Driven dynamics: A photodriven Frenkel-Kontorova model

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In this study, we examine the dynamics of a one-dimensional Frenkel-Kontorova chain consisting of nanosize clusters (the ''particles'') and photochromic molecules (the ''bonds''), also being subjected to a periodic substrate potential. Whether the whole chain should be running or be locked depends on both the frequency and the wavelength of the light (keeping the other parameters fixed), as observed through numerical simulation. In the locked state, the particles are bound at the bottom of the external potential and vibrate backwards and forwards at a constant amplitude. In the running state, the initially fed energy is transformed into directed motion as a whole. It is of interest to note that the driving energy is introduced to the system by the irradiation of light, and the driven mechanism is based on the dynamical competition between the inherent lengths of the moving object (the chain) and the supporting carrier (the isotropic surface). However, the most important feature is that the light-induced conformational changes of the chromophore lead to the time-and-space dependence of the rest lengths of the bonds.

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The driven dynamics of a system of interacting particles in atomic or mesoscopic scale has been attracting much attention. It is very important in technology, very rich in physics, and widely applicable in many fields, such as mass transport, conductivity, tribology, etc. As far as we know, one of the most typical examples conducted on the driven dynamics has been the driven Frenkel-Kontorova-type systems biased by dc, and ac external forces, respectively.

The Frenkel-Kontorova (FK) model [1] may describe, for example, a closely packed row of atoms in crystals, a layer of atoms adsorbed on crystal surface, a chain of ions in a ''channel'' of quasi-one-dimensional conductors, hydrogen atoms in hydrogen-bonded systems, and so on. In general, such a system can be treated with two parts in the driven dynamical model: the moving object and the supporting carrier. First, the moving object is considered an atomic subsystem, in which the interparticle interaction is taken as a harmonic interaction between the nearest neighbors. Second, the action of the supporting carrier to the moving object is modeled as an external potential, a damping constant, and a thermal bath. When, for instance, an external dc driving force f is applied to such a system, its response can be very nonlinear and complex. The overdamped case ($\eta \gg \omega_0$, where η is the external damping and ω_0 is the vibrational frequency at the bottom of the periodic potential), has been studied in a number of papers [2–4]. When the driving force f changes, the multistep and the hysteretic transition of the system from the locked state to the sliding state in the underdamped case ($\eta \ll \omega_0$) has also been delineated in detail [5,6]. At the same time, various intermediate regimes can be described by resonance phenomena [7] and by the moving quasiparticle excitation, kinks [8].

A theoretical demonstration of driven dynamical behavior, as a steady-state response to an applied driving force, must be well verified in laboratory. It is of interest to note that a Josephson junction array is just a technically and physically excellent demonstration, of many typical nonlinear features of the driven FK-type systems biased by, for instance, dc forces [9] and ac forces [10].

In this paper, we propose a photo-driven Frenkel-Kontorova model, which may be realized through experiment. The basic challenge of our proposal is to keep the time-and-space dependence of the rest lengths of the harmonic oscillator, as was suggested originally by Proto *et al.* [11] when discussing the atomic scale engines. In this model system, the supporting carrier is taken as an isotropic surface, and the moving object (a FK chain) consists of nanosize clusters (the ''particles'') and photochromic molecules [12] (the ''bonds''). The particles are identical with mass m; the bonds are flexible with elastic strength k and photoactive with sensitive coefficient b; the time-and-space dependence of the free equilibrium rest lengths is due to the light-induced conformational changes of the chromophore. In contrast to the particles, the bond mass is so small that it can be neglected. For simplicity, we restrict the discussion to one dimension at zero temperature. The N equations of motion read as

$$m\ddot{x}_n + \eta\dot{x}_n + \frac{\partial\Phi(x_n)}{\partial x_n} + \sum_{\delta} \frac{\partial\Psi[x_n, x_{n+\delta}, a_{n,n+\delta}(t)]}{\partial x_n} = 0, \tag{1}$$

where x_n is the coordinate of the nth particle with $1 \leqslant n \leqslant N$. The second term of Eq. (1) describes the dissipative interaction (damping) between the particles and the surface.

