Unlocking mechanism in the ac dynamics of the Frenkel-Kontorova model

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The dissipative dynamics of commensurate structures of the one-dimensional Frenkel-Kontorova model submitted to dc and ac forces is studied. The average velocity varies with the average external force as a staircase (dynamical mode locking). We characterize the unlocking transition as a transition from temporal periodicity to quasiperiodicity by using standard tools of the theory of dynamical systems. This transition is phenomenologically described as the generation of coherent, time-localized, and regularly-distributed increases of the particle velocities (instantons), which carry out a topological charge, the origin of which is the discrete character of the symmetry group of transformations of the locked steady state.

The dissipative dynamics of many-body models with competing interactions has been recently studied in connection with some interesting problems in condensed matter such as density-wave transport (either charge- or spin-density wave),[1-3] Josephson-junction arrays (JJA),[4] or flux-line motion in layered type-II superconductors.[5] In particular, when these systems are submitted to *ac forces,* they show a staircase macroscopic response, i.e., the response function locks at certain resonant values, when the average driving force varies. This dynamical mode locking appears to be a universal feature of the competition of time scales. The material systems mentioned above are rather complicated and the various interactions which give rise to the observed behavior are yet imperfectly understood. Hence it seems natural to focus on simple many-body models in order to gain some insight into the problem. In this respect, the Frenkel-Kontorova (FK) model seems one of the simplest capable of exhibiting not only a rich variety of commensurate and true incommensurate static structures,[6] but also, when submitted to both dc and ac forces, the complexity of dynamical mode locking.[7,8]

In this paper we address the problem of the mechanism of the locking-unlocking transition and its characterization, using molecular-dynamics simulations. We characterize the unlocking transition in the ac driven dissipative dynamics of commensurate structures of the FK model as a transition to quasiperiodicity. This transition is driven by the generation of coherent, time localized and regularly distributed in time disturbances (instantons) which produce a quantized increase of the mean velocity. The "topological charge" or "phase shift" carried out by an instanton is a consequence of the discrete character of the symmetry group of transformations of the locked trajectory. Moreover, these instantons are particular instances of intermittencies of type I.[9] The interpretation of the numerical results makes use of various well-known and powerful concepts and tools of the theory of dynamical systems.

We study the dissipative (overdamped) dynamics of an array of coupled harmonic oscillators u_j in a periodic substrate (pinning) potential V:

$$V(u)=[K/(2\pi)^2][1-\cos(2\pi u)] \tag{1}$$

(Frenkel-Kontorova model), submitted to dc and ac driving forces, $F(t)=\bar{F}+F_{ac}\cos(2\pi\nu_0 t)$. The equations of motion are

$$\dot{u}_j=u_{j+1}+u_{j-1}-2u_j-[K/(2\pi)]\sin(2\pi u_j)+F(t)\ , \tag{2}$$

where $j=-N/2,\ldots,N/2$; and we are interested in the thermodynamic limit ($N\to\infty$), as well as the asymptotic behavior (steady state). Equations (2) have been integrated using a fourth-order Runge-Kutta code. Given a steady-state solution of (2), $\{u_j(t)\}$, the transformation $\sigma_{r,m,s}$,

$$\sigma_{r,m,s}\{u_j(t)\}=\{u_{j+r}(t-s/\nu_0)+m\}=\{u_j'(t)\}\ , \tag{3}$$

(r,m,s arbitrary integers) produces another steady-state

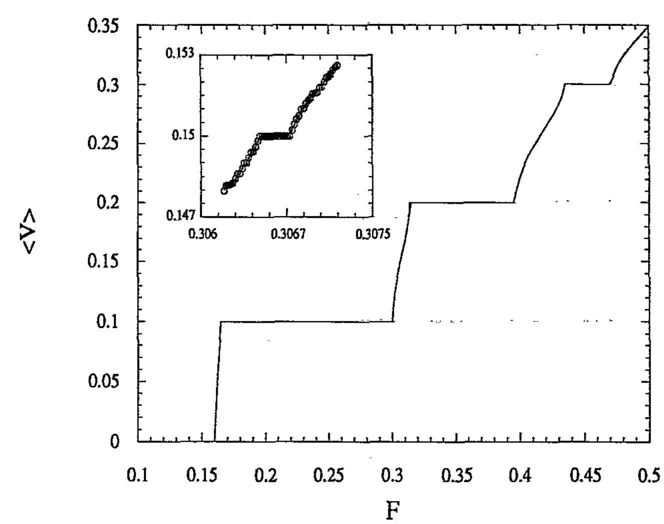

FIG. 1. Staircaselike response function $\bar{v}(\bar{F})$ for $\omega=\frac{1}{2}$, $F_{ac}=0.2$, $\nu=0.2$, and $K=4.0$. The inset shows a subharmonic step ($s=2$).

