Hysteresis in the Underdamped Driven Frenkel-Kontorova Model

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We study a commensurate chain of atoms subject to a periodic substrate potential, damping, and a thermal bath, and driven by an external dc force. In the underdamped case the average system velocity as a function of adiabatically varying force exhibits hysteresis at nonzero temperatures. The hysteresis exists due to the instability of the driven motion of kinks at high velocities. In the force-decreasing process, the system passes through two regimes: the "cavity-mode" regime (a standing wave superimposed on the state of running atoms) and the "traffic-jam" regime, where the mobility is due to kink-antikink pairs, the kinks being bunched into compact groups. [S0031-9007(97)04430-X]

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Nonequilibrium dynamics of simple systems of interacting atoms subjected to an external periodic potential, damping, and a thermal bath, 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, conductivity, tribology, Josephson transmission lines, etc.

Two limiting situations have already been studied in detail. The *first* one corresponds to a system of noninteracting atoms; this case was studied, in particular, by Risken *et al.*, and the results are summarized in the monograph [1]. Under the influence of a dc force F a Brownian particle in a sinusoidal potential preferentially diffuses in the direction of the force and on average there is a drift velocity $\langle v \rangle$ which depends on F. The mobility B is then defined as $B = \langle v \rangle / F$. For small forces, B is independent of F (the linear response regime), but for larger ones a nonlinear response takes place. The total potential experienced by the particle is the sum of the periodic potential and the potential $-Fx$ due to the driving force, i.e., it corresponds to a corrugated surface, whose average slope is determined by F. At small forces the potential has local minima, therefore the particle is static and its mobility is zero at temperature $T = 0$. On the contrary, for large forces there are no stable positions, and the particle slides over the corrugated potential, reaching its maximum mobility $B_f = (m\eta)^{-1}$, where m is the mass of the particle and η is the viscous friction coefficient. Denoting by ε the height of the periodic potential and by a the lattice constant, the critical force for which the stable positions disappear is $F_f^{(0)} = \pi\varepsilon/a$.

In the underdamped case, however, the system may have a running solution even if the minima of the potential exist. Indeed, because of its momentum the particle may overcome the next hill, which is lower than the one from which it was falling due to the $-Fx$ contribution to the potential, if the gain in potential energy is greater than the energy dissipated during this motion. One finds that this second critical force is $F_b^{(0)} = (4/\pi)\eta\sqrt{m\varepsilon}$. As the particle is either locked or running, depending on its initial velocity, the system exhibits bistability and the transition between these two states shows hysteresis. However, for a single particle the bistability disappears in the presence of an external noise, because the fluctuations can kick the particle out of the locked state. Thus, the Brownian motion of a single particle driven by an external force shows hysteresis only for $T = 0$.

The *second* limiting case corresponds to the overdamped Frenkel-Kontorova (FK) model [2], when $\eta \gg \omega_0$ (ω_0 is the vibrational frequency at the bottom of the periodic potential). Interesting results were obtained by reducing the time-independent Schmoluchowsky equations for a steady state of the driven system to a one-particle equation with an effective on-site potential, which then was solved numerically by the transfer-integral method [3]. This problem was also studied by an approximate solution of the many-particle Schmoluchowsky equation in configuration space [4]. The results show that there is a region of highly nonlinear mobility, but without any bistability phenomenon.

However, simulation results [5] have shown that in the *underdamped* Frenkel-Kontorova model hysteresis exists even at nonzero T. *The goal of the present work is to find conditions under which hysteresis persists at nonzero T for the one-dimensional case.* We shall show that hysteresis does exist at $T \neq 0$ due to the instability of high-speed kink motion.

First of all, recall that in the FK model mass transport along the chain is carried out by kinks, the topologically stable quasiparticles which describe a local compression (or extension in the case of antikink) of the chain. Motion of a single kink which starts with a high speed in the highly discrete undamped FK model was studied by Peyrard and Kruskal [6]. They found two important phenomena. First, during its motion the kink experiences a strong interaction with phonons; therefore, at resonance conditions (i.e., with kink velocities in certain intervals) the kink motion is strongly damped and its velocity

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decreases quickly, while outside these resonance intervals the damping is very low, and the kink moves with such a velocity for a long time. The velocity-locking effect for a driven kink was studied recently in detail by Watanabe *et al.* [7]. Second, Peyrard and Kruskal observed that the very fast kink is unstable, while a pair of two coupled kinks can be stable and move as a whole with very high velocity and practically without damping.

