Hysteresis from dynamically pinned sliding states

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Abstract

We report a surprising hysteretic behavior in the dynamics of a simple one-dimensional nonlinear model inspired by the tribological problem of two sliding surfaces with a thin solid lubricant layer in between. In particular, we consider the frictional dynamics of a harmonic chain confined between two rigid incommensurate substrates which slide with a fixed relative velocity. This system was previously found, by explicit solution of the equations of motion, to possess plateaus in parameter space exhibiting a remarkable quantization of the chain center-of-mass velocity (dynamic pinning) solely determined by the interface incommensurability. Starting now from this quantized sliding state, in the underdamped regime of motion and in analogy to what ordinarily happens for static friction, the dynamics exhibits a large hysteresis under the action of an additional external driving force $F_{\text{ext}}$. A critical threshold value $F_c$ of the adiabatically applied force $F_{\text{ext}}$ is required in order to alter the robust dynamics of the plateau attractor. When the applied force is decreased and removed, the system can jump to intermediate sliding regimes (a sort of “dynamic” stick-slip motion) and eventually returns to the quantized sliding state at a much lower value of $F_{\text{ext}}$. On the contrary no hysteretic behavior is observed as a function of the external driving velocity.

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1 Introduction

Nonlinear systems driven far from equilibrium exhibit a very rich variety of complex spatial and temporal behaviors [1]. In particular, in the emerging field of nanoscale science and technology, understanding the nonequilibrium dynamics of systems with many degrees of freedom which are pinned in some external potential, as is commonly the case in solid state physics, is becoming more and more often an issue. Friction belongs to this category too, because the microscopic asperities of the mating surfaces may interlock. It has been frequently shown [2] that simple phenomenological models of friction give good qualitative agreement with experimental results on nanoscale tribology or with more complex simulation data of sliding phenomena. In this kind of simplified approaches, studies are typically restricted to describing microscopic dynamics in one (1D) or two (2D) spatial dimensions. The substrates defining the moving interface are modelled in a simplified, although often effective, way as purely rigid surfaces or as one- or two-dimensional arrays of particles interacting through simple (e.g., harmonic) potentials. Despite this crude level of description, this approach has frequently revealed the ability of modelling the main features of the complex microscopic dynamics, ranging from regular to chaotic motion.

One of the pervasive concepts of modern tribology – with a wide area of relevant practical applications as well as fundamental theoretical issues – is the idea of free sliding connected with \textit{incommensurability}. When two crystalline workpieces with lattices that are incommensurate (or commensurate but not perfectly aligned) are brought into contact, the minimal force required to achieve sliding, i.e. the static friction, should vanish, provided the two substrates are stiff enough. In such a geometrical configuration, the lattice mismatch can prevent asperity interlocking and collective stick-slip motion of the interface atoms, with a consequent negligibly small frictional force. Experimental observation of this kind of \textit{superlubric} and anisotropic regime of motion has recently been reported [3,4]. The remarkable conclusion of frictionless sliding can be drawn, in particular, in the context of the Frenkel-Kontorova (FK) model (see [5] and references therein). Since however the physical contact between two solids is generally mediated by so-called “third bodies”, the role of incommensurability has been recently extended [6] in the framework of a driven 1D confined model inspired by the tribological problem of two sliding interfaces with a thin solid lubricant layer in between. The moving interface is thus characterized by three inherent length scales: the periods of the bottom and top substrates, and the period of the embedded solid lubricant structure. In particular, in the presence of a uniform external driving, the interplay between these incommensurate length scales can give rise to intriguing dynamical phase locking phenomena and surprising velocity quantization effects [7,8].
Extending a previous study of this confined tribological model [7], here we focus on the remarkable hysteretic behavior that this system exhibits starting now from this quantized sliding state. We find a strictly analogy to what ordinarily happens for static friction in the underdamped regime of motion [9]. The lubricant center-of-mass (CM) velocity turns out to be robustly locked to the quantized plateau value (dynamic pinning) which is only abandoned above a critical force. As long as inertia effects are not negligible compared to dissipative forces, the adiabatic variation (increase and decrease) of the external applied force shows a large hysteresis loop in the $V_{cm} - F_{ext}$ characteristics. Some differences between this dynamic locking and the usual static pinning are also briefly discussed.