solution. If a solution is invariant under a particular symmetry operation (3), it will be called resonant and its (particle and time) average velocity is then given by $\bar{v}/\nu_0=(r\omega+m)/s$, where $\omega=\langle(u_{j+1}-u_j)\rangle$ is the interparticle average distance, fixed by the appropriate boundary conditions. Commensurate structures are characterized by a rational value of ω, this value being irrational for an incommensurate structure. For commensurate structures, which is the case we will consider hereafter,[10] the response function $\bar{v}(\bar{F})$, at any nonzero value of the pinning strength K, is a staircase function with steps at every resonant value of the velocity. A particular example of this response function for $\omega=\frac{1}{2}$, $K=4$, $\nu_0=0.2$, and $F_{ac}=0.2$ is shown in Fig. 1, where several steps corresponding to values of $s=1$ are clearly visible. The inset in Fig. 1 shows a step with $s>1$. The existence of subharmonic ($s>1$) steps has been a matter of controversy: Renné and Polder[11(a)] and Waldram and Wu[11(b)] proved that for $\omega=1$ they do not exist. But, for noninteger values of ω, Inui and Doniach[12] gave some evidence as well as plausibility arguments for the existence of subharmonic steps. We have carefully checked this issue for many different fractional values of ω, and have always found numerical evidence of subharmonic steps (as well as no subharmonics for integer values of ω).

The largest Lyapunov exponent[13] of the steady-state trajectories reveals in a most sensitive way the existence of subharmonic steps. The trajectories in the steps are resonant and, consequently, periodic in time, so that the Lyapunov exponent takes on negative values in the steps (Fig. 2). Outside the steps, the trajectories are quasiperiodic, as suggested by the computed zero Lyapunov exponent, and confirmed by the inspection of Poincaré sections: An example of it is shown in Fig. 3(a), for a time interval between sections of $1/\nu_0$, the period of the external force. The section has the topology of a circle, which reveals that the unlocking transition is a transition from periodic to quasiperiodic behavior.

This characterization of the dynamical locking-unlocking transition in the Frenkel-Kontorova model is further confirmed by inspection of the power spectrum of the (particle) average velocity $v(t)$: It shows peaks only

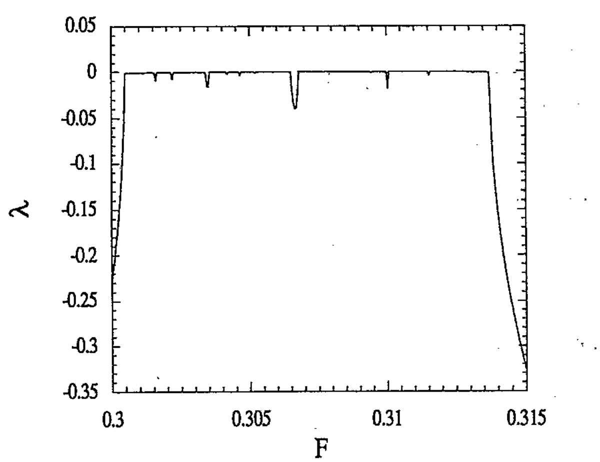

FIG. 2. Lyapunov exponent for a detail of the response function between the first and second steps.

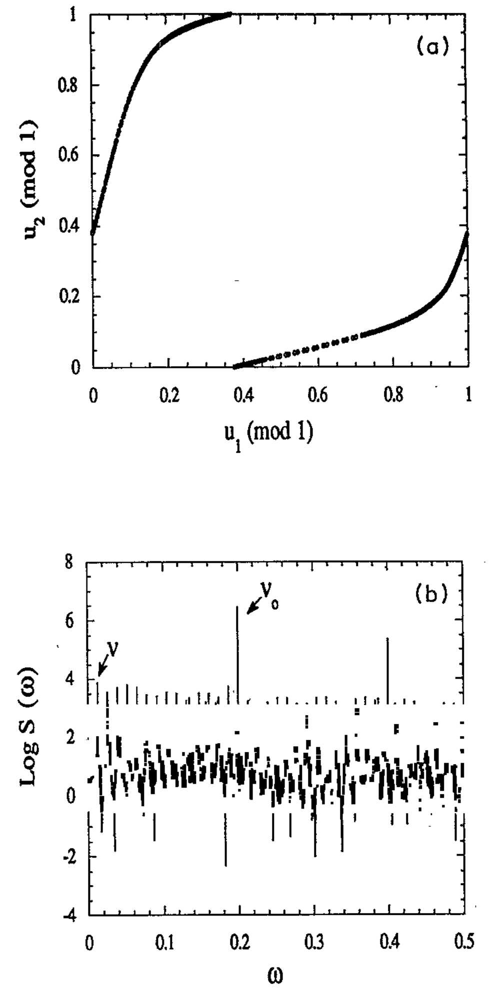

FIG. 3. Poincaré section (a) and power spectrum (b) of $v(t)$ for an unlocked steady state at $\bar{F}=0.3006$ close to the right edge of the first harmonic step. The logarithm is to base 10.

