Driven, underdamped Frenkel-Kontorova model on a quasiperiodic substrate

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We consider the underdamped dynamics of a chain of atoms subject to a dc driving force and a quasiperiodic substrate potential. The system has three inherent length scales which we take to be mutually incommensurate. We find that when the length scales are related by the *spiral mean* (a cubic irrational) there exists a value of the interparticle interaction strength above which the static friction is zero. When the length scales are related by the *golden mean* (a quadratic irrational) the static friction is always nonzero. From considerations based on the connection of this problem to standard map theory, we postulate that zero static friction is generally possible for incommensurate ratios of the length scales involved. However, when the length scales are quadratic irrationals, or have some commensurability with each other, the static friction will be nonzero for all choices of interaction parameters. We also comment on the nature of the depinning mechanisms and the steady states achieved by the moving chain.

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INTRODUCTION

Recent advances in technology, notably the use of the quartz crystal microbalance, the friction force microscope, etc. [1], have provided data on the frictional process at the nanoscale. This progress has stimulated attempts to understand the fundamental processes involved via the use of simple low-dimensional models, in particular those based on one-dimensional, driven Frenkel-Kontorova (FK) type models [2]. In these models a certain density of interacting particles is made to slide over a periodic substrate potential by the application of an external driving force. There are two inherent length scales: the periodicity of the substrate potential, a, and the natural equilibrium distance between the particles, b. If we consider the case where $a/b=1$, we would model the case of sliding between two identical, perfectly aligned crystalline workpieces. In general one does not expect the two workpieces to be perfectly aligned, and so one would need to consider $a/b\neq 1$. This would also be the case for workpieces with two different atomic spacings. It has been noted [3], that unless one has very well controlled conditions, one would expect that a and b be mutually incommensurate.

In this paper we shall examine the case of a one-dimensional array of particles sliding over a *quasiperiodic* substrate potential. This may be considered as a simple model of friction between a quasicrystalline and crystalline solid, or between two quasicrystals. Recent experiments [4] have demonstrated that quasicrystals have a particularly low coefficient of friction and so may be useful in technological applications [5]. The case of a quasiperiodic potential can also be viewed as an intermediate case between periodic order and a disordered substrate. The quasiperiodic potential is not translationally invariant: the maxima of the potential are no longer evenly spaced, nor are they of equal height. Hence we might hope to gain an insight into the more complex problem of sliding between two disordered solids from the study of this precisely defined problem, not complicated by randomness.

In this article we shall consider a driven, underdamped chain of N particles, interacting via a potential $V(r)$, where r is the interparticle separation, and subject to a quasiperiodic substrate potential. The behavior of the system will be controlled by the relative strengths of substrate and interaction potential. Here we chose to fix the amplitude of the substrate potential and vary the interparticle interaction strength. We shall characterize this by $K=V''(b)$. In constructing the quasiperiodic substrate we introduce a third length scale, so that the substrate is defined by *two* mutually incommensurate lengths a and c. (In this work we shall restrict ourselves to the case where c is also incommensurate with b.)

From the following considerations, it becomes clear that the choice of the irrational values of these three lengths may strongly affect the behavior of the system.

As pointed out in the pioneering work of Aubry [6], the problem of the standard FK model (with two competing length scales a and b) is closely connected to the theory of the two-dimensional Hamiltonian standard map. In particular this link is related to the problem of finding the ground state and possible metastable states of the FK model by recursive iterations of this area-preserving map.

