Incommensurability of a Confined System under Shear

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We study a chain of harmonically interacting atoms confined between two sinusoidal substrate potentials, when the top substrate is driven through an attached spring with a constant velocity. This system is characterized by three inherent length scales and closely related to physical situations with confined lubricant films. We show that, contrary to the standard Frenkel-Kontorova model, the most favorable sliding regime is achieved by choosing chain-substrate incommensurabilities belonging to the class of cubic irrational numbers (e.g., the spiral mean). At large chain stiffness, the well known golden mean incommensurability reveals a very regular time-periodic dynamics with always higher kinetic friction values with respect to the spiral mean case.

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One of the pervasive concepts of recent physics with a wide area of practical applications as well as fundamental theoretical issues is the idea of free sliding connected with *incommensurability.* Especially from a practical point of view, this issue has found intriguing and relevant applications in the field of nanotribology, i.e., the science of friction, lubrication, and wear at the nanoscale (e.g., see [1]). When two crystalline workpieces with incommensurate lattices (or commensurate but not perfectly aligned) are brought into contact, then the minimal force required to achieve sliding, known as the static frictional force f_s, vanishes, provided the two substrates are stiff enough (a typical situation). This remarkable conclusion can be drawn, in particular, in the context of the Frenkel-Kontorova (FK) model (see [2] and references therein), where a chain of harmonically interacting atoms with the natural lattice constant b is made to slide over a rigid sinusoidal potential of spatial period a. In the case of incommensurate length scales (i.e., a/b irrational), the FK ground state undergoes a transition by breaking of analyticity if the chain stiffness K drops below a critical value K_c (*Aubry transition* [3]). From a physical point of view, this means that for $K > K_c$ there exists a continuum of ground states that can be reached by the chain through nonrigid displacements of its atoms with no energy cost. This sliding mode corresponds to the regime of zero static friction. On the contrary, below K_c, the chain and substrate become pinned with nonzero static friction, irrespective of incommensurability. The threshold K_c depends on the mathematical properties of the irrational winding number a/b.

In real situations, however, such a case of "dry" friction is exceptional. A physical contact between two solids is generally mediated by so-called "third bodies," which act like a lubricant film. Therefore, the sliding interface corresponds, in fact, to a system with three inherent lengths: the periods of the bottom and top substrates (here, a and c, respectively), and the period of the lubricant structure (here b).

Analogously to the Aubry transition in the standard FK model, where the best choice of the winding number a/b (i.e., the one leading to the lowest value for the threshold K_c) is known to be the golden mean $\phi \equiv (\sqrt{5}+1)/2$, it is now relevant and interesting for the three-length system to wonder which incommensurabilities a/b and c/a will lead to the most favorable sliding behavior. Guided by a similarity with the recent study of the driven quasiperiodic FK model [4], we show that, for sufficiently stiff chains, the best low-friction regime is achieved for incommensurabilities related to cubic irrational numbers (as, for example, the spiral mean [5]) rather than to quadratic irrationals (e.g., the golden mean). This result demonstrates how the kind of incommensurability of the contact interface can dramatically influence, both quantitatively and qualitatively, the tribological behavior of the system during sliding.

Model.—We consider a one-dimensional system of two rigid sinusoidal substrates and a chain of interacting particles embedded between them as shown in Fig. 1. The top substrate of mass M is pulled through a spring, of elastic constant $K_{\rm ext}$, connected to a stage that moves with a velocity $V_{\rm ext}$. The system dynamics is described by

$$m\ddot{x}_i + \gamma\dot{x}_i + \gamma(\dot{x}_i - \dot{X}_{\rm top}) + \frac{d}{dx_i}\sum_{i\neq j} V(|x_i - x_j|) + \frac{1}{2}\left[\sin\frac{2\pi x_i}{a} + \sin\frac{2\pi(x_i - X_{\rm top})}{c}\right] = 0, \quad (1)$$

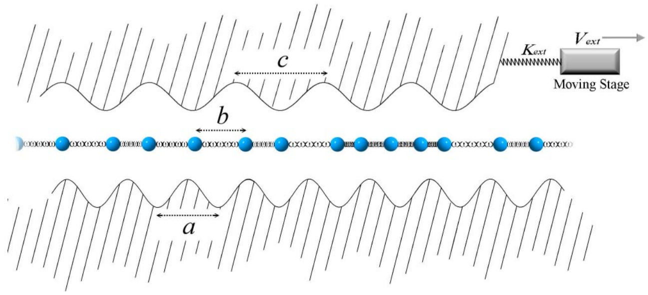

FIG. 1 (color online). Schematic drawing of the model with three characteristic length scales.