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It is proportional to the relative velocities of the particles, with proportionality constant η. The static interaction between the particles and the surface is represented by the periodic substrate potential

$$\Phi(x_n)=\Phi_0\left(1-\cos\frac{2\pi x_n}{\lambda_1}\right). \tag{2}$$

Concerning the interparticle interaction, we take the form of the nearest neighboring harmonic interaction

$$\Psi[x_n,x_{n+\delta},a_{n,n+\delta}(t)]=\frac{k}{2}[|x_n-x_{n+\delta}|-a_{n,n+\delta}(t)]^2. \tag{3}$$

Due to the light sensitivity, the bond lengths change with the irradiation of light. The free equilibrium rest lengths $a_{n,n+\delta}(t)$ depend on both the bond's position, specified by the indices n, $n+\delta$, ($\delta=\pm1$), and time t. We restrict ourselves to a certain choice for $a_{n,n+\delta}(t)$:

$$a_{n,n+\delta}(t)=a_0(1+b\cos[qx_{n,n+\delta}-\omega t)]$$
$$=a_0\left[1+b\cos\left(\frac{2\pi}{\lambda_2}\frac{x_n+x_{n+\delta}}{2}-\omega t\right)\right], \tag{4}$$

where b ($b<1$) is an absorption coefficient (amplitude) less than one, a_0 is the rest length of the harmonic interaction, and λ_2 and ω are the wavelength and frequency of external irradiated light, respectively. Obviously, a_0 and b are intrinsic parameters, and λ_2 and ω are externally adjustable. Light energy, if pumped into the system in an irradiating manner, may produce spatially and temporally correlated changes of the lengths $a_{n,n+\delta}(t)$. Then, the dynamical local competition between the periodicity λ_1 and the rest lengths $a_{n,n+\delta}(t)$ may induce a driving power, which will impel the chain into motion in some manner. Granted, this power must be strong enough to overcome the resistance.

After introducing dimensionless parameters $x_n\rightarrow(2\pi/\lambda_1)x_n$, $t\rightarrow(2\pi/\lambda_1)\sqrt{\Phi_0/m}t$, and the renormalized parameters $\omega\rightarrow[(2\pi/\lambda_1)\sqrt{\Phi_0/m}]^{-1}\omega$, $\eta\rightarrow[(2\pi/\lambda_1)\sqrt{m\Phi_0}]^{-1}\eta$, $k\rightarrow(1/\Phi_0)(\lambda_1/2\pi)^2k$, $a_0\rightarrow(2\pi/\lambda_1)a_0$, the motion equation reads as follows:

$$\ddot{x}_n=-\eta\dot{x}_n-\sin x_n+k\left[x_{n+1}-2x_n+x_{n-1}+2a_0b\sin\left(\frac{\lambda_1}{\lambda_2}\frac{x_{n+1}-x_{n-1}}{4}\right)\sin\left(\frac{\lambda_1}{\lambda_2}\frac{x_{n+1}+2x_n+x_{n-1}}{4}-\omega t\right)\right]$$
$$-\frac{ba_0}{2}\frac{\lambda_1}{\lambda_2}k\left\{(x_n-x_{n-1}-a_0)\sin\left(\frac{\lambda_1}{\lambda_2}\frac{x_n+x_{n-1}}{2}-\omega t\right)-\frac{ba_0}{2}\sin\left[2\left(\frac{\lambda_1}{\lambda_2}\frac{x_n+x_{n-1}}{2}-\omega t\right)\right]\right\}$$
$$-\frac{ba_0}{2}\frac{\lambda_1}{\lambda_2}k\left\{(x_{n+1}-x_n-a_0)\sin\left(\frac{\lambda_1}{\lambda_2}\frac{x_{n+1}+x_n}{2}-\omega t\right)-\frac{ba_0}{2}\sin\left[2\left(\frac{\lambda_1}{\lambda_2}\frac{x_{n+1}+x_n}{2}-\omega t\right)\right]\right\}. \tag{5}$$

In the present survey, the mass of the particle is $m=1$, the period and amplitude of the external sinusoidal potential are $\lambda_1=2\pi$ and $\Phi_0=1$, respectively. So, if we take the natural unit like this, i.e., the time scaled by $(2\pi/\lambda_1)\sqrt{\Phi_0/m}$, the length scaled by $(2\pi/\lambda_1)$, and the mass scaled by $(1/m)$, then the physical quantities, time, velocity and so on, become dimensionless. And one should, in order to restore them, multiply spatial variables by $(\lambda_1/2\pi)$, times by $(\lambda_1/2\pi)\sqrt{m/\Phi_0}$, mass by m, and energies by Φ_0, etc.