In the case of incommensurate length scales, it is well-known [6] that the FK ground state undergoes a transition (usually referred to as TBA, i.e., transition by breaking of analyticity) that can be related to the stochasticity threshold which is observed in the standard map. For a fixed amplitude of the substrate potential, the critical value K_c of the interatomic interaction strength at which the TBA takes place, depends on the mathematical properties of the irrational *winding number* $\omega=b/a$, so that there is a relation $K_c=K_c(\omega)$. Above the transition ($K>K_c$), in the map representation, the FK ground state corresponds to a trajectory in phase space that is rotating with winding number ω on a closed, smooth curve (Kolmogorov-Arnold-Moser- or KAM-*torus*), while below the transition ($K<K_c$) it is still rotating with the same ω but on a Cantor set (*cantorus*). 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 (*sliding mode*); on the other hand for $K<K_c$ the atoms are trapped close to the minima of the substrate potential and, because of the discontinuity of the trajectory, they require a finite amount of energy (the *Peierls-Nabarro barrier*) to be moved. (Here we shall consider fixing the amplitude of the substrate potential and varying K. The location of the TBA is, in fact, controlled by the *effective elastic constant* $g_{eff}=b^2K/2\pi^2\lambda$, where λ is the amplitude of the substrate potential [7]. Hence, it is also possible to fix K and vary λ as is done in [8]).

The breakup of the *last* and *most robust* invariant torus in KAM theory, which is one of the key mechanisms of the transition to chaos in Hamiltonian dynamics, takes place when the trajectory in phase space possesses the ''most'' Diophantine irrational winding number. For the standard FK model this can be shown to be the *golden mean* $\omega=(\sqrt{5}-1)/2$. For this specific winding number, K_c takes the minimal possible value; local minima appear also corresponding to the other *noble frequencies*, which belong to the class of quadratic irrationals with a continued fraction expansion whose elements are all one beyond some level.

In a similar way our problem can be related to Hamiltonian systems with *three* incommensurate frequencies or equivalently four-dimensional maps. Though KAM theory guarantees stability only for systems with two degrees of freedom, and there has been limited success in determining the existence of invariant tori for three or more frequency dynamical systems, there is some evidence that [9,10], for four-dimensional maps, cubic irrationals replace the quadratics. In the generalized Ostlund-Kim version of the Farey tree construction [11], the cubic irrational satisfying the equation $\omega^3-\omega-1=0$ (the *spiral mean*), has been introduced, for its specific Diophantine properties, as a possible analog of the golden mean. However, there is no direct proof that this cubic irrational is more robust (in the sense of a KAM theorem) than others.

A recent study of the undriven, quasiperiodic FK model [8] noted distinct behaviors for particular cubic and quadratic irrational winding numbers: (i) For the case where the lengths a,b, and c were related by the spiral mean (cubic) a sliding mode was present for sufficiently strong interparticle interaction ($K>K_c$). This case is analagous to the case of the standard FK model with a and b incommensurate, where the TBA is observed. (ii) For cases where the lengths were connected by the relation $m/a+n/b+p/c=0$, with m,n,p integer (as, for example, for the golden mean and all other quadratic irrationals) no sliding mode was found for any strength of the interparticle interaction.

Here, we report our numerical observation of different behaviors for these two types of irrational winding numbers in a *driven system*. This is manifested by a vanishing static friction force (the force required to initiate motion) for the case of lengths connected by the spiral mean and sufficiently strong interaction strength and a nonzero static friction for smaller K and for all K for the golden mean ratio.

THE MODEL

Our model consists of a one-dimensional array of N particles, with positions u_i $(1\leqslant i\leqslant N)$, which satisfy the following equations of motion:

$$\ddot{u}_i+\gamma\dot{u}_i+\frac{1}{2}\left\{\sin\frac{2\pi u_i}{a}+\sin\frac{2\pi\beta u_i}{a}\right\}+\frac{d}{du_i}\left[\sum_{j\neq i}V(|u_i-u_j|)\right]=F, \tag{1}$$

where γ is a phenomenological viscous damping coefficient, chosen such that we are in the underdamped regime, and F is the driving force. γ can be thought of as representing degrees of freedom inherent in real, physical systems which are not included in our model (e.g., vibrational or electronic excitations in the substrate). $V(r)$ was chosen to have a minimum at $r=b$, where the system size $L=bN$. For the simulations shown we used the Morse potential, $V(r)=K/2[1-e^{(b-r)}]^2$.

