Dc-Driven Diatomic Frenkel-Kontorova Model

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We investigate the resonance steps, spatiotemporal dynamics, and dynamical phase diagrams of the dc-driven diatomic Frenkel-Kontorova model. The complete resonance velocity spectrum is given. The diatomic effects result in each resonant state being characterized by two integer pairs, \((k_1, k_2)\) and \((k_1, k'_2)\). In the high-velocity region the linear response of the average velocity, \(v\), of the chain to the driving force \(F\) is often punctuated by subharmonic resonances \((k_1 > k_2)\). There are two kinds of nonlinear response regions in the high-velocity region. A new physical interpretation of the mean-field treatment is presented.

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The static and the transport properties of Frenkel-Kontorova (FK) [1] systems have been subjects of intensive studies [2–4]. In these studies, one of the most important parameters is the winding number $\omega$ [5]. Starting from uniform sliding states, Strunz and Elmer [6] presented the main, superharmonic resonant conditions while Zheng et al [7] gave the complete resonance condition. The main studies in Refs. [6] and [7] are limited to the region of low velocity and to the case where the chain is composed of the same atoms.

In this paper, we study the dc-driven FK system where the chain is composed alternatively of two different kinds of atoms. The response of the average velocity of the system to the driving force, the resonant steps, and the spatiotemporal dynamics are studied analytically and numerically. Our studies shed some different light on the dynamical behavior of the driven FK systems because (i) diatomic effects which result in new resonance modes are shown; (ii) regions far away from those addressed in previous investigations are treated; and (iii) a new physical interpretation of the mean-field treatment is presented.

We consider a uniform, quasi-static force field $F(t)$ acting on a FK system in the presence of a damping proportional to the velocity and where the atoms can exchange energy with a thermal bath. When the FK chain is composed of more than one kind of atoms, the motion equation of the system may be expressed as

$$m_j \ddot{x}_j = -m_j \eta \dot{x}_j + (x_{j-1} - 2x_j + x_{j+1})$$

$$- \frac{K}{2\pi} \sin(2\pi x_j) + F.$$  \hspace{1cm} (1)

In this paper, we choose $m_1 = m_3 = \cdots = 1$, $m_2 = m_4 = \cdots = m$ where $m \geq 1$. The ground states of this diatomic FK model have been studied in one of our previous papers [8]. The diatomic effect results in a second critical point.

When $K = 0$, there is no nonlinear interaction in the system, and the system mobility shows a linear response $B = 1/\eta$. When $K > 0$, the interactions between the atoms and the external potential are nonlinear. The commensurate ground states are always pinned. For an incommensurate ground state with the winding number $\omega$, there exists a critical value $K_C(\omega)$ at which the Aubry transition occurs [9]. When $K < K_C(\omega)$, the system is
unpinned; when \( K > K_C(\omega) \), the system is pinned. For the latter case, when \( F \) is less than the depinning force \( F_d \), the system is in the locked state. When \( F > K/(2\pi) \), the system should behave approximately as a homogeneous one, and \( B(F) \) reaches the final value \( B^f = 1/\eta \) (linear response). For an intermediate force, the mobility depends on the driving strength (nonlinear response).

The average sliding velocity of the chain reads

\[
v = \lim_{T \to \infty} \frac{1}{T} \int_0^T \frac{1}{N} \sum_{j=1}^N \dot{x}_j dt.
\]

For an incommensurate structure with winding number \( \omega \), when \( K < K_C(\omega) \) at which the transition by breaking of analyticity occurs [9], \( \frac{1}{N} \sum_{j=1}^N \sin(2\pi x_j) = 0 \), so in the case of no dissipation, the chain may slide without any applied force. If the particles are charged, this state corresponds to the superconductivity state.