In our model, parameters η, k, b, λ_2, and ω are all very

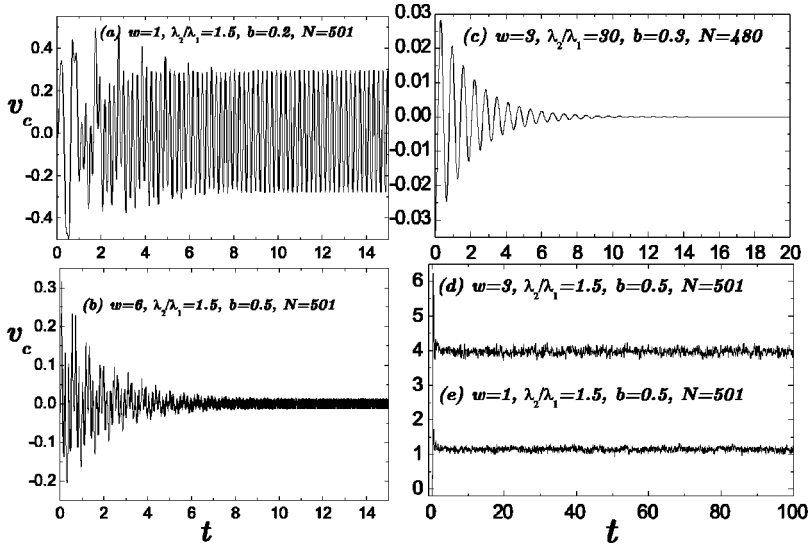

FIG. 1. Velocity of the centre of mass v_c of chain as a function of time t. For different parameters, the system turns quickly into a steady-going locked state [(a)–(c)] or a steady-going running state [(d),(e)] passing through a transitory relaxation.

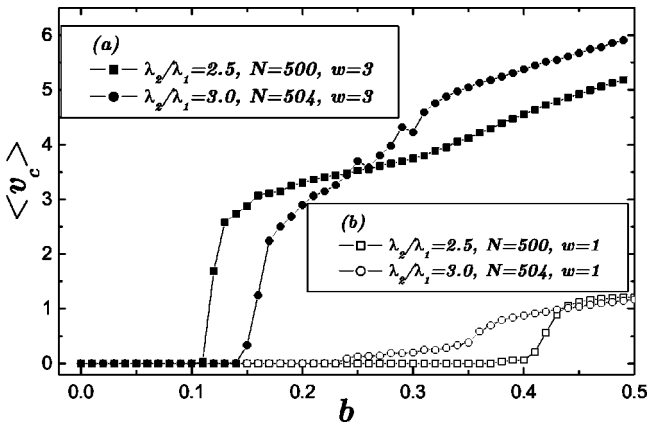

FIG. 2. Average velocity of the center of mass $\langle v_c \rangle$ of chain as a function of the amplitude b.

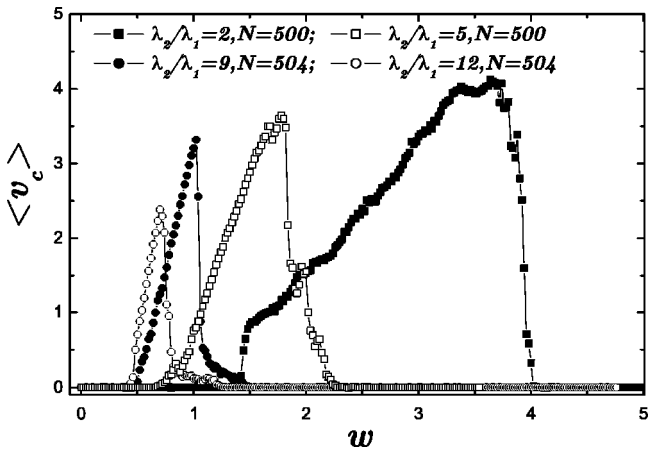

FIG. 3. Average velocity of the center of mass $\langle v_c \rangle$ of chain as a function of the driving frequency ω.