2 Confined model and numerical method

Like in Ref. [7], we consider a simplified one-dimensional generalized FK model consisting of two rigid sinusoidal substrates, of spatial periodicity $a_+ \text{ and } a_-$, and a chain of harmonically interacting particles, of equilibrium length $a_0$, mimicking the sandwiched lubricant layer, as schematically shown in the inset of Fig. 1. The two substrates move at a constant relative velocity $V_{ext} = V_- - V_+$. (In particular we set in full generality $V_+ = 0$ and $V_- = V_{ext}$). In order to probe the robustness of quantized dynamics of $V_{cm}$, an additional constant force $F_{ext}$ is applied adiabatically to all chain particles. The equation of motion of the $i$-th lubricant particle becomes:

$$m\ddot{x}_i = -\frac{1}{2} \left[ F_+ \sin \frac{2\pi}{a_+} x_i + F_- \sin \frac{2\pi}{a_-} (x_i - V_{ext} t) \right]$$

$$+ K(x_{i+1} + x_{i-1} - 2x_i) - \gamma (2\dot{x}_i - V_{ext}) + F_{ext},$$

where $m$ is its mass. $F_\pm$ are the amplitudes of the forces due to the sinusoidal corrugation of the substrates. Presently we set $F_-/F_+ = 1$ as the least biased choice. $K$ is the chain spring constant defining the harmonic nearest-neighbor interparticle interaction. The penultimate damping term in Eq. (1) originates from two frictional contributions of the form $-\gamma (\dot{x}_i - V_+) - \gamma (\dot{x}_i - V_-)$, where $\gamma$ is a viscous friction coefficient accounting phenomenologically for degrees of freedom inherent in the real physical system (such as substrate phonons, electronic excitations, etc.) which are not explicitly included in the model. The infinite chain size is managed – in the general incommensurate case – by means of periodic boundary conditions (PBC) and finite-size scaling (see, for example, Refs. [7,8]). We finally take $a_+ = 1$, $m = 1$, and $F_+ = 1$ as basic dimensionless units.

The detailed behavior of the driven system in Eq. (1) depends crucially on the
relative (in)commensurability of the substrates and the chain. The relevant length ratios are defined by $r_{\pm} = a_{\pm}/a_0$; we assume, without loss of generality, $r_- > r_+$, focusing mostly on the case $r_+ > 1$. In particular, in order to make a comparison with previous tribological studies [7,8], we shall restrict our present analysis to the incommensurate golden-mean case $\phi \equiv (\sqrt{5} + 1)/2 \approx 1.6180$ with ratios $(r_+, r_-) = (\phi, \phi^2)$. Since the qualitative features of velocity quantization phenomena were proved [7] to survive for much more general values of $r_+$ and $r_-$, this specific choice of incommensurability should not be considered too restrictive.

The equations of motion (1) are integrated using a standard fourth-order Runge-Kutta algorithm. The system is initialized with the chain particles placed at rest at uniform separation $a_0$. After relaxing the starting configuration and selecting a reference frame in which the bottom substrate is at rest ($V_+ = 0$), the top substrate starts sliding at the imposed constant velocity $V_- = V_{\text{ext}}$. For a very wide range of model parameters the system reaches, after an initial transient, the quantized “dynamical stationary” state with $V_{\text{cm}}/V_{\text{ext}} = V_{\text{plateau}}/V_{\text{ext}} = 1 - r_+^{-1}$, that depend solely on the chosen incommensurability ratio $r_+$. In order to investigate the possibility for the system to exhibit hysteresis starting now from this quantized sliding state, at which the confined layer is robustly pinned, the additional constant force $F_{\text{ext}}$ acting on all chain particles is now varied upward and downward adiabatically.

3 Results and discussion

After stationarity has been reached, Fig. 1 shows the striking behavior of the normalized time-averaged CM velocity of the sandwiched lubricant chain, $V_{\text{cm}}/V_{\text{ext}}$, as a function of the stiffness $K$, for the two incommensurate case of golden mean (GM) and spiral mean (SM) 1.

As discussed in previous works [7,8], the crucial feature is the presence of perfectly flat $V_{\text{cm}}/V_{\text{ext}}$ plateaus, whose precise value $(1 - r_+^{-1})$ is independent not only of $K$, but also of $\gamma$, $V_{\text{ext}}$, and even of $F_-/F_+$. Their occurrence was ascribed to the intrinsic topological nature of this quantized dynamics. The phenomenon is explained by one confining substrate rigidly dragging the topological solitons (kinks) that the embedded chain forms with the other substrate.