For a numerical solution to Eq. (1), we use the standard fourth-order Runge-Kutta method. Periodic boundary conditions, \( x_{N+1} = x_1 + M \), \( x_0 = x_N - M \), \( \dot{x}_0 = \dot{x}_N \), \( \dot{x}_{N+1} = \dot{x}_1 \), are imposed, where \( M, N \) are positive integers and \( N \) is an even number. In the simulation, we start with the ground state and \( F = 0 \). We increase the dc force \( F \) by small steps \( \Delta F \) up to a value \( F_{\text{max}} \). Then, we decrease it to zero with the same steps. At each step, we wait long enough to allow the system to reach a stationary state. Then, for the discrete times \( t_i = i\Delta t \), we measure system characteristics such as the average velocity \( <v> \).

The symmetries of the equation of motion lead to the existence of nonstationary solutions called uniform sliding states. They are characterized by the fact that every odd-numbered (or even-numbered) atom performs the same motion, but is shifted in time. That is, \( x_{2n+1}(t) = x_{2n-1}(t + T_1) \) (or \( x_{2(n+1)}(t) = x_{2n}(t + T_2) \)) for \( n = 1, 2, \ldots \). It is clear that \( T_1 = T_2 \), \( v_1 = v_2 = v \), where \( v_1 \) and \( v_2 \) are the average velocities of the odd-numbered and the even-numbered atoms, respectively. Thus, we need only two dynamical hull functions, \( f_1 \) and \( f_2 \), to describe the motions of all atoms:

\[
x_{2n-1}(t) = \psi_0 + \psi + (2n - 1)\omega + vt + f_1[\psi + (2n - 1)\omega + vt],
\]

(3)
\[ x_{2n}(t) = \psi + 2n\omega + vt + \]

\[ f_2(\psi + 2n\omega + vt), \]  

\text{(4)}

where \( \psi_0 + \psi + (2n-1)\omega + vt \) and \( \psi + 2n\omega + vt \) are the positions of the \((2n-1)\)th and \((2n)\)th atoms for the case of \( K = 0 \). The dynamical hull functions \( f_1 \) and \( f_2 \) describe the modulations of the external potential to the atomic positions, \( \psi \) is an arbitrary phase, and \( \psi_0 \) is a constant phase. Because of the discrete translation symmetry of Eq. (1), the hull functions are periodic, and their periods may be any positive integer \( n_1 \); i.e.

\[ f_1(\varphi_{2n-1} + n_1) = f_1(\varphi_{2n-1}), \]  

\text{(5)}

\[ f_2(\varphi_{2n} + n_1) = f_2(\varphi_{2n}). \]  

\text{(6)}

It should be noted that \( f_1(\varphi_{2n-1} + n_1 - 1) \neq f_1(\varphi_{2n-1}) \) and \( f_2(\varphi_{2n} + n_1 - 1) \neq f_2(\varphi_{2n}) \) when we say the period is \( n_1 \). That is to say, uniform sliding states have infinite kinds of modes. This fact is of key importance in obtaining the complete resonance condition.

In the frame of the mass center which moves with the average sliding velocity \( v \), the external potential leads to a time-periodic force acting on the atoms. The frequency of this force, the so-called “washboard frequency,” is given by the velocity of the mass center divided by the period of the potential; i.e., \( \Omega_w = 2\pi v \). A resonance may occur if the washboard frequency \( \Omega_w \) and the eigenfrequencies \( \Omega_{p\pm} \) of the phonon satisfy the condition  

\[ k_1\Omega_{p+} = k_2\Omega_w \quad \text{or} \quad k_1\Omega_{p-} = k_2\Omega_w, \]  

where \( k_1 \) and \( k_2 \) are positive coprime integers. To see this and to find the eigenfrequencies \( \Omega_{p\pm} \) of the phonon, we (i) use the linear approximations  

\[ \sin\{2\pi[\varphi_{2n-1} + f_1(\varphi_{2n-1})]\} \approx \sin(2\pi\varphi_{2n-1}) + 2\pi \cos(2\pi\varphi_{2n-1})f_1(\varphi_{2n-1}) \]  

and  

\[ \sin\{2\pi[\varphi_{2n} + f_2(\varphi_{2n})]\} \approx \sin(2\pi\varphi_{2n}) + 2\pi \cos(2\pi\varphi_{2n})f_2(\varphi_{2n}), \]  