As was mentioned in [8] and will be discussed in detail in the present work, it is this instability of the motion of fast kinks that is responsible for the hysteresis, i.e., the sharp transition from the low-B motion to the high-B sliding regime is solely a dynamical effect which exists only in the underdamped system.

In our simulation we studied a chain of $N = 128$ atoms subjected to a sinusoidal potential with amplitude $\varepsilon = 2$ and period $a = 2\pi$, the atomic mass was $m = 1$ (this defines our system of units). The equations of motion for the displacements x_i are

$$\ddot{x}_i + \eta\dot{x}_i + \sin x_i + \frac{d}{dx_i}\left[\sum_{j(j\neq i)} V(|x_i - x_j|)\right] = F, \tag{1}$$

with $1 \leq i \leq N$. We used periodic boundary conditions, the potential has $M = 128$ wells on the chain length, i.e., the ground ($T = 0$) state is trivial (commensurate). For convenience (in order to study later the generalized FK model with a transverse degree of freedom [9] with the same model parameters) we used the Toda interaction potential, with the amplitude $V_0 = 4\pi^2 e$ and the exponent $\beta = 1/2\pi$. This choice corresponds to the dimensionless elastic constant (which is defined as $g = a^2 V''(a)/2\pi^2\varepsilon$; see, e.g., [10]) $g = 1$, i.e., to the intermediate case between the strong coupling (sine-Gordon) case and a weakly coupled chain. (Recall that the Aubry transition from the pinned to sliding state takes place at $g \approx 1$ for the golden-mean case [11].)

To all atoms we applied the dc force F which was adiabatically changed (the details of simulation procedure are described in [12]), and calculated the average system velocity $\langle v \rangle$. The damping coefficient was taken as $\eta = 0.1$ (recall that the frequency of atomic vibrations in the external potential is $\omega_0 = 1$ in our system of units), and the temperature was $T = 0.7$ (compare with the barrier height $\varepsilon = 2$).

The results are presented in Fig. 1. One can see that during the force-increasing process the system jumps at $F_f \approx 0.53$ from the $B \approx 0$ (locked) state directly to the $B \approx 1$ (sliding) state, while when the force is decreased, starting from the sliding state, B begins to decrease at $F < 0.5$, and reaches the "force-increasing" values only at $F < F_b \approx 0.2$, so the system dynamics shows a large hysteresis. To compare, we plot also the $B(F)$ dependence for the noninteracting system for $T = 0$, where $F_f^{(0)} = 1$ and $F_b^{(0)} \approx 0.18$, and the hysteresis disappears at $T > 0$.

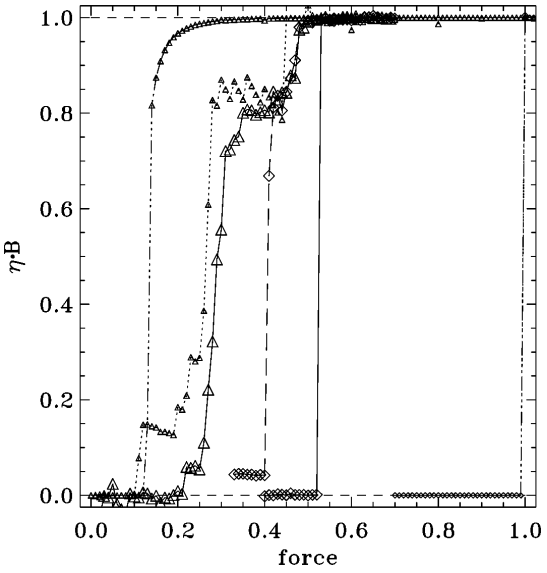

FIG. 1. $B(F)$ dependences: solid curve for $T = 0.7$ and $g = 1$, dotted curve for $T = 0$ and $g = 1$, dot-dashed curve for $T = 0$ and $g = 0$, and dashed curve for $T = 0.7$ and $g = 1$ for the initial configuration with one kink-antikink pair. (For the last case we show the forward transition only.) Adiabatic increase and decrease of the force is denoted by diamonds and triangles, respectively. Notice that the $T = 0$ forward transition takes place at $F = 1$ for both noninteracting ($g = 0$) and interacting ($g = 1$) cases.