The two lengths defining the quasiperiodic substrate potential are a and $c=a/\beta$. We used periodic boundary conditions, which means that one is forced to approximate the desired incommensurate winding numbers by ratios of integers. We considered the two cases discussed in [8]. In the case of the golden mean, the lengths are given by ratios of Fibonacci numbers, so that, in particular, we have chosen $a=1$, $b=144/233$, and $c=a/\beta=144/89$. For the spiral mean one uses the series of integers generated by the recursion relation $G_{n+1}=G_{n-1}+G_{n-2}$, with $G_{-2}=G_0=1$, $G_{-1}=0$, to make the approximation, $a=1$, $b=265/351$, and $c=a/\beta=265/200$. We have checked that the approximations we have taken are of sufficiently high order to produce behavior characteristic of the ratios we wish to consider.

NUMERICAL METHOD

The equations of motion were solved numerically using a fourth-order Runge-Kutta algorithm. The following scheme was used to vary the driving force: the system was initialized with the particles placed at rest at a uniform separation b. The dc-force, F, was then increased adiabatically from 0 to 1 with a step $dF=0.005$. For every value of F, and with a time step $dt=0.006$, Eqs. (1) were integrated over a time $t=300$, which we believe is long enough to eliminate transient behavior and reach a steady state. The average system velocity $\langle v\rangle=1/NT\int_0^T\Sigma_{i=1}^N\dot{u}_i dt$ was then calculated over a time $T=150$. The final chain configuration (positions and velocities) obtained at one value of F was used as the initial condition for the integration of the dynamics for the next value of the driving.

RESULTS

Spiral mean

In Fig. 1 we show the mobility of the chain $\mu\equiv\langle v\rangle/F$ as a function of the driving force for the case of the spiral mean winding number and two values of K. For $K=1$ the chain remains pinned until the driving force exceeds the static friction $F_s=0.185$. 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_s 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.

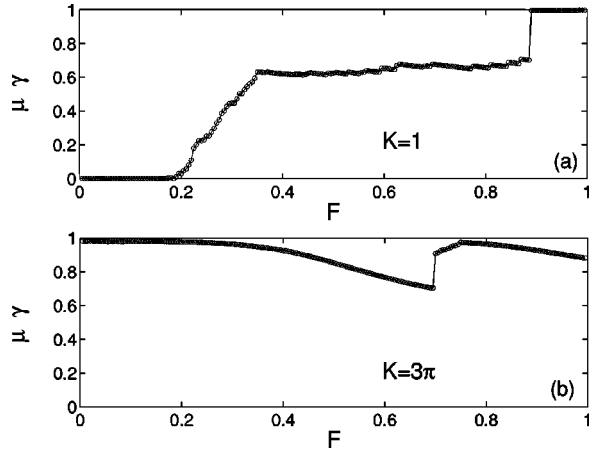

FIG. 1. (Spiral mean) Dependence of the chain mobility μ on the driving force F for two different values of the interaction strength: (a) $K=1<K_c$; (b) $K=3\pi>K_c$ ($\gamma=0.7$).

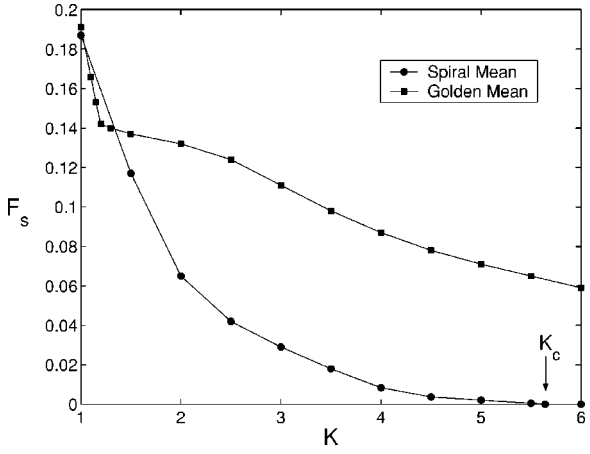

FIG. 2. Static friction force F_s as a function of the interparticle interaction strength K. We observe the existence of a critical value K_c (above which the chain supports a sliding mode) only in the spiral mean case. To obtain a higher precision plot, here the driving has been increased with a step size $dF=0.001$.

