Can aperiodicity cause superlubricity?

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Abstract

The ground state of incommensurate structures is determined by the modulation due to the substrate potential. This causes an interplay between the motion of the center of mass and frequencies related to the modulation wavevector q. We build for the one-dimensional Frenkel-Kontorova model an analytical framework which enables us to interpret the initial behavior of the system for a broad range of initial velocities in terms of these relevant phonon modes, and to investigate the occurrence of superlubricity.

1. Introduction

The Frenkel-Kontorova (FK) model[1] is a powerful tool in the study of many interesting systems in solid-state physics and nonlinear dynamics; in particular, it has been applied in the study of atomistic friction and of the role that incommensurability plays[2]. The ground state properties of the model are by now very well understood[3], and interesting predictions and experimental observation of a frictionless regime in the dynamical version of the model have been made[4,5].

We have recently shown[6] how it is possible to work out, in the framework of the incommensurate, undamped and undriven dynamical FK model, an analytical framework which allows us to accurately reproduce the initial phases of the time evolution of the system in terms of minimal sets of equations. We also elucidated how friction sets in in the system via a two-stage process involving the resonant excitation of phonons caused by the coupling of the center of mass Q (c.m.) to the phonon modes with wavevector related to the modulation potential. Here we aim at showing how our approach can be used to identify the phonon modes which are relevant for the time evolution of the system. Our analysis also allows us to make precise statements about the occurrence of superlubricity.

2. Model and numerical results

In its one-dimensional formulation, the FK model describes the interaction of a chain of atoms with a rigid, modulated substrate potential. Atoms within the chain interact via a first-neighbor harmonic potential. In order to study the dynamics of the system, we add a kinetic term to the potential energy. The dynamical version of the model is described by the following Hamiltonian:

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

where N is the number of particles in the chain, u_n are the lattice positions and the substrate potential strength λ is rescaled to the harmonic spring constant. We define the modulation wavevector $q = 2\pi l/m$, where m is the modulation period of the potential. The equilibrium spacing l between atoms can have any real value, but, as far the ground state of the model is concerned, it has been proved[3] that, if the ratio between l and m is incommensurate, the system undergoes a transition for a critical value $\lambda = \lambda_c$, known as *breaking of analyticity* and characterized by a passage from a *sliding* to a *pinned* state.

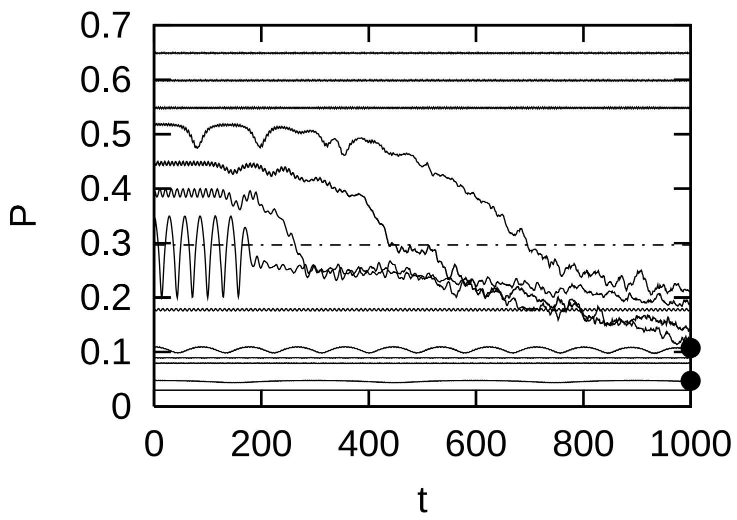

Figure 1: Time dependence of the c.m. velocity for several values of the initial c.m. momentum P_0, $\lambda = 0.05$, N=144.The dashed line corresponds to $P_0 = \frac{\omega_q}{2\pi} = 0.2966$. The solid dots indicate higher resonances.

We consider the case where an initial velocity $P(t=0) = P_0$ is given to all particles in the chain. By writing $u_n = nl + x_n + Q$, where $Q = \frac{1}{N}\sum x_n$, the following equations of motion for the deviations from the rigid displacement x_n can be derived:

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

Fig. 1 shows the behavior of the c.m. velocity P of the chain (defined as $P = \frac{1}{N}\sum p_n$) for a value of the substrate potential $\lambda \sim \frac{\lambda_c}{3}$ and for various values of P_0, as obtained by numerically solving Eq.(2), with $m = 1$ and $l = F_{13}/F_{12} = 233/144 \simeq \frac{\sqrt{5}+1}{2}$, F_n being the nth Fibonacci number. Depending on the initial value P_0, the time behavior of P exhibits oscillations of very different amplitude and period. For some values of P_0 we observe a quick decay which corresponds to a frictional behavior. We will now briefly show how all the features in the initial phase of the time evolution can be well explained by a Fourier analysis of the equations of motion (2) in the regime $\lambda << \lambda_c$.

3. Analytical results and discussion

The equations of motion (2) can be rewritten in the Fourier space as:

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

whence

$$\ddot{Q} = \frac{\lambda}{2N}\sum_n \left[e^{i2\pi Q}e^{iqn}e^{i2\pi x_n} + c.c.\right] \tag{4}$$

where $\omega_k = 2|\sin\left(\frac{k}{2}\right)|$ is the phonon spectrum of the chain for $\lambda = 0$.