The detailed behavior at the locked-to-running transition is clear from Fig. 2, where we plot the atomic trajectories just at the transition point. As seen, the scenario starts with the creation of one kink-antikink pair. The kink and antikink move in opposite directions, quasielastically collide (because of the periodic boundary conditions), and quite soon a new kink-antikink pair is created in the tail of the primary kink and then another pair in the tail of

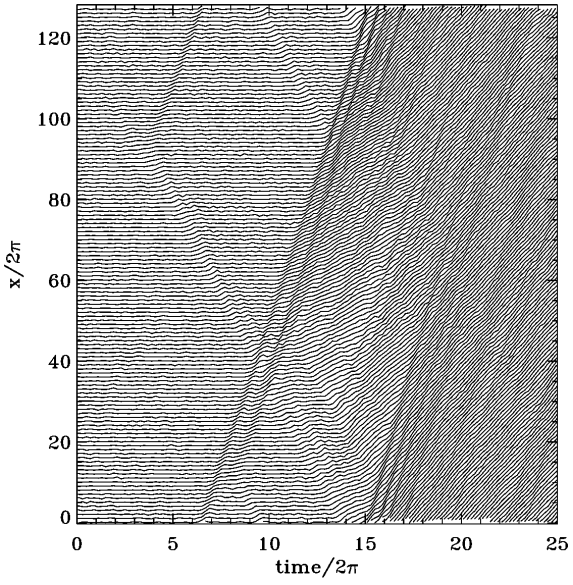

FIG. 2. Atomic trajectories for $F = 0.53$.

the new kink. This process continues, resulting in an exponential (avalanchelike) growth of the kink-antikink pair concentration, finishing in the totally running state.

For the chosen model parameters, the kink-antikink creation energy is $\varepsilon_{\text{pair}} \approx 31.7$ (this value is higher than $\varepsilon_{\text{pair}}^{(\text{SG})} = 16$ the value for the SG system; the difference is due to the exponential interaction used in the present simulation), so that the expected number of kink-antikink pairs is [13] $n_{\text{pair}} \lesssim 10^{-9}M$, i.e., it is negligible for the chosen system size at $T = 0.7$. When F increases, the barrier for kink-antikink creation decreases, and at large forces it disappears completely (this scenario is described in detail in [4]). To check if the pair creation event plays the dominant role, we started with the initial state which already has one kink-antikink pair at small $F = 0.23$ (this state was taken from the backward trajectory of Fig. 1) and then adiabatically increased the force. Again, the above scenario repeated (although the locked-to-running transition takes place now at $F \approx 0.41$): the atomic trajectories at the transition look like those in Fig. 2 except that the kink-antikink pair exists much earlier. From this we may conclude that the main mechanism responsible for the transition is not the creation of a pair, but the kink motion itself.

To check the last assumption, we studied the system with $N/M = 129/128$, where one (residual) kink exists from the beginning. Now the low-F mobility is determined by motion of this kink, which is activated (Arrhenius-like) at small F and unactivated at $F > 0.08$, when the Peierls-Nabarro potential for the kink motion is suppressed due to the force F. However, at $F \approx 0.42$ the system exhibits the transition to the totally running state just as was described above. The atomic trajectories at the transition are shown in Fig. 3. As seen, new kink-antikink pairs are generated in the kink tail, and this results in the avalanche leading to the running state. Notice also that the kinks (the primary kink and the kinks from the newly created kink-antikink pairs) are bunched, and move together as an entity. We note that the kink-antikink pair generation behind a moving domain wall was observed in the 2D FK model [14], and kink bunching was also observed in [5].