(ii) introduce the mean-field treatment, i.e., the term \( \cos(2\pi\varphi_j) \) is replaced by an averaged quantity  

\[ \beta = \lim_{T \to \infty} \frac{1}{T} \int_0^T \frac{1}{N} \sum_{j=1}^N \cos(2\pi\varphi_j) dt, \]  

\text{(7)}

(iii) consider a small vibration \( \varepsilon_j(t) \) of the atoms around their positions, and (iv) use the Fourier expansion
\[ f_1(\varphi) = \sum_{n_2} C_{n_2} \exp(i \frac{2\pi n_2}{n_1} \varphi), \]  
(8)

\[ f_2(\varphi) = \sum_{n_2} D_{n_2} \exp(i \frac{2\pi n_2}{n_1} \varphi). \]  
(9)

Finally, we obtain the resonance velocity

\[ v_\pm = \frac{n_1}{2\pi n_2} \left\{ \frac{1}{2m} \left[ (2 + K\beta)(1 + m) \pm \gamma \right] \right\}^{1/2}, \]  
(10)

where \( \left\{ \frac{1}{2m} (2 + K\beta)(1 + m) \pm \gamma \right\}^{1/2} = \Omega_p \), \( \gamma = [(2 + K\beta)^2(m - 1)^2 + 16m \cos^2 \left( \frac{2\pi n_2}{n_1} \omega \right)]^{1/2} \), and \( 2\pi v_\pm = \Omega_w \). It is clear that \( k_1/k_2 = n_1/n_2 \). This is a complete resonance velocity spectrum which relates only to the winding number, i.e., the commensurability, implies that the resonance is not a finite-size effect, but a discreteness effect. From Eq. (10), it is clear that the resonance behavior of the present model is very different from that of the standard driven FK model. For a given integer pair \( (k_1, k_2) \), the present model has two possible resonance states. For a given resonance state, the value of the average velocity \( v \) is fixed, so if the value of \( k_1 \) is fixed, then \( k_2 \) should have two possible values which correspond to the two cases where the “+” and “−” signs are taken. So one resonance state should be characterized by two integer pairs, \( (k_1, k_2) \) and \( (k_1, k'_2) \). That is to say, there are two kinds of resonance modes in one state.

When \( m = 1 \), we can reduce Eq. (10) to a simpler form:

\[ v_+ = \frac{n_1}{2\pi n_2} \sqrt{K\beta + 4 \cos^2 \left( \frac{\pi n_2}{n_1} \omega \right)}, \]

\[ v_- = \frac{n_1}{2\pi n_2} \sqrt{K\beta + 4 \sin^2 \left( \frac{\pi n_2}{n_1} \omega \right)}, \]  
(11)

where \( v_- \) is the real resonance velocity while \( v_+ \) is a fake one. From Eqs. (10) and (11), we can clearly find that the external potential not only leads to a periodic driving force but also leads to a modulation to the eigenfrequencies. In the high-velocity region, the standard FK model shows a behavior similar to that of the diatomic FK model. It is clear that \( E'_p = -\beta/(4\pi^2) = \lim_{T \to \infty} \frac{1}{T} \int_0^T E'(p) dt \) is the average external potential energy experienced
by an atom. In the following, we will see that the dependence of $E'_p$ on $F$ helps us to understand better the resonance steps.

Figure 1 shows the response of the average velocity $v$ of the system to the driving force $F$, where $\omega = 3/8$, $\eta = 0.1$, $K = 1$, $0 < F < 0.1$, $\Delta F = 0.001$, and the integral step $\Delta t = 0.01$. The line with solid squares and the dotted squares without a line are for the case of $m = 2$. The line with solid circles and the dotted circles without a line are for the standard FK model which is plotted for comparison. It is clear that for the diatomic FK model, each resonance state is characterized by two pairs of integers, $(k_1,k_2)$ and $(k_1,k'_2)$, which are for small and large atoms, respectively. The main property of a resonance step is characterized by one kind of resonance state, but some other resonance states may occur at the edges of the step. The ratio $k_1/k_2$ is always smaller than $k_1/k'_2$, which implies that the frequency of the small atom is larger than that of the large one. Figure 2 shows an example of the corresponding dynamical behavior in a resonance state for the case of $m = 2$, where $F = 0.015$. The thin line is for small atoms and the thick line is for large ones. The high peaks are due to hopping from one well to another well, and the low peaks are due to neighboring-particle hopping. In this case, the time between two neighboring high peaks for the thin line (or the thick line) equals the period of the washboard, and there are four small oscillations for the thin line and three small oscillations for the thick line, so the resonance state is characterized by $(1,4), (1,3)$.