$$M\ddot{X}_{\rm top} + \sum_{i=1}^{N} \gamma(\dot{X}_{\rm top} - \dot{x}_i) + K_{\rm ext}(X_{\rm top} - V_{\rm ext}t) + \sum_{i=1}^{N} \frac{1}{2}\left[\sin\frac{2\pi(X_{\rm top} - x_i)}{c}\right] = 0, \quad (2)$$

where x_i ($i = 1, \ldots, N$) and $X_{\rm top}$ stand for the coordinates of the N chain particles and the top substrate, respectively.

The damping γ terms in Eqs. (1) and (2) describe the dissipative forces that are proportional to the relative velocities of the atoms with respect to both rigid substrates. The coefficient γ (we chose $\gamma = 0.2$ in our numerical examples, so that the system is in the underdamped regime) represents degrees of freedom inherent in the real physical system, which are not explicitly included in the model (e.g., substrate phonons, electronic excitations, etc.). Simulations [6] have provided indirect evidence that such phenomenological viscosity terms serves well this purpose. We use dimensionless units with chain atom mass $m = 1$ and a bottom substrate period $a = 1$. The last (sinusoidal) terms in Eqs. (1) and (2) represent the on-site interaction between the particles and the substrates. The magnitudes of these rigid potentials are chosen such that the same factor (1/2) sits in front of their derivatives in the equations of motion. The interparticle chain interaction [fourth term in Eq. (1)] is harmonic with strength K and equilibrium spacing b.

In this work we focus on the most generic and physically interesting case of incommensurability among the three inherent lengths a, b, c. Experimentally, commensurability can be achieved only under well-controlled operating conditions [7], although thermal expansion and epitaxy may hamper a precise choice of incommensurability. Theoretically, when simulating an infinite system, we are forced by the periodic boundary constraints to approximate the desired irrational winding numbers a/b, c/a by ratios of integers. The continued fraction expansion technique [8] allows us to check quantitatively that a given rational approximant is of sufficiently high order to model the desired incommensurability. The chain of N atoms and length $L = Nb$ is thus confined between the bottom and top substrates with $N_a = L/a$ and $N_c = L/c$ minima, respectively. For specificity, we consider here two irrational cases already discussed in the context of the driven quasiperiodic FK model [4], namely, the golden mean and the spiral mean.

The equations of motion are integrated using the standard fourth-order Runge-Kutta algorithm. The system is initialized with the chain particles placed at rest at uniform separation b. After relaxing the starting configuration, the stage attached to the top substrate via the spring $K_{\rm ext}$ begins to move at the constant velocity $V_{\rm ext}$. After reaching the steady state, we measure the system characteristics of relevant physical interest.

In tribology applications, the main issue is the kinetic friction force $F_{\rm kin}$, which describes the energy losses inside the contact layer when the substrates move relative to each other. In our model, $F_{\rm kin}$ can be easily evaluated from the energy balance. When the bottom substrate is fixed and the top substrate moves for a distance $\Delta X_{\rm top} = \dot{X}_{\rm top}\Delta t$, the system loses, due to the friction force, an energy

$$E_{\rm loss} = F_{\rm kin}\Delta X_{\rm top} = F_{\rm kin}\dot{X}_{\rm top}\Delta t. \quad (3)$$

In the regime of steady motion, this must balance the losses due to the dissipation generated by the γ-damping terms in the chain, i.e.,

$$E_{\rm loss} = \sum_{i=1}^{N} \int_{t_1}^{t_2} dt \gamma[\dot{x}_i^2 + (\dot{x}_i - \dot{X}_{\rm top})^2], \quad (4)$$

where $\Delta t = t_2 - t_1$. Thus, for the kinetic friction force, we obtain

$$F_{\rm kin} = \sum_{i=1}^{N} \lim_{\Delta t\to\infty} \int_{t_1}^{t_2} \frac{dt}{\Delta t} \gamma[\dot{x}_i^2 + (\dot{x}_i - \dot{X}_{\rm top})^2]\frac{1}{\dot{X}_{\rm top}}. \quad (5)$$