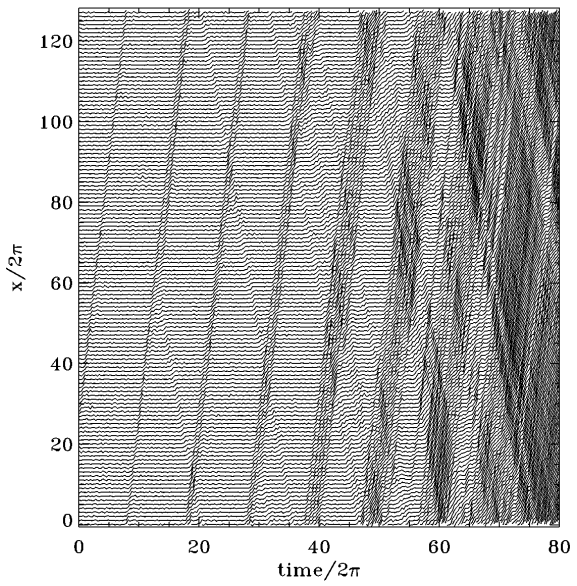

FIG. 3. Trajectories for the system with one residual kink at $F = 0.42$.

The critical kink velocity causing the avalanche is estimated as $v_c \sim 12$ (this value may be found in two ways: from the slope of the kink trajectory in Fig. 3, and from the B value at the threshold F_f if we suppose that $v_c \approx N\langle v \rangle$). Note that the sound velocity for the chosen system parameters is $c = 2\pi$; recall also that in the SG system the kink cannot move faster than with the velocity c.

Thus, we conclude that a sharp locked-to-running transition exists in systems for which the driven kink reaches the critical velocity v_c before the atomic motion becomes significant (i.e., it is still activated and may be neglected compared with the kink-antikink contribution to B). The origin of this "primary" kink is insignificant; it may be either a thermally excited kink-antikink pair, or it may be created at an impurity site (both processes are stimulated by the force which decreases the creation barriers). The only difference may emerge in a finite system, when $n_{\text{pair}} \ll 1$; in this case the initiating event may be the creation of an initial kink-antikink pair.

We emphasize that the sharp locked-to-running transition of necessity leads to hysteresis in the $B(F)$ dependence; clearly the avalanche cannot go backwards, and the system cannot jump back to the low-B state when F is slightly decreased below F_f.

Finally, we briefly discuss the backward $B(F)$ dependence. The transition from the running to locked state for the underdamped SG model at $T = 0$ was studied in [15]. As was shown there, it proceeds first through a series of "cavity-mode" states, and then a series of kink-antikink wave train states (in an infinite system this sequence should be infinite, so the transition is continuous). A similar scenario is exhibited by our discrete FK system (see Fig. 1). First, the system passes through the "cavity-mode" states. For the $T = 0$ case one may clearly resolve five steps on the $B(F)$ curve; each step is characterized by an approximately constant velocity ($\langle v \rangle \approx 3.43, 3.18, 2.88, 2.63$, and 2.34). Note that the discrete system differs from the continuous SG one in that the former may have resonances with phonons, and this may result in locking of some states.

After the cavity-mode regime, the system jumps to the kink-antikink-pair regime. An important difference from the SG case is that in the discrete system the kinks have a tendency to be bunched and to move in groups. A typical example of such a state is shown in Fig. 4; as seen it resembles a "traffic jam." Contrary to the $N < M$ case studied in Ref. [5], in the present work we did not observe bunching of antikinks.

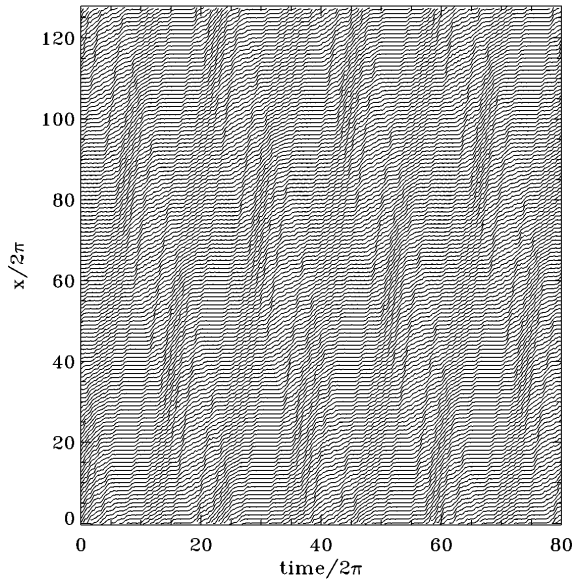

FIG. 4. Atomic trajectories in the "traffic-jam" regime at $F = 0.24$.

