giving a detailed account of the numerical result as shown in Fig. 4b. This mechanism where a parametric resonance is enhanced by coupling to near-resonant modes is quite general in systems with a quasicontinuous spectrum of excitations and is related to the one proposed [15] in explaining instabilities in the FPU chain in a different physical context.

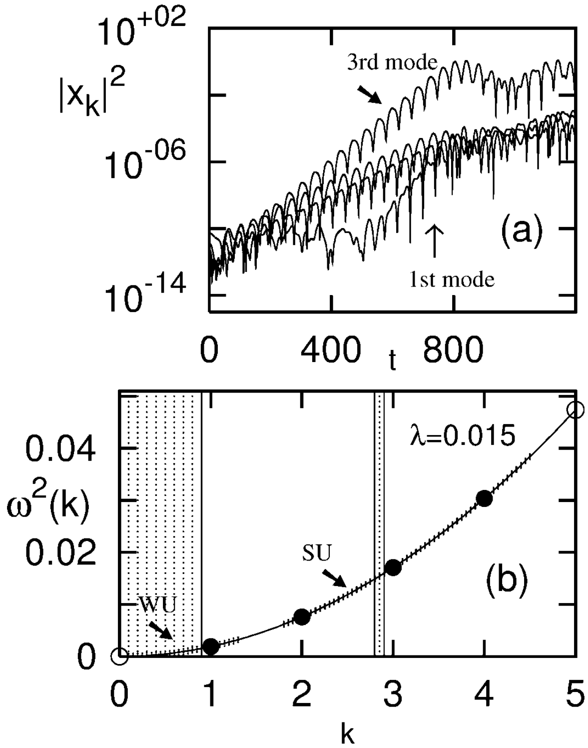


FIG. 4. (a) $|x_k(t)|^2$ of the first four modes from Eq. (2) with $N = 144$, $\lambda = 0.015$, and $P_0 = 0.29$. Note that the first mode has a longer rise time and that the third mode is the most unstable. (b) Dispersion relation for a chain of 144 atoms [$k$ values in units of $(\frac{2\pi}{144})$]. Unstable modes resulting from the full simulation are represented by solid dots. The shaded $k$ ranges give the instability windows resulting from the Mathieu-type Eq. (13) and cannot explain the simulation. Conversely the wiggled ranges of the phonon dispersion (WU = weakly unstable, SU = strongly unstable) are the instability windows predicted by Eqs. (5a), (5b), (15a), and (15b). They explain all instabilities as well as the long rise time of the first mode (WU) and the shortest one of the third mode which falls in the middle of the SU range.

The number of particles $N$ is an important parameter. When this number is very small, the chain is in fact commensurate and the phase of the c.m. is locked (the gap scales as $\lambda^N$ due to umklapp terms). Next, one enters a stage of apparent superlubric behavior due to the fact that the spectrum is still discrete on the scale of the size of the instability windows discussed above. For $N = 144$ and $\lambda = \frac{1}{3}\lambda_c$ (Fig. 1) we only begin to see the decay for values of $P_0$ close to resonances. The experimentally observed superlubricity in [14] could then be due either to the finiteness of the system or to the low sliding velocities.

The above described multiple parametric excitation gives rise to an effective damping for the system via a cascade of couplings to more and more modes via the nonlinear terms in Eq. (4). It remains an open question if this mechanism will eventually lead to a full or partial equilibrium distribution of energy over the normal modes [18], although our preliminary results support the former hypothesis even at weak couplings.

In summary, we have described in detail the mechanism which gives rise to friction during the sliding of a harmonic system onto an incommensurate substrate. The onset of friction occurs in two steps: the resonant coupling of the c.m. to modes with the wave vector $q$ leads to long wavelength oscillations which in turn drive a complex parametric resonance involving several resonant modes. This mechanism is robust in that it leads to wide instability windows and represents a quite general mechanism for the onset of energy transfer in systems with a quasicontinuous spectrum of excitations.

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