In order to highlight in the kinetic friction force the dissipative part resulting from the internal dynamics of the confined chain, we wash out the systematic contribution arising from the motion of the top substrate, and also normalize $F_{\rm kin}$ to the number of particles N, i.e.,

$$f_{\rm kin} = \frac{F_{\rm kin}}{N} - \frac{1}{2}\gamma\dot{X}_{\rm top}. \quad (6)$$

Results.—In the range of the model parameters considered, our numerical simulations reveal a strikingly different behavior of the system dynamics depending on incommensurability. In particular, it is not sufficient to distinguish simply between commensurate and incommensurate periodicities. The "degree" of incommensurability (as measured by continued fraction expansion) plays a fundamental role as well. Here the mathematical properties of the ratio among different length scales leave the realm of abstract number theory to become physically relevant.

Figure 2 shows the kinetic friction force $f_{\rm kin}$ as a function of the interparticle interaction strength K for different values of the velocity of the moving stage. The plots are given for two irrational choices of the three length scales:

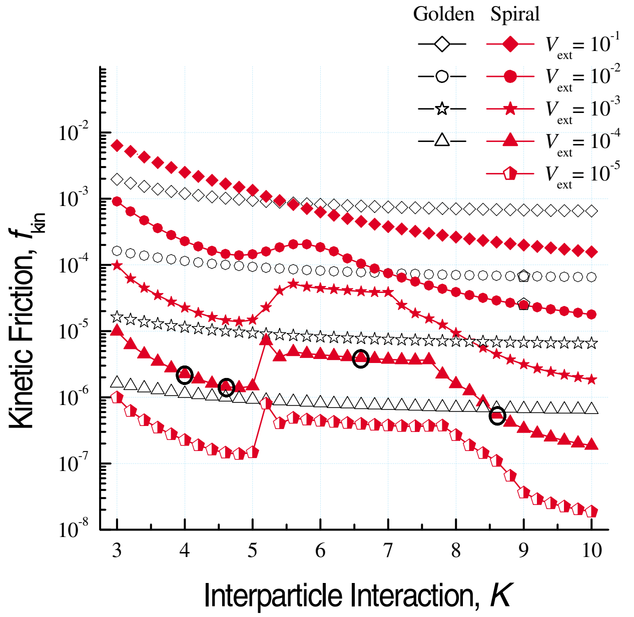

FIG. 2 (color online). Dependence of the kinetic friction force f_{kin} on the chain stiffness K for different values of the external driving velocity. Both cases of golden and spiral incommensurability are shown.

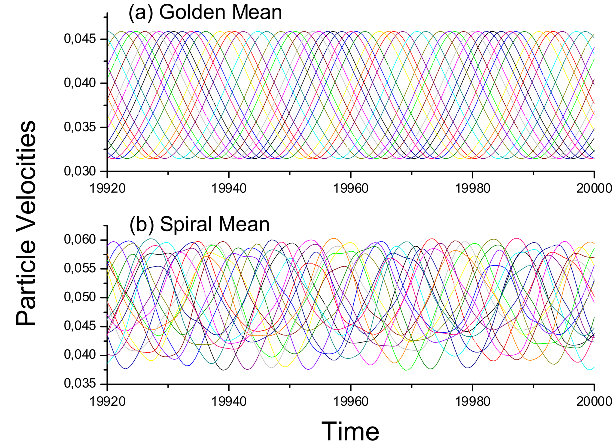

FIG. 3 (color online). Atomic velocities versus time for (a) golden incommensurability $a/b = 233/144$, $c/a = 144/89$; (b) spiral incommensurability $a/b = 351/265$, $c/a = 265/200$. Only a limited portion (20 adjacent particles) of the chain is shown. The model parameters are $K = 10$, $\gamma = 0.2$, $V_{\text{ext}} = 0.1$, and $K_{\text{ext}} = 0.0003N_c$.

the golden mean ($N_a = 144$, $N = 233$, $N_c = 89$) and the spiral mean ($N_a = 265$, $N = 351$, $N_c = 200$). By simulating larger systems, we checked that these rational approximants [5] are of sufficiently high order to mimic the selected incommensurabilities.