One may expect that temperature should not modify this scenario seriously, because the system kinetic energy in the running state is much larger than the thermal energy. Indeed, the simulations confirm this expectation (see Fig. 1), although the peculiarities of the $B(F)$ curve are smoothed. It is important to note that the continuous or discontinuous nature of the transitions in this nonequilibrium situation has nothing in common with continuous or discontinuous equilibrium phase transitions, i.e., has no bearing on the existence of hysteresis.

Note that the cavity-mode and traffic-jam states are characterized by different symmetries. Therefore the system can pass from one state to the next state only at the points where the previous state becomes unstable. Besides, a typical scenario for a first-order transition, where different states (phases) coexist, is forbidden here due to the one dimensionality of the system. Each state is characterized by a different average velocity. As the system is one dimensional, it is therefore impossible for two different phases to coexist as a steady state.

To conclude, our simulation results have shown that the underdamped discrete SG system at low temperatures should exhibit hysteresis in its $B(F)$ dependence. A study of the nature of the forward and backward transitions shows that this hysteresis exists in both *finite* and *infinite* systems. (That it is not merely a finite-size effect has been verified in a simulation of the $N = M = 256$ system [16].) The reason for the sharp locked-to-running transition is the existence of a critical kink velocity v_c, above which the kink destroys itself and causes an avalanche driving the whole system to the totally running state. The nature of this critical velocity merits a more detailed study.

[1] H. Risken, *The Fokker-Planck Equation* (Springer, Berlin, 1984).
[2] Ya. Frenkel and T. Kontorova, Phys. Z. Sov. **13**, 1 (1938).
[3] S. E. Trullinger, M. D. Miller, R. A. Guyer, A. R. Bishop, F. Palmer, and J. A. Krumhansl, Phys. Rev. Lett. **40**, 206 (1978); **40**, 1603 (1978).
[4] M. Büttiker and R. Landauer, Phys. Rev. A **23**, 1397 (1981); M. Büttiker and T. Christen, Phys. Rev. Lett. **75**, 1895 (1995).
[5] O. M. Braun, T. Dauxois, M. V. Paliy, and M. Peyrard, Phys. Rev. Lett. **78**, 1295 (1997); Phys. Rev. E **55**, 3598 (1997).
[6] M. Peyrard and M. D. Kruskal, Physica (Amsterdam) **14D**, 88 (1984).
[7] S. Watanabe, H. S. J. van der Zant, S. H. Strogatz, and T. P. Orlando, Physica (Amsterdam) **97D**, 429 (1996).
[8] M. Paliy, O. Braun, T. Dauxois, and B. Hu (to be published).
[9] O. M. Braun and Yu. S. Kivshar, Phys. Rev. B **44**, 7694 (1991).
[10] O. M. Braun and Yu. S. Kivshar, Phys. Rev. B **50**, 13 388 (1994).
[11] S. Aubry, Physica (Amsterdam) **7D**, 240 (1983); M. Peyrard and S. Aubry, J. Phys. C **16**, 1593 (1983).
[12] O. M. Braun, T. Dauxois, M. V. Paliy, and M. Peyrard, Phys. Rev. B **54**, 321 (1996).
[13] J. F. Currie, M. B. Fogel, and F. L. Palmer, Phys. Rev. A **16**, 796 (1977).
[14] J. Pouget, S. Aubry, A. R. Bishop, and P. S. Lomdahl, Phys. Rev. B **39**, 9500 (1989).
[15] J. C. Ariyasu and A. R. Bishop, Phys. Rev. B **35**, 3207 (1987).
[16] O. M. Braun, A. R. Bishop, and J. Röder (unpublished).