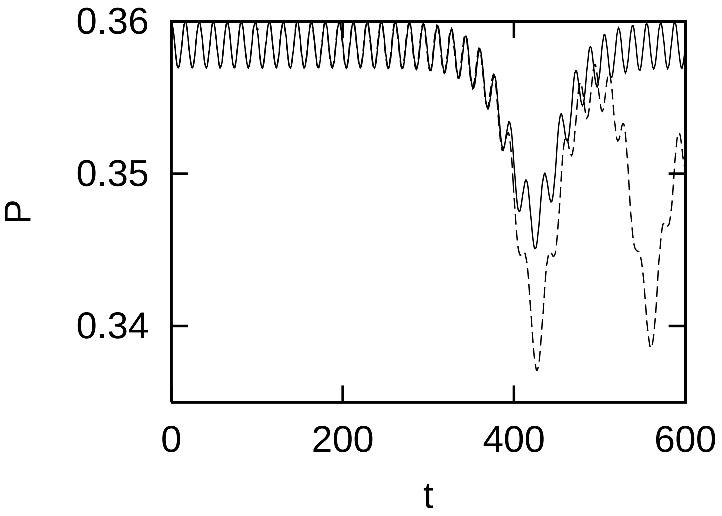

Figure 2: Comparison between the numerical solution of Eq.(2) (solid line) and of Eq.(6) (dashed line) for N=144, $P_0 = P(\omega_{M1}) \simeq 0.36$, $\lambda = 0.015$. An analogous behavior is found at $P_0 = P(\omega_{M2}) \simeq 0.53$.

Expanding the terms $e^{i2\pi x_n}$ gives:

$$\ddot{x}_k = -\omega_k^2 x_k + \frac{\lambda}{2}\sum_{m=0}^{\infty}\frac{(i2\pi)^m}{m!}\sum_{k_1\ldots k_m}\left[e^{i2\pi Q}x_{k_1}\cdots x_{k_m}\delta_{k_1+\cdots+k_m,-q+k}\right. \tag{5}$$
$$\left.+(-1)^m e^{-i2\pi Q}x_{k_1}\cdots x_{k_m}\delta_{k_1+\cdots+k_m,q+k}\right]$$

In the ground state the only modes present in order λ are $x_{\pm q}$; therefore, the behavior of the c.m. is determined, up to second order in λ, only by the resonant coupling to those modes. In Ref. 6 we compare the solution of the full system of Eq.(2) and of the set of equations obtained by Eq.(5) for the aforementioned modes $x_{\pm q}$ and their coupling to the c.m.. The agreement is very good for values of the initial momentum close to the resonance $P_0 \simeq \frac{\omega_q}{2\pi}$, where a long wavelength oscillation around an average value Ω is observed in the initial phase. The later onset of friction cannot of course be reproduced by this dissipationless coupling, and it is explained by subsequent couplings with other modes, which cause complex parametric resonances. A similar behavior is observed at superharmonic resonances for $nP_0 \simeq \frac{\omega_{nq}}{2\pi}$. We give in Ref. 6 an extensive treatment of the problem.

Here we concentrate on another type of resonances which also lead to decay of the initial momentum. Based on our expansion (5) we find that modes $x_{\frac{q}{2}}$ are parametrically excited by the oscillatory motion of the c.m.:

$$\begin{aligned} \ddot{x}_{\frac{q}{2}} &= -\omega^2_{\frac{q}{2}} x_{\frac{q}{2}} + i\lambda\pi \left(e^{i2\pi Q} x_{-\frac{q}{2}} - e^{-i2\pi Q} x_{\frac{3}{2}q} \right) \\ \ddot{Q} &= i\lambda\pi \left(e^{i2\pi Q} x_{-q} - e^{-i2\pi Q} x_q \right) - \lambda\pi^2 \left(e^{i2\pi Q} x^2_{-\frac{q}{2}} + e^{-i2\pi Q} x^2_{\frac{q}{2}} \right) \end{aligned} \tag{6}$$

These resonances give instability regions (thus frictional behavior) centered around the values $\omega_{M1} = 2\omega_{\frac{q}{2}}$ and $\omega_{M2} = 2\omega_{\pi-\frac{q}{2}}$. Fig.2 shows a comparison between the full system (2) and the numerical solution of Eqs.(6). The features of the initial behavior are also in this case remarkably well reproduced. When compared to the standard Mathieu equation, the parametric resonances described by Eq.(6) can be considered peculiar for two reasons: firstly, the equation for mode $x_{\frac{q}{2}}$ is in fact a set of two coupled equations (x_k being a complex number). Secondly, the back coupling to the resonant mode $x_{\frac{q}{2}}$ in the equation for the c.m. motion drives Q inside and outside the instability window (see Fig.2), which is not a standard feature of this type of phenomena.

In conclusion, we can state that, starting with the ground state of the one-dimensional FK model we have studied, a frictionless superlubric regime cannot exist because the resonant coupling of the c.m. to the modes nq or $(\frac{q}{2}, \pi - \frac{q}{2})$ gives raise to an effective damping for the system via a cascade of couplings to more and more modes via the non-linear terms in Eq.(5). An *apparent superlubricity* can arise in numerical calculations (thus with finite N), and can be attributed to the discreteness of the spectrum on the scale of the size of the instability windows.

4. References

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