Numerical results show that in the high-velocity region, the linear response of $v$ to $F$ is often punctuated by nonlinear response regions. Figure 3 shows an example for the response of $v$ to $F$ in the high velocity region, where only the process of increasing $F$ is shown: $m = 2$, $\omega = 1/8$, $\eta = 0.1$, $K = 1$, $\Delta F = 0.002$, and the integral step $\Delta t = 0.1$. It is clear that the linear response of $v$ to $F$ is punctuated by resonance steps which result from sub-harmonic resonances ($k_1 > k_2$). The distances between two successive nonlinear response regions are nearly equal. A nonlinear response region is usually composed of one large step and several smaller ones. The main resonance properties are characterized by the large step. There are two kinds of nonlinear response regions in the high-velocity region. The two kinds of
nonlinear response regions occur alternatively.

To understand better the resonant steps in the high-velocity region, in Fig. 4 we show the average external potential energy $E_p'$ experienced by an atom. The values of the parameters are same as those used for Fig. 3. From Figs. 4(a) and 4(b), we can easily find that $E_p'$ usually oscillates and has different properties for the two kinds of nonlinear responses, which correspond to two kinds of dynamical configurations of the moving chain. In one kind of the nonlinear response, the time-averaged value of $E_p'$ is higher than that in its vicinity. In the other kind of nonlinear response, the time-averaged value of $E_p'$ is lower than that in its vicinity. Other interesting phenomena are the facts that the average kinetic energy $E_k$, the average interparticle potential $E_p$, and $E_p'$ are all constants in the cases of $F = 1.5, 3.0, 4.5, 6.0, \cdots$, which implies that the moving chain does not feel the existence of the external potential in these cases. The results given in this letter also can be used to describe an dc-biased one-dimensional Josephson-junction array.

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Fig. 1. Response of the average velocity $v$ of the system to the driving force $F$ for increasing $F$, where $\omega = 3/8$, $\eta = 0.1$, $K = 1$, $0 < F < 0.1$, $\Delta F = 0.001$, and the integral step $\Delta t = 0.01$.

Fig. 2. Dynamical behavior in a resonance state, where $m = 2$, $F = 0.015$. The thin line is for small states, and the thick line is for large ones. The high peaks are due to hopping from one well to another well, and the low peaks are due to neighboring-particle hopping. In this case, the time between two neighboring high peaks for the thin line (or the thick line) equals the period of the washboard. There are four small oscillations for the thin line and three small oscillations for the thick line, so the resonance state is characterized by $(1,4)$, $(1,3)$.

Fig. 3. Response of the average velocity $v$ of the system to the driving force in the high velocity region, where only the process of increasing $F$ is shown, $m = 2$, $\omega = 1/8$, $\eta = 0.1$, $K = 1$, $\Delta F = 0.002$, and the integral step $\Delta t = 0.1$.

Fig. 4. Average external potential energy $E'_p$ experienced by an atom. The values denoted in the figure are for the external force. The values of the parameters are the same as those used for Fig. 3.
dc-driven FK model, $\omega=3/8, \eta=0.1, K=1$
\[ m=2, \omega=\frac{3}{8}, K=1, \eta=0.1, F=0.015, T_w=14.75, (1,4), (1,3) \]
This process is for a diatomic FK chain and an increasing driving force, where $m=2$, $\omega = 1/8$, $\eta=0.1$, $K=1$, $\Delta F=0.002$, $\Delta t=0.1$. 