at $(n/s)\nu_0$ (n integer) when computed in the steps, whereas out of the steps [Fig. 3(b)] one observes peaks at linear combinations of two frequencies ν_0 and ν, a well-known feature of a quasiperiodic temporal series. This new frequency ν comes into scene when crossing the unlocking transition, grows with $\bar{F}$, and is directly related to the temporal distribution of intermittencies, already mentioned in the introduction, which we discuss in the following.[14]

Figure 4(a) shows the computed $v(t)$ for a value of $\bar{F}=0.3006$, close to the right edge ($\bar{F}_c\approx0.30047$) of the step corresponding to $r=-1$, $m=1$, $s=1$. It presents long time intervals of periodic oscillations (essentially indistinguishable from the time series inside the nearby step), but this regular behavior is suddenly disrupted by bursts of short duration, after which the regular periodic oscillations are restored. We are seeing what is commonly termed as intermittencies [9]. Unlike the behavior observed in the intermittent transition to turbulence in convective fluids or to chaos in dissipative dynamical systems of a few degrees of freedom, the occurrence of intermittencies in Fig. 4(a) is regular and never random; the system being in a quasiperiodic attractor, the signal $v(t)$ is

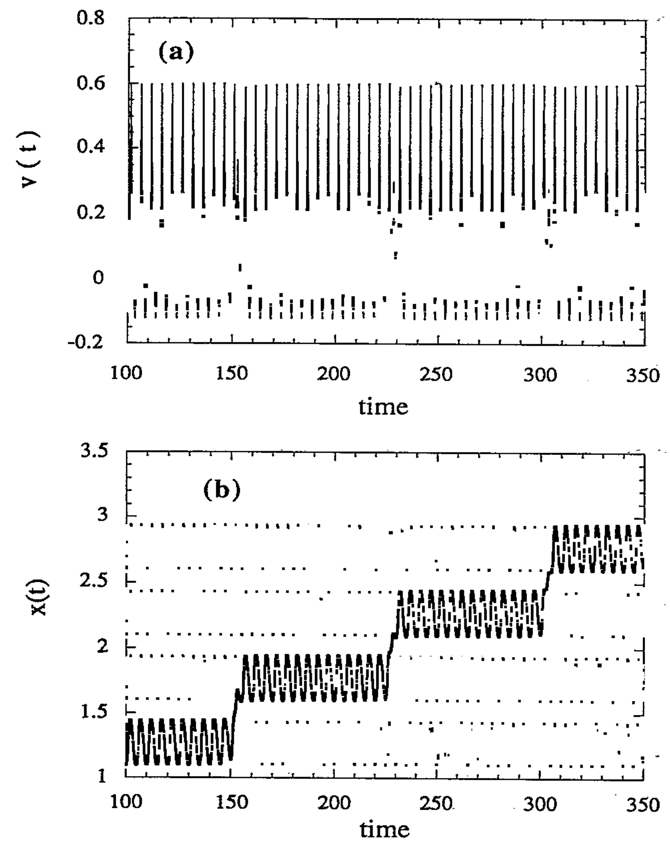

FIG. 4. (a) Particle average velocity vs time in an unlocked state near the right border of the first step, $\bar{F}=0.3006$. (b) Plot of centroid $x(t)$ (see text for details) in the unlocked steady state (solid line). Instantons are given by jumps in the figure. Dotted lines correspond to different steady-state (locked) trajectories in the first step ($\bar{F}=0.3004$).

quasiperiodic.