For the *golden* incommensurability, the qualitative (monotonic) behavior of the kinetic friction does not depend significantly either on K or on V_{ext}. For the same value of the chain stiffness, f_{kin} decreases with decreasing driving velocity. The chain dynamics exhibits an asymmetric sliding with respect to the two sinusoidal substrates, moving as expected with an intermediate mean velocity, but always faster with respect to the sinusoidal substrate with the longer spatial period. We checked that the asymmetry persists when the amplitudes of the substrate potentials are equal (instead of their derivatives being equal as above). The golden incommensurability sliding is characterized by a regular time-periodic dynamics as demonstrated in Fig. 3(a). One may suppose that this regular motion results in parametric resonances inside the chain [9], thus converting the kinetic energy of the center of mass motion into internal vibrational excitations and making the golden irrationality less favorable to sliding than the spiral one at high K values.

For inherent lengths related by the cubic *spiral* mean, the function $f_{\text{kin}}(K)$ displays a nonmonotonic and much richer behavior, although at high driving velocities, $V_{\text{ext}} > 0.01$, these exotic features diminish and eventually disappear. A chaotic temporal dependence of atomic velocities in the stiff spiral chain [see Fig. 3(b)] probably destroys parametric resonances inside the confined layer as possible channels for energy dissipation, making the spiral chain more effective as compared to the golden case.

The change in the sliding behavior of the spiral chain occurs at $K_c \approx 5.6$, i.e., at the value when the Aubry transition for the quasiperiodic FK model was previously found [4]. When the driving velocity decreases (see lower curves in Fig. 2), a plateau region in $f_{\text{kin}}(K)$ starts to develop. The location of its left edge is, in fact, almost independent of V_{ext} and centered around the value K_c. This point marks a gradual transition from a stick-slip dynamics at small K towards an almost frictionless smooth sliding at large K. The intermediate plateau, with large friction but without stick slip, is a new spiral feature whose existence and extension depends significantly on the external driving velocity V_{ext} but, as we checked, only weakly on the pulling spring constant K_{ext}. At large and increasing chain stiffness, the spiral friction drops considerably as compared to the golden tribological dissipation, which retains, instead, quite large values in its regular time-periodic sliding.

In order to get insight into different regions to the left, in between, and to the right of the plateau, we analyzed in detail the four points circled in black in Fig. 2, all belonging to the same driving velocity $V_{\text{ext}} = 0.0001$. The four upper panels of Fig. 4 show the time evolution of the spring force $F_{\text{ext}} \equiv K_{\text{ext}}(X_{\text{top}} - V_{\text{ext}}t)$; the lower panels display the corresponding velocities of the top substrate, of the center of mass of the chain, and of one generic atom. The first upper panel for $K = 4.0$ clearly displays a typical sawtooth dependence of $F_{\text{ext}}(t)$, the hallmark of stick-slip motion. At $K = 4.6$ the slip events are prevailing, but the stick-slip regime of the chain is still clearly visible. The next value examined, $K = 6.6$, lies in the plateau region. Here the chain stiffness is too high to support stick slip, and