important. For example, when the external viscous damping coefficient η is overdamped $\eta \gg \omega_0$, underdamped $\eta \ll \omega_0$, or other intermediate regions, the driven system exhibits very different dynamical behavior, which has been studied in a number of papers as mentioned above. Note that in the present survey, the characteristic frequency of particle vibration at the minimum of the external potential is $\omega_0 = 1$. To simplify the problem, we keep the damping coefficient and the elastic strength fixed as $\eta = 0.1$ and $k = 1$. Here, the value of k also corresponds to the intermediate case between a strong coupled (sine-Gordon) and a weakly coupled chain. Thus, we focus on the parameters b, λ_2, and ω, all of which definitely characterize how the free equilibrium rest lengths $a_{n,n+\delta}(t)$ depend on the time and position of the bonds.

Our simulation of the Runge-Kutta iteration method starts when the particles are at the bottom of the substrate potential well at rest, and the boundary condition is chosen to be the simplest, as $x_{j+N} = x_j + 2\pi N$ (periodic boundary condition). In this way, $a_0 = \lambda_1 = 2\pi$. Only a finite system possible, its size should be appropriate to ensure that M waves (M is the wave number) can be inserted into the background structure of N-particles system; the integers N and M must satisfy the relation: $N/M = \lambda_2/\lambda_1$. In all calculations, we took the natural unit ($m = 1$, $\lambda_1 = 2\pi$ and $\Phi_0 = 1$) and kept $\eta = 0.1$ and $k = 1$, as mentioned above.

In Fig. 1, we show the velocity of the center of mass of the system v_c [$v_c = (\Sigma_{i=1}^N m_i \dot{x}_i)/(\Sigma_{i=1}^N m_i) = (\Sigma_i \dot{x}_i)/N$, $m_i = m$] as a function of time t for some different parameters. The results tell us the following: (1) after passing through a transitory relaxation, the system turns quickly into a steady state; (2) there are two types of steady states, the locked state [Fig. 1(a–c)] and the running state [Fig. 1(d–e)]. In the locked state, the particles are bound at the bottom of the substrate potential and vibrate backwards and forwards at a constant amplitude. In the running state, the initially fed energy is transformed into directed motion as a whole, with almost constant speed except for a little undulation. With different parameters, there are different oscillating amplitude (in the locked state) or running speed (in the running state). On the whole, the system exhibits interesting and parameter-dependent dynamical behavior.

The amplitude b intrinsically characterizes the light sensitivity of the photochromic molecules (bonds) and determines the elastic energy stored. To find more about it, we started from $b = 0$, slowly increased it by small steps $\Delta b = 0.01$. With every b value, we let the system relax to 10^4 time steps, 10^{-3} each, to ensure a stationary state. We then calculated the average velocity of the center of mass $\langle v_c \rangle$ over the time period of 10^4–10^6 steps. The results for $\lambda_2/\lambda_1 = 2.5$, 3 and $\omega = 1$, 3, respectively, are shown in Fig. 2(a) and 2(b). The processes both have a $\langle v_c \rangle$ increasing from zero as soon as the amplitude exceeds a critical value b_c. At zero speed, each particle is locked in one external potential well without any observable macroscopic motion, expecting its emancipation as the driving energy exceeds a certain value. This is easy to understand for a dissipation system.

It is no surprise as well, that each particular situation is unique, given different frequencies and wavelengths as temporal and spatial modulations. To get further information of their effects, our next simulation was focused on the external photo-driving parameters. Figure 3 presents $\langle v_c \rangle$ as a function of the driving frequencies ω for a fixed value of the wavelength λ_2. From these numerical results, three things are note worthy. First, as the magnitude of frequency slowly increases from $\omega = 0$, a dynamical transition occurs, from an initially locked state to a running state, and finally back to a locked state again. Second, there exits a peak of maximal velocity. Third, as the wavelength increases, the running state has a lower maximal velocity and exists in a narrower span of frequency with lower values. The same is true for $\langle v_c \rangle$ as a function of wavelength, as is presented in Fig. 4.

Finally, we present a dynamical phase diagram in Fig. 5, where we plot the driving frequency vs the ratio of the optical wavelength to the period of the substrate potential. The figure shows that, within a finite range of driving frequencies and wavelengths, the system as a whole will be running; otherwise, the particles will be locked at the bottom of the substrate potential, permanently.