Eventually (around F=0.35) there are enough defects that, even though they are very narrow, they begin to overlap. At a second threshold force $F=0.89$, the chain motion changes to the high driving running state where $\gamma\langle v\rangle=F$. For $K=3\pi$, the chain is never pinned, and motion of the chain is initiated by even the smallest driving force, i.e., $F_s=0$. The chain jumps directly to the running state. (The dips in the curve around $F=0.7$ and $F=1$ are due to parametric resonances [12].)

In Fig. 2 we show F_s as a function of the strength of the interparticle interaction, K. We have determined the static friction from our simulations as the driving force at which the chain first has nonzero mobility. The static friction is zero for interaction strengths above a critical value $K_c=5.6$. Below this value the static friction increases with decreasing K. Near K_c we estimate the dependence as $F_s\sim(K_c-K)^{\alpha}$, with $\alpha\sim2.4$. For the standard FK model, from a numerical evaluation of the Peierls-Nabarro barrier [13], one finds $\alpha\approx3$.

Golden mean

Plots of mobility against driving force are given for two values of K for the golden mean winding number in Fig. 3. For $K=1$ the plot resembles that for the spiral mean case. The chain is pinned until a force $F_s=0.19$ and then depins via motion of a few isolated defects. Again the chain jumps to the running state for higher driving. At larger K, however, we always observed a nonzero static friction. The case $K=3\pi$ is shown in Fig. 3.

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 more extended and tend to overlap. One no longer observes isolated defects; there is instead an appreciable background drift velocity on top of which the inhomogeneities occur. Hence, even just above F_s, we observe a relatively large mobility.

The static friction for the golden mean case is shown, as a function of K, in Fig. 2. Again F_s decreases as one increases K, although we found $F_s>0$ for all values of K we considered. The bend in the curve around $K=1.2$ is due to an abrupt restructuring of the pinned state of the chain. As we steadily increase the driving force from zero, the pinned state of the chain adjusts to adopt the conformation locally lowest in energy. Usually a small change in F produces a small change in the optimal conformation of the chain. However, it is possible for the optimal pinned state of the chain to change discontinuously. When $K<1.2$, the chain restructures dramatically at a force below the depinning threshold. This restructuring is illustrated in Fig. 4. Hence, the chain depins from a very different state than was the case for $K>1.2$, where the chain starts to move before such a restructuring is advantageous.

C. Other ratios

We have also carried out simulations for other choices of the ratios between a, b, and c. All our simulations agree with

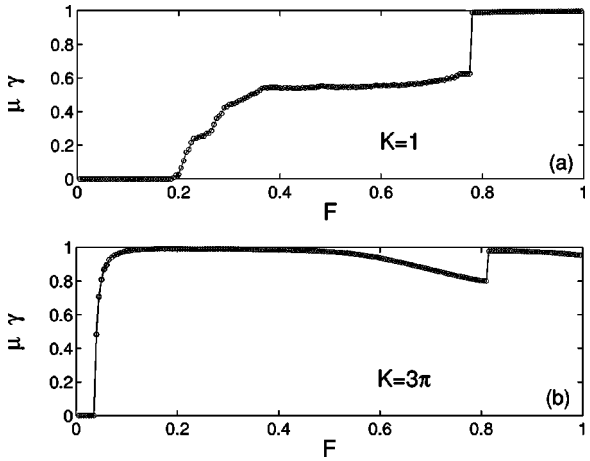

FIG. 3. (Golden mean) Dependence of the chain mobility μ on the driving force F for two different values of the interaction strength: (a) $K=1$; (b) $K=3\pi$ ($\gamma=0.7$).

