Modelling study of microscopic sliding on irregular substrates

Andrea Vanossi a, Alan R. Bishop b, Anna Franchini a,*, Virginio Bortolani a

a INFM-S3 e Dipartimento di Fisica, Università di Modena e Reggio Emilia, Via Campi 213/A, 41100 Modena, Italy
b Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

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Abstract

In connection with microscopic solid friction phenomena, we study the underdamped dynamics of a driven Frenkel–Kontorova chain subject to a substrate potential defined by the sum of two sinusoidal function with different periodicity. We simulate microscopic sliding over quasiperiodic and multiple-well (periodic) substrates. We comment on the nature of the particle dynamics in the vicinity of the pinning–depinning transition point and consider the role played by the coverage variable on the depinning mechanism. We also investigate on the different nonlinear excitations forming during sliding and characterizing the dynamical states observed at different strengths of the imposed driving. The dependence of the static friction on the ratio of the model interaction strengths is analyzed.

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1. Introduction

Nonequilibrium dynamics of simple systems of interacting particles subjected to an on-site potential, a damping and driven by an external force, is a very rich and interesting theoretical problem, as well as having many important applications in such areas as mass transport, charge-density waves, Josephson junctions, etc. These systems, with many degrees of freedom, are usually pinned in the external potential and exhibit, once driven, a strongly nonlinear mobility as a function of the applied force. Also dry (i.e., solid–solid) friction belongs to this class of systems because the asperities of the surfaces may interlock.

The recent acquisition, for tribological phenomena, of experimental (AFM, FFM, SFA, QCM) and computational (realistic MD simulations) data at the nanoscale [1], has stimulated modelling studies, as those based on the driven Frenkel–Kontorova (FK) type models [2], able to capture the essential physics involved in the atomistic dynamics of interfaces in relative motion. In these one-dimensional models, a certain density of particles is made to slide, by the application of an external driving and in the presence of dissipation, over a rigid substrate. The shape of the substrate potential, assumed purely sinusoidal in the standard FK chain [3,4], is a factor of particular importance when modelling physical systems. Its introduction, justified via a self-consistent microscopic model [5] where only interparticle interactions are considered, can be viewed as an effective potential produced by the coupling of the
chain atoms with other degrees of freedom such as, the substrate atoms.

Some important generalizations of the geometry of the on-site potential have already been considered, as, for example, those proposed for systems of adsorbed atoms [6,7], or those introduced in the theory of solitons in hydrogen-bonded chains [8].

In this work, in order to model the chain sliding on irregular interfaces [9,10], we chose to define the on-site potential by the sum of two sinusoidal function with different spatial periodicity. The quasiperiodic or multiple-well periodic feature of the substrate depends, respectively, on the mutually incommensurate or commensurate choices for the inherent system length scales. This study may well be relevant in the two, distinct, real physical situations of friction dynamics between quasicrystal surfaces (for the quasiperiodic case), or between lattices with a complex unit cell (for the multiple-well periodic choice).

2. Model and numerical procedure

We consider a FK-type chain, whose \( N \) particle positions \( \{ x_i \} \) satisfy the following equations of motion:

\[
\ddot{x}_i + \gamma \dot{x}_i + \frac{1}{2} \left[ \sin \left( \frac{2\pi}{a} x_i + \frac{2\pi \beta}{a} x_i \right) \right] + \frac{d}{dx_i} \left[ \sum_{i \neq j} V(|x_i - x_j|) \right] = F
\]

where \( \gamma \) is a phenomenological viscous damping coefficient [11], chosen such that we are in the underdamped regime, and \( F \) is the external driving force. The numerical simulations of Eq. (1) are performed choosing, for the interatomic interaction \( V \), both a simple harmonic interaction and a Morse-type potential, with strength \( K \) and natural equilibrium spacing \( b = L/N \), where \( L \) is the chain length. The two lengths \( a \) and \( c = a/\beta \) define the geometry of the substrate potential. Periodic boundary conditions are imposed on the system.

The essential physical feature of the model consists in the interaction length scale competition, resulting in a rich complexity of spatially modulated structures for the chain particles.

The three lengths \( a, b \) and \( c \) are chosen to be:

- \textit{mutually incommensurate} so to study the friction dynamics [9] of a FK model over quasiperiodic substrate potentials (quasicrystals);
- \textit{mutually commensurate} so to consider the possible formation of commensurate dynamical structures [10] during sliding (lattices with a complex unit cell).

A fourth-order Runge-Kutta algorithm is implemented to solve numerically the equations of motion (1). The system is initialised with the particles placed at rest at the uniform separation \( b \). The dc-force, \( F \), is then increased adiabatically. For every value of \( F \), the Eq. (1) are integrated over a time period \( [0, T] \) long enough to eliminate transient behavior and reach a steady state for which the system mobility \( \mu \equiv \langle v \rangle / F \) is then calculated, \( \langle v \rangle \) being the average center of mass velocity of the chain.

3. Results and discussion

3.1. Quasiperiodic case

For \textit{incommensurate} choices among \( a, b, \) and \( c \) (Fig. 1a and b), we find that when the three length scales are related by cubic irrational numbers, e.g. the spiral mean (Fig. 1a), there exists a critical value \( K_c \approx 5.6 \) of the interparticle interaction strength \( K \) above which the static friction (the minimal force required to initiate the chain motion) is zero. On the other hand, when the length scales are related by quadratic irrationals, e.g. the golden mean (Fig. 1b), we always observe a nonzero static friction in order to start the dynamics (\( \mu \neq 0 \)).