Let us now turn to consider specifically the GM case only. Fixing a value of

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1 The golden mean $\phi \equiv (\sqrt{5} + 1)/2$ is the solution of the quadratic equation $\phi^2 - \phi - 1 = 0$; the spiral mean, $\sigma \approx 1.3247$ satisfying the equation $\sigma^3 - \sigma - 1 = 0$, belongs to the class of cubic irrationals.
the chain stiffness $K$ lying approximatively in the middle of the plateau of Fig. 1 and considering a sufficiently small value of the damping coefficient $\gamma$ (underdamped regime), we start investigating the hysteresis by applying an external force $F_{\text{ext}}$ to all the chain particles through an adiabatic increase and decrease process.

The results are displayed in Fig. 2 for two different external driving velocities. A clear hysteretic loop emerges, with qualitative similar features for high (upper panel) and low (lower panel) $V_{\text{ext}}$. Surprisingly, the cycle is broader for larger velocities. We will return to this point later on.

The finding of exact plateaus implies a kind of “dynamical incompressibility”, namely, identically null response to perturbations or fluctuations trying to deflect the CM velocity away from its quantized value. What is now the effect of the additional force $F_{\text{ext}}$? We find that as long as $F_{\text{ext}}$ remains below a critical threshold $F_c$, it does perturb the single-particle motions but has no effect whatsoever on $V_{\text{cm}}$, which remains exactly pinned to the quantized value, as could indeed be expected of an incompressible state. This picture is analogous to the pinning-depinning transition in static friction, where a minimum force (the static friction) is required in order to start the motion. Thus the sudden change of $V_{\text{cm}}$ taking place at $F_{\text{ext}} = F_c$ can be termed a “dynamical depinning”. The value of $F_c$ is a nontrivial function of the parameters, and vanishes linearly when $K$ approaches from below the upper border $K_c$ of the plateau. The depinning transition line $F_c$, ending at $K = K_c$, appears as a “first-order” line, with a jump $\Delta V$ in the average $V_{\text{cm}}$ and a clear hysteretic behavior as $F$ crosses $F_c$. As expected, we find that $\Delta V$ decreases to 0 as $K$ increases towards $K_c$ (not shown). Thus $K = K_c$ represents a sort of non-equilibrium critical point, where the sliding chain enters or leaves a dynamical orbit. The precise value of $K_c$ depends on parameters such as $V_{\text{ext}}$ and $\gamma$; however, its properties do not. Fig. 3(a) displays the general decreasing behavior of $K_c$, and thus the corresponding diminishing extension of the plateau, as a function of the external driving $V_{\text{ext}}$ (no applied force $F_{\text{ext}}$). As shown in Fig. 3(b), and contrary to what could be intuitively expected, no straightforward relation seems to exist between the plateau extension in $K$ and its robustness against the external perturbing force $F_{\text{ext}}$. At a fixed chain stiffness, quite large values of $F_c$ are found even for very high sliding velocities, where the plateau extension has already been reduced significantly.

Depending on model parameters such as chain stiffness and external driving velocity, the dynamical depinning off the quantized sliding state takes place through different kinds of mechanisms, ranging from a series of intermittencies with a well-defined temporal periodicity to more chaotic and irregular jumps [7]. As displayed in Fig. 4, when the applied force is decreased and removed, the system may jump to intermediate sliding regimes and eventually returns to the quantized sliding state at a much lower value of $F_{\text{ext}}$. As for the forward
dynamical depinning transition, the details of these backward steps in the $V_{cm} - F_{ext}$ characteristics strongly depend on the parameters of the model. At high values of $F_{ext} (= 0.07$, left panels) the confined layer moves almost freely with a large sliding velocity depending on the damping coefficient $\gamma$. For intermediate force ($F_{ext} = 0.045$, middle panels), simulations reveal the intriguing occurrence of a sliding regime closely reminiscent of a dynamic stick-slip motion. This intermittent dynamics is seen with particular clarity by plotting the particle trajectories in the reference frame which slides at the quantized velocity value of the plateau. A further reduction of $F_{ext} (= 0.02$, right panels) brings the system back to the time-periodic dynamics of the quantized sliding state.

The above picture of dynamical depinning as a first order transition is valid for weak dissipation. For strong dissipation, when the viscous damping coefficient $\gamma$ is much larger than the characteristic vibrational frequencies of the system (overdamped motion) the dynamical depinning is likely to be of second order: The forward and backward trajectories become indistinguishable, and hysteresis disappears, as shown in Fig. 5(a). In this strongly dissipative regime, we found instead of the hysteretic jumps a nonlinear mobility region of $V_{cm}$ versus $F_{ext}$, but without any bistability phenomenon.