In order to illustrate the nature of these intermittencies, it is convenient to examine with some detail the structure of the set of steady states $\{u_{j_{\rm step}}(t)\}$ in the close resonance (step) characterized by

$$\bar{v}_{\rm step}=v_0(r\omega+m)/s$$

(Ref. 15). Consider the center-of-mass position (centroid) of a given unit cell, relative to an inertial frame moving at the step velocity:

$$x(t)=q^{-1}\sum_{j=1}^{n}u_j(t)-\bar{v}_{\rm step}t \ , \qquad (4)$$

where q is the number of particles in a unit cell ($\omega=p/q$). For $\{u_{j_{\rm step}}(t)\}$, the corresponding $x_{\rm step}(t)$ oscillates around some average value $\bar{x}_{\rm step}$. Different steady-state trajectories

$$\{u'_{j_{\rm step}}(t)\}=\sigma_{r',m',s'}\{u_{j_{\rm step}}(t)\} \ ,$$

can be obtained by using the invariance of the equations of motion under transformations $\sigma_{r',m',s'}$ [Eq. (3)]. One easily finds that the average $\bar{x}'_{\rm step}$ of the center of mass for $\{u'_{j_{\rm step}}(t)\}$ is related to $\bar{x}_{\rm step}$ by

$$\begin{aligned}\bar{x}'_{\rm step}-\bar{x}_{\rm step}&=\Delta(r',m',s')\\&=(qs)^{-1}[s(r'p+m'q)-s'(rp+mq)]\\&=n_{r',m',s'}(qs)^{-1} \ . \end{aligned} \qquad (5)$$

Provided p and q are relatively prime and[15] that $(rp+mq)$ and s have no common factors, $n_{r',m',s'}$ can take on any integer value. Consequently the "phase shift" Δ between consecutive steady-state trajectories is $(qs)^{-1}$, as shown in Fig. 4(b), where dotted curves are plots of $x_{\rm step}(t)$ for different resonant steady states in the step associated to $r=1$, $m=0$, $s=1$.

The (heavy line) curve in Fig. 4(b) shows $x(t)$ for a steady-state trajectory outside (but very close to) the step mentioned above. It clearly shows that instantons connect consecutive trajectories and then carry a topological charge of $(qs)^{-1}$. The unlocked state can be described as a temporal array of instantons superimposed to the locked periodic near state. This description shares the spirit of the familiar phenomenological description of a (static) incommensurate structure as an array of spatial discommensurations superimposed to a commensurate near structure. In both cases there is a topological charge (or phase shift) associated to the defect (discommensuration in one case, instanton in our case) whose origin lies in the discrete character of the symmetry group corresponding to the locked state (commensurate structure or periodic trajectory).

The numerical observations (in rather different circumstances) of unlocked states always reveal that instantons occurs at regular intervals of time, a fact that can be related to the convexity of the interparticle potential. If we denote by τ_u the width of such intervals, its inverse $\nu=\tau_u^{-1}$, is the additional frequency revealed by the power spectrum of the unlocked trajectory, and the average velocity $\bar{v}$ satisfies

$$|\bar{v}-\bar{v}_{\rm step}|=\nu(qs)^{-1} \ .$$

This characteristic time τ_u diverges as the locking transition is approached with a classical exponent: $\tau_u\approx|\bar{F}-\bar{F}_c|^{-1/2}$. This scaling is predicted from general arguments, which are applicable here, developed in the study of type-I intermittencies,[9] and is very well fitted by our numerical results. When the transition is approached from the resonant state, another characteristic time, τ_1, diverges: it is the inverse of the Lyapunov exponent, which measures the rate of decay of transients. The scaling is the same, $\tau_1\approx|\bar{F}-\bar{F}_c|^{-1/2}$. These diverging time scales at the locking-unlocking transition[16] play the same role as the correlation length at the critical point in equilibrium phase transitions.

Although these results have been obtained for a particular one-dimensional (1D) model, they are based on rather general features: the discrete symmetries of the steady states and the convex interaction between particles. Recent studies on charge-density wave (CDW) systems show a suggestive parallelism with the results reported here: Careful analysis on dc and ac excited $NbSe_3$ crystals shows transition to quasiperiodicity driven by "dynamical solitons" (i.e., instantons)[17(a)] as well as "frequency pulling" behavior near subharmonic steps.[17(b)] In 2D superconducting systems (JJA or layered type-II superconductors), vortex motion has the same type of discrete symmetries[18] as the one studied here. In spite of the fact that the superconducting phase interaction is nonconvex, the pinning seems to be low enough there so that only the convex part of the interaction would be relevant. Indeed, our own preliminary numerical simulations on 2D JJA confirm that the scenario for the unlocking transition shown here is applicable to this system.

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[15]It is important to realize that one can choose r,m,s, so that $(rp + mq)$ and s have no common factors, and that this condition fixes uniquely the value of s for a given $\bar{v}_{\text{step}}$. Otherwise the topological charge of the instanton $(qs)^{-1}$ we talk about below would not be well defined.

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