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The dynamic characters of excitations in a one-dimensional Frenkel–Kontorova model*

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A one-dimensional (1D) Frenkel–Kontorova (FK) model is studied numerically in this paper, and two new analytical solutions (a supersonic kink and a nonlinear periodic wave) of the Sine–Gordon (SG) equation (continuum limit approximation of the FK model) are obtained by using the Jacobi elliptic function expansion method. Taking these new solutions as initial conditions for the FK model, we numerically find there exist the supersonic kink and the nonlinear periodic wave in these systems and obtain a lot of interesting and significant results. Moreover, we also investigate the subsonic kink and the breather in these systems and obtain some new feature.

Keywords: Sine–Gordon equation, Frenkel–Kontorova model, kink, breather
PACC: 4610, 4630L, 4660D

1. Introduction

More than 60 years ago, Frenkel and Kontorova introduced a simple model which has become very popular in many branches of solid state physics and nonlinear physics. They developed a model in order to describe the motion of a dislocation in a crystal. Meanwhile, the Frenkel–Kontorova (FK) model has also become a model for an adsorbate layer on the surface of a crystal, for ionic conductors, for glassy materials, for charge-density-wave (CDW) transport, and for chains of coupled Josephson junctions. Especially, a number of current researches, such as sliding friction,[1−8] heat conduction,[9−13] chaos control[14,15] and nonlinear coupled pendulum[16] are also carried out with the help of the model.

The standard FK model describes a chain of particles that are interacting with the nearest neighbours and subjected to a periodic substrate potential. The essential physical feature of the model consist of the competition between these two types of interactions: one is favourable for a uniform separation among particles and the other tends to pin the atom positions to the bottom of the substrate wells. This competition, often referred to as frustration or, more specifically, length scale competition, results in a rich complexity of spatially modulated structures. The model and its generations have been extensively explored over the past few decades.[17−21] The dynamics of diverse FK models has also aroused the remarkable interest in the recent years. Zolotaryuk and Salerno investigated the damped and the ac driven one-dimensional (1D) FK models, showing that if the driving field broke certain time–space symmetries, the kink could perform a unidirectional motion.[22] In the overdamped case, Hu and Tekić[23] first examined the dynamics in a commensurate structure of the 1D periodically driven FK model subjected to a parametrized deformable periodic substrate potential, and drew a conclusion that when the shape of the substrate potential started to deviate from the standard one, new subharmonic steps appeared in a response function even in the structures with an integer value of average interparticle distance, while the critical depinning force can even decrease for some values of system parameters. Then, they studied the dependence of amplitude on frequency for dynamical mode locking phenomena under the drive of dc and ac forces and found that the Shapiro steps and the critical depinning force exhibited very complex behaviour.[24] Besides 1D map, Tekić *et al*[25] also studied the nonlinear dc response of a two-dimensional (2D) underdamped system of interacting atoms sub-

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jected to an isotropic periodic external potential with a triangular symmetry. Furthermore, among a variety of behaviours of the lattice nonlinear dynamics, some attention was concentrated on the so-called "discrete breather" (DB). For example, Zueco *et al* studied numerically synchronization phenomena of mobile discrete breathers in dissipative nonlinear lattices periodically forced, and gave an explicit dynamic picture of the relation between the breather speed and the drive force.[26]

In the continuum limit approximation, which can be used for a large number of coupled elements, the FK model can be reduced to the well-known Sine–Gordon (SG) equation

$$u_{tt} + \sin u = u_{xx}, \tag{1}$$

which allows exact solutions describing different types of nonlinear waves. As is well known, elementary excitations of an SG system are kinks, breathers and phonons. In general, the SG kink has the following form:

$$u(x,t) = 4\arctan\left[\exp\frac{\pm(x - v_{\rm kink}t)}{\sqrt{1 - v_{\rm kink}^2}}\right], \tag{2}$$

where $v_{\rm kink}$ is the kink speed which is measured in units of the sound speed c in the chain, and the signs $\pm$ correspond to kink and antikink configurations, respectively. As can be seen from Eq.(2), the kink cannot propagate with a speed large than sound speed c because of Lorentz contraction of kink's width, d ($d = \sqrt{1 - v_{\rm kink}^2}$), i.e. it is subsonic. The breather has the form

$$u(x,t) = 4\arctan\left[\frac{\sqrt{1-\Omega^2}}{\Omega}\sin(\Omega t)\,\mathrm{sech}\left(x\sqrt{1-\Omega^2}\right)\right]. \tag{3}$$

However, due to the discreteness effects, the FK system can present different nonlinear dynamic features compared with the SG model. The SG kink can move freely through the chain without loss of their energy for dissipation but the FK kink cannot. In the SG model, the breather describes a nonlinear oscillating state with an internal frequency, however exact time-periodic space-localized solutions are absent in the FK model. Moreover, other type of nonlinear waves such as peaked solitary wave and saw-tooth wave can exist in the SG system, while in the FK model there are no such waves.