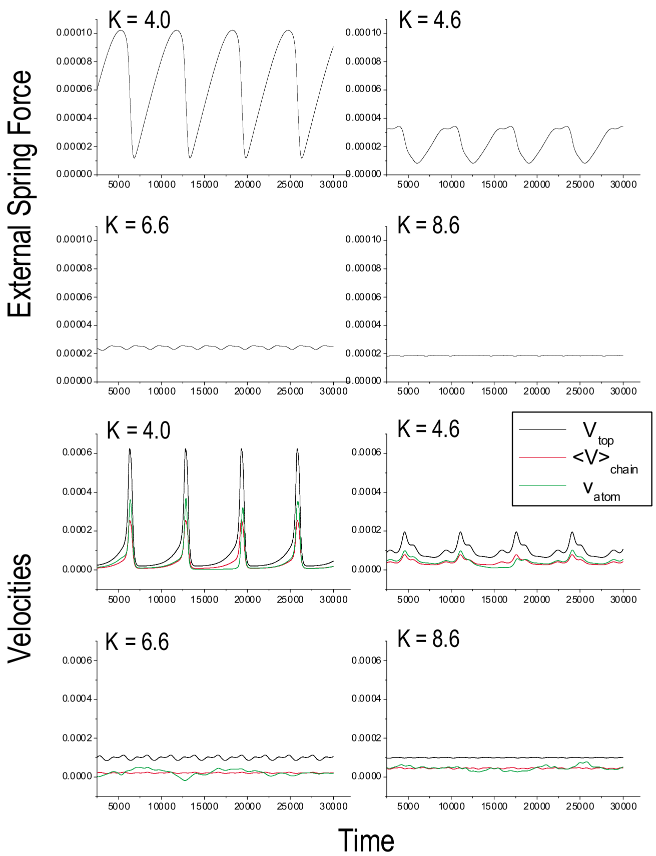

FIG. 4 (color online). Dynamics of the four sliding states marked by the black circles in Fig. 2. The four upper panels show the temporal behavior of the spring force, with the characteristic transition from the stick-slip motion at low K to the smooth sliding at high K. The lower panels display the corresponding time dependences of the velocities of the top substrate, of the chain, and of one generic atom.

the confined layer motion reaches a sliding regime with an almost constant value of the pulling spring force, and the velocity of the top substrate exhibiting only very tiny oscillations around $V_{\rm ext}$. The increase in the average kinetic friction $f_{\rm kin}$ of the plateau states (relative to the contiguous stick-slip dynamics region) can be ascribed to the asymmetric chain motion with respect to the two substrates in this regime. We suppose that in this range of stiffness and driving velocity values, a better dynamical phase matching is possible between the confined layer and the two sinusoidal substrates, making easier (similar to the golden case) the excitation of dissipative parametric resonances. Finally, at $K = 8.6$ the confined layer slides almost freely with a very low value of $f_{\rm kin}$. The sliding is symmetric in this regime, i.e., the average chain velocity is equal to half of the relative velocity between the two rigid substrates.

Thus, we have shown that for stiff confined chains, $K \gg K_c$, the standard golden mean incommensurability always reveals higher kinetic friction than the spiral one. This conclusion can be generalized to a three length-scale sliding system with incommensurability defined by a generic quadratic, rather than cubic, irrational number. Quite notably, these results show that, at least for a three-length contact interface (a typical physical situation), there is no quantitative and qualitative uniformity of behavior in incommensurate sliding friction, and that certain irrationals slide systematically better than others. It is not clear at the moment whether this conclusion can be generalized from the present one-dimensional case to a more realistic two-dimensional interface. In a similar way to what has been recently done for just a two-length sliding contact [10], such a situation could, in principle, be accessed experimentally by driving, for example, a graphite flake between two different crystalline surfaces.

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[1] B. N. J. Persson, *Sliding Friction: Physical Principles and Applications* (Springer-Verlag, Berlin, 1998); Surf. Sci. Rep. **33**, 83 (1999).

[2] O. M. Braun and Yu. S. Kivshar, *The Frenkel-Kontorova Model: Concepts, Methods, and Applications* (Springer-Verlag, Berlin, 2004); Phys. Rep. **306**, 1 (1998).

[3] S. Aubry, Physica (Amsterdam) **7D**, 240 (1983); S. Aubry and P. Y. Le Daeron, Physica (Amsterdam) **8D**, 381 (1983).

[4] A. Vanossi *et al.*, Phys. Rev. E **63**, 017203 (2001).

[5] The spiral mean (≈ 1.3247) belongs to the class of cubic irrationals, satisfying the equation $\omega^3 - \omega - 1 = 0$. Its rational approximants can be generated by the recursion relation $G_{n+1} = G_{n-1} + G_{n-2}$ with $G_{-2} = G_0 = 1$, $G_{-1} = 0$. For the golden mean ϕ, the needed rational approximants are provided instead by the famous Fibonacci sequence, $F_{n+1} = F_n + F_{n-1}$ with $F_0 = F_1 = 1$.

[6] J. Röder *et al.*, Physica (Amsterdam) **142D**, 306 (2000).

[7] E. D. Smith, M. O. Robbins, and M. Cieplak, Phys. Rev. B **54**, 8252 (1996).

[8] A. Ya. Khinchin, *Continued Fractions* (Dover, New York, 1997).

[9] T. Strunz and F.-J. Elmer, Phys. Rev. E **58**, 1601 (1998).

[10] M. Dienwiebel *et al.*, Phys. Rev. Lett. **92**, 126101 (2004).