Finally, independently of the value of the chain stiffness, no hysteresis has been found in the underdamped regime by varying the external driving velocity with time with a gentle enough rate of increase and decrease. Panels (b) and (c) of Fig. 5 show, for two different $K$ inside the quantized plateau region, the nonlinear, but not bistable, behavior of $V_{cm}/V_{ext}$ as a function of adiabatic variation of $V_{ext}$.

### 4 Conclusions

We have shown that starting from the quantized $V_{cm}$ sliding state, previously found for a simple tribological model of a confined layer, the layer sliding dynamics exhibits a large hysteresis under the action of an additional external driving force $F_{ext}$ trying to change $V_{cm}$ away from its quantized value. In analogy to depinning in ordinary static friction, the hysteretic dynamical behavior depends strongly on whether the system degrees of freedom have sufficient inertia (underdamped regime) or if, on the contrary, the inertia is negligible (overdamped regime).

The robustness of quantized dynamics is proved by the existence of a finite critical threshold $F_c$ needed to move the chain CM velocity away from the plateau value (dynamical depinning). When the applied force is decreased and removed, the system may jump to intermediate sliding regimes (a sort
of dynamic stick-slip motion) and eventually returns to the quantized sliding state at a much lower value of $F_{\text{ext}}$.

There are however nontrivial differences from static friction. The first is that the dynamical pinning hysteresis cycle may be larger in situations where the pinning itself could be intuitively considered more fragile, e.g., for larger external velocity. Another feature (presently under investigation, not discussed above) is that the sudden application of an external force can leave $V_{\text{cm}}$ locked to the quantized value, even if the applied force is larger than the dynamic depinning threshold $F_c$, obtained instead through the adiabatic procedure sketched above. Once again, this is different from static depinning, usually requiring smaller force (than $F_s$) if applied suddenly.

A final open question concerns the effect of a finite temperature on the dynamical hysteresis. Preliminary results obtained through a Langevin dynamics indicate that, so long as the thermal energy is much smaller than an effective dynamical barrier (gap) preserving the incompressible plateau state, the velocity quantization is still observed. We expect, therefore, that the qualitative dynamical hysteretic behavior should not change too much. These aspects are currently under investigation.

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Fig. 1. (Color online) Normalized velocity of the center of mass, $V_{cm}/V_{ext}$, as a function of the chain stiffness $K$, for the golden mean $(r_+, r_-) = (\phi, \phi^2)$ and spiral mean $(r_+, r_-) = (\sigma, \sigma^2)$ incommensurability. Here $\gamma = 0.1$ and $V_{ext} = 0.1$. Note the logarithmic scale in the abscissa. A sketch of the driven 3-length scale confined model is shown in the inset.
Fig. 2. (Color online) Hysteresis in the $V_{\text{cm}} - F_{\text{ext}}$ characteristics for the GM case and a relatively soft ($K = 4$) confined chain. The behavior is shown for high ($V_{\text{ext}} = 0.1$, upper panel) and low ($V_{\text{ext}} = 0.01$, lower panel) applied driving velocities. Adiabatic increase and decrease of $F_{\text{ext}}$ is denoted by triangles and circles, respectively. A characteristic multi-step feature appears when decreasing adiabatically the external force.
Fig. 3. (Color online) (a) \((V_{\text{ext}}; K)\) phase diagram, with no additional force applied, for the GM incommensurability. At a fixed value of the external driving velocity, \(K_c\) marks the point above which the quantized sliding regime of the chain breaks down. (b) Irregular dependence of the dynamical depinning force \(F_c\) upon the driving velocity \(V_{\text{ext}}\) for chain stiffness \(K = 4\).

Fig. 4. (Color online) Time evolution of the velocities \(v_i\) (upper panels) and of the corresponding rescaled coordinates \(x_i - (V_{\text{plateau}} \cdot t)\) (lower panels) of seven contiguous chain particles. The plots refer to three different dynamical regimes observed in the adiabatic decrease process of the external force: free sliding at \(F_{\text{ext}} = 0.07\) (left), dynamic stick-slip at \(F_{\text{ext}} = 0.045\) (middle), and quantized sliding state at \(F_{\text{ext}} = 0.02\) (right). Note the different scale in the ordinate of the \(v_i\)-plots. Here \(\gamma = 0.1, K = 4,\) and \(V_{\text{ext}} = 0.1\).
Fig. 5. (Color online) No hysteretic behavior of $V_{cm}/V_{ext}$ is observed in leaving the $V_{cm}$ quantized plateau as a function of: (a) the external applied force in the overdamped regime; (b)-(c) the driving velocity, for different values of $K$. 