For small values of \( K \) (e.g., \( K = 1 \)), from examination of the particle trajectories, we see that the chain depins via the motion of a small number of isolated defects (kinks) along the chain. At forces just above \( F_c \), the steady states consist of mainly stationary particles, with a small number of
kinks moving around the chain. This produces the low mobilities observed. The number of kinks present increases as one raises the driving force. Eventually there are enough defects that, even though they are very narrow, they begin to overlap. At a second threshold force, the chain motion changes to the high driving running state where \( \gamma(v) = F \).

For large values of \( K \) (e.g., \( K = 3\pi \)), the chain is never pinned for the spiral mean case, and motion is initiated by even the smallest driving force, i.e., \( F_s = 0 \). The chain jumps directly to the running state (see low panel of Fig. 1(a)). For the golden mean case (low panel of Fig. 1(b)), on the contrary, the static friction is smaller than at \( K = 1 \), but clearly nonzero. The first steady states above the depinning threshold are again spatially inhomogeneous. However, now that \( K \) is large, defects are extended and no more isolated with an immediate tendency to overlap. Hence, even just above \( F_s \), we observe a relatively large mobility.

### 3.2. Multiple-well periodic case

The rational choice among \( a, b \) and \( c \) results in a periodicity of the substrate \( T = M_2a = M_1c \), with \( M_1 \) and \( M_2 \) integer numbers. We fix \( a = 1 \), and vary the parameter \( \beta \). Due to the imposed periodic boundary conditions, the chain length \( L \) must be an integer multiple, \( Q \), of the substrate period \( T \), i.e., \( TQ = L = bN \). In principle, we may simulate the dynamics over \( L \) different substrates (\( \beta = M_1/L \), with \( M_1 = 1, \ldots, L \)). Obviously, we consider just a few examples, in an attempt to infer some general qualitative behavior connected to the commensurability of the system length scales. Let us now analyse, for example, the specific value \( \beta = 24/30 \), allowed by the imposed periodic boundary conditions for a system of length \( L = 30 \), for which the substrate potential have five wells for each of its six unit cells of period \( T = 5 \). Once we tilt the on-site potential by the application of \( F \), the lowest minima, having a height much smaller than the others, soon disappear and each substrate cell then contains only four wells.

Fig. 2 shows the mobility \( \mu \) as a function of \( F \), for chains with different numbers \( N \) of particles. As far as the depinning transition is concerned, we notice that for \( N = 24 \), there are no extra particles in place (with respect to the number of substrate wells) to initiate the motion when the Peierls–Nabarro (PN) barrier disappears. Consequently, without any thermal noise to create a kink, the chain motion does not start when we exceed the PN barrier and dynamics is delayed. Then, as the number of particles \( N = 25, 26, \ldots \), etc., is increased, each extra particle provides one more “intrinsic” kink, and the depinning transition occurs at a lower value of the driving, i.e., as soon as the PN barrier is exceeded. We observe a rise in the
mobility that is approximately proportional to the number of these intrinsic kinks, up until \( N = 30 \) (see inset of Fig. 2).

Because of the complex substrate potential, it is not easy to determine a precise relation between the steps shown in the curves of \( \mu \) vs. \( F \), above the depinning threshold, and the various dynamical behaviours observed during the chain motion. Moreover, these regimes, characterized by spatial rearrangements of particle configurations with different periodicities and amplitudes, turn out to be strongly dependent also on the number of system particles, \( N \), and on the chain stiffness, \( K \). For the choice of the parameters \( \beta = 24/30 \) and \( N = 30 \), Fig. 3 shows four dynamical commensurate structures (corresponding to four different values of the driving) with periodicities 5, 10, 15, and 30. From these snapshots, one observes that the structures moving around the chain often display smaller superimposed decorations of period \( T = 5 \).

We have also investigated the dependence of the static friction \( F_s \) on the interatomic strength \( K \) for various numbers \( N \) of particles. In general, it is possible to prove [10] that, in the limit for large \( K \),
there is no possible stable solution for $F > 0$ and so $F_s$ vanishes. However, see Fig. 4, whenever $N$ is a factor of $M$ or $L$, stable configurations do exist and a nonzero static friction results. $F_s$ will then be, either 0.5, if $N$ is a factor of either $M$ or $L$ (e.g., $N = 24$ or 30), or 1, if $N$ is a factor of both $M$ and $L$ (e.g., $N = 6$). One notable feature of these curves is that, in contrast to the standard FK model, they can be nonmonotonic. A study of the pinned configurations shows that a restructuring occurs in the stable state at the value $K = 1$, leading to the characteristic downward spike in the static friction at $K = 1$. It is the complex, multiple-well nature of the substrate that allows for a discontinuous change [9] in the stable particle positions as one varies the elastic constant, so permitting the nonmonotonic behavior.

4. Conclusions

We have studied the sliding dynamics of an interacting chain of atoms driven by a dc external force over a complex substrate potential and subject to a weak viscous damping.

In order to model the friction behavior between two quasicrystal surfaces, we considered an irrational choice among the three inherent length scales of the system, finding zero static friction for the case of cubic irrational numbers (e.g., spiral mean) at sufficiently strong interparticle interactions, whereas for quadratic irrationals (e.g., golden mean) $F_s$ was always found to be nonzero.

For mutually rational choices instead, relevant, e.g., in the real physical situation of friction dynamics between lattices with a complex unit cell, we have observed the formation of commensurate dynamical structures during the motion over the on-site potential. These moving entities (often “decorated” by the substrate periodicity) characterize the different spatially inhomogeneous stable states, giving rise to the multiple steps found in the chain mobility as a function of the driving. We have also illustrated the role played by the coverage variable in the depinning mechanism and the peculiar nonmonotonic dependence of the static friction on the ratio of the model interaction strengths.

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