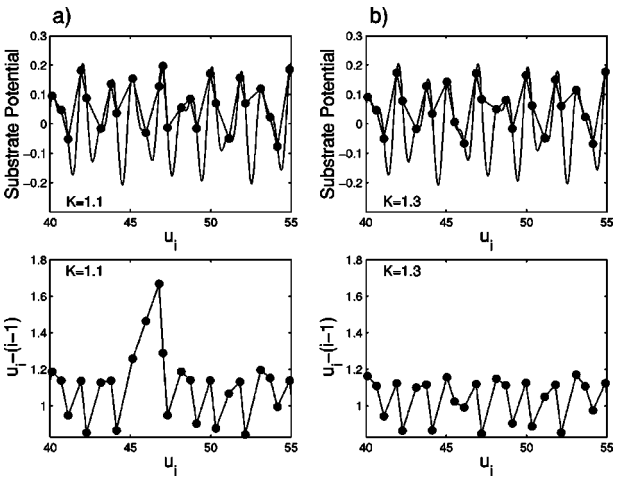

FIG. 4. (Golden mean) Pinned state configurations observed just below the depinning transition for: (a) $K=1.1$; (b) $K=1.3$. Only a limited portion of the chain is displayed for clarity.

the following postulate [8]: Choosing a, b, and c so that $m/a+n/b+p/c\neq 0$, for any set of integers m,n,p, one obtains behavior in the class of the spiral mean. For partially commensurate choices, e.g., $a=b=1$, a/c incommensurate, or even irrational choices such that $m/a+n/b+p/c=0$ (e.g., all systematic approximations to quadratic irrationals) behavior in the golden mean class is observed.

CONCLUSIONS

We have studied the underdamped dynamics of an interacting chain of particles subject to a quasiperiodic substrate potential and dc driving force for particular values of the ratios of the length scales involved. We observed zero static friction for the case of the spiral mean at sufficiently strong interparticle interactions, whereas for the golden mean F_s was always found to be nonzero. This is consistent with the recent observations made for the undriven quasiperiodic FK model [8]. As in Ref. [8] we have postulated that for any approximation to incommensurate winding numbers not satisfying $m/a+n/b+p/c=0$, for any nonzero integers m,n,p, $F_s=0$ is possible for strong enough K. Only for special choices satisfying the above condition will one obtain $F_s\neq 0$ for all K. Whether the spiral mean plays the role for the quasiperiodic substrate that the golden mean does for the periodic substrate, i.e., gives the smallest K_c for zero static friction, is an open question.

Hence, using these systems as models of sliding quasicrystals, one would expect that, for sufficiently strongly coupled systems, zero static friction could be attained. Only with certain specially selected atomic spacings and orientations would this not be possible. Even though a zero static friction may be obtained, this does not mean that nonzero *dynamic* friction (a superlubric state) is possible. For our model $F\geqslant \gamma v$. Even when $\gamma=0$, it has recently been demonstrated, for the standard, incommensurate FK model [14], that a superlubric state is only possible for very small systems. As soon as the phonon spectrum of the chain becomes quasicontinuous, energy will always be transfered from the center of mass motion of the chain to excite phonon modes via high-order resonances with the washboard driving frequency. The same kind of process should also hold for our model in the undamped limit, even though our substrate is defined by two length scales.

It would probably be necessary to generalize this model to at least two dimensions to obtain a more realistic model which one could relate to experiment. In two dimensions it would be possible for the sliding particles to avoid passing over the highest barriers in the substrate potential, which they have to negotiate in one dimension. The present experimental data on quasicrystal tribology does not clearly link their desirable frictional properties with their unique atomic arrangements. We hope that sufficiently well-controlled experiments can be carried out in the future to determine if the particular quasicrystalline arrangement of atoms has any special signature in their frictional properties.

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