In conclusion, we would like to emphasize several points. First, a reasonable explanation for the photo-driven FK model seems to be that temporal and spatial modulations both result in the resonant absorption of optical energy. And,

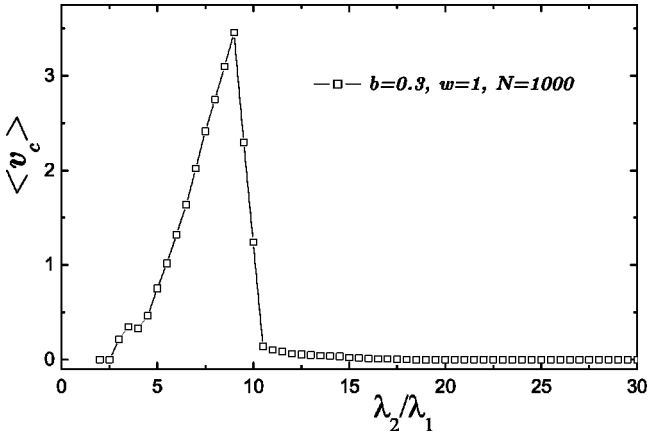

FIG. 4. Average velocity of the centre of mass $\langle v_c \rangle$ of chain as a function of λ_2/λ_1 that denotes the ratio of the optical wavelength to the period of the substrate potential. (Although the relation $N/M=\lambda_2/\lambda_1$ is not satisfied everywhere, the result is still credible with the large system size of $N=1000$.)

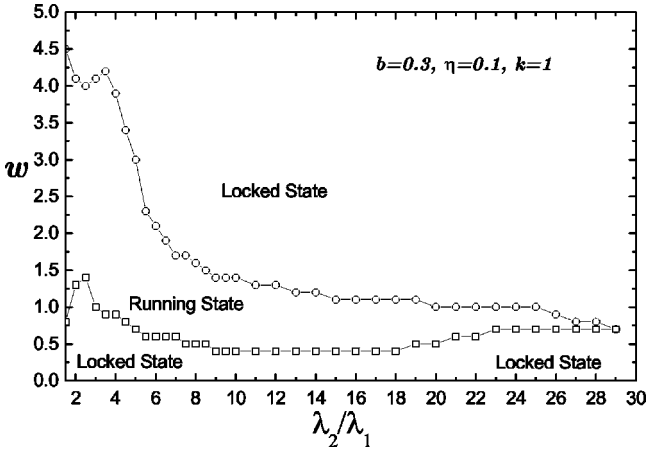

FIG. 5. Dynamical phase diagram in the $(\omega,\lambda_2/\lambda_1)$ plane for the photo-driven one-dimensional FK model. Here parameters are fixed at $b=0.3$, $\eta=0.1$ and $k=1$, respectively. And the particle number N is chosen in 450–550 to ensure that M waves (M is an integer, N and M satisfy the relation: $N/M=\lambda_2/\lambda_1$) can be inserted into the commensurate background structure of N-particle system from first to last.

the dynamical competition between the inherent lengths of the moving object (the chain) and the supporting carrier (the isotropic surface) leads to the transformation of fed energy to directed motion. Second, the light-induced conformational changes of the photochromophore leads to the time-and-space dependence of the rest lengths of the bonds, which is the most important in this model. Third, according to our calculations, the steady state of the system is not affected by the initial conditions. The drift direction of the chain lies only on the sign in front of ω in the expression $a_{n,n+\delta}(t)=a_0[1+b\cos(qx_{n,n+\delta}\mp\omega t)]$. Namely, "$-$" and "$+$" correspond to a motion in positive and negative x direction, respectively. Therefore, the motion of the system can be easily controlled. Fourth, the "springs" connecting the "particles" are light-sensitive molecules (photochromic molecules) and can expand or shrink with light reversibly [13] adjusting the frequency or the wavelength of the light wave may produce spectacular motions. We believe that the concept presented in this paper is simple and robust enough to be realized in actual experiments, and may demonstrate many interesting and typical nonlinear features of a system of interacting particles. However, we would like to further state that the connection between the model and photochromic chains stands at the level of speculation, being an interesting open question or idea, still to be proved.

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