In spite of a number of studies of spatiotemporal dynamics of the FK model, they are all about subsonic kink. In fact, as will be shown in Section 2.1 of the present paper, the supersonic speed kink does also exist in the SG model. Of course, the exploration of this kink in the FK model is still lacking. Moveover, for an integrable SG model, any localized excitation can be presented as an asymptotic superposition of elementary excitations of three kinds, i.e. kinks, breathers and phonons. The nonlinear periodic solution of the SG equation can also be found explicitly, for example, a chain of kinks is given by Eq.(12) in Section 2.2. And in the FK chain, for this nonlinear periodic wave, no studies have been found till now. So it is our task in this paper to obtain the supersonic kink solution and the nonlinear periodic wave solution for SG equation, and then explore the dynamic features of the two excitations in different FK systems. The subsonic and the breather are also studied by using the FK model. Our results accord with Braun's explorations[17] in the ground state. Furthermore, we find some new issues, when we consider the peculiar anharmonic interaction between atoms.

2. New excitations in SG equation

Due to the wide application of SG equation, many solutions to it have been obtained in different functional forms, such as 'arctan cosh', 'arctan tanh', 'arctan sech', 'arctan sn' and so on. In this paper, we follow the method of Liu *et al*[27] to gain two new solutions (supersonic kink and nonlinear periodic wave) for the SG equation.

2.1. Supersonic kink (antikink)

We can use the transformation $\xi = \frac{1}{2}(x - t)$ and $\eta = \frac{1}{2}(x + t)$ to reduces SG equation (1) to the form

$$u_{\xi\eta} = \sin u. \tag{4}$$

In order to solve Eq.(4), we introduce the transformation $u = 2\sin^{-1} v$ or $v = \sin\frac{u}{2}$, and rewrite Eq.(4) as

$$(1 - v^2)v_{\xi\eta} + vv_\xi v_\eta - v(1 - v^2)^2 = 0. \tag{5}$$

Equation (5) can be solved in the frame

$$v = v(\zeta) \qquad \text{and} \qquad \zeta = k(\xi - c\eta). \tag{6}$$

Substituting expression (6) into Eq.(5), we have

$$k_2 c(1 - v^2)\frac{\mathrm{d}^2 v}{\mathrm{d}\zeta^2} + k^2 cv\left(\frac{\mathrm{d}v}{\mathrm{d}\zeta}\right)^2 + v(1 - v^2)^2 = 0, \tag{7}$$

which can be solved directly by using the Jacobi elliptic function expansion method. The ansatz solution can be written as

$$v = a_0 + a_1 \mathrm{sn}\zeta, \tag{8}$$

where $\mathrm{sn}\zeta$ is the Jacobi elliptic sine function. Substituting expression (8) into Eq.(7), we can determine a_0 and a_1. When $\mathrm{sn}\zeta$ modulus $m \to 1$, we obtain the supersonic kink (antikink) solution to Eq.(1) as follows:

$$u(x,t) = \pm 2 \arcsin \tanh[k_{\mathrm{kink}}(x - v_{\mathrm{kink}}t)], \tag{9}$$

where $k_{\mathrm{kink}} = \dfrac{k^2-1}{2k}$ and $v_{\mathrm{kink}} = \dfrac{k^2+1}{k^2-1}$ are wave number and wave speed of the kink respectively, and the signs $\pm$ correspond to kink and antikink configurations, respectively.

2.2. Nonlinear periodic wave

For Eq.(4), if we introduce another transformation $u = 2\arctan v$ or $v = \tan\dfrac{u}{2}$, Eq.(4) will reduce to the form

$$(1+v^2)v_{\xi\eta} - 2vv_\xi v_\eta - v - v^3 = 0. \tag{10}$$

In the travelling wave frame of expression (6), Eq.(10) can be rewritten as

$$k_2 c(1+v^2)\frac{\mathrm{d}^2 v}{\mathrm{d}\zeta^2} - 2k^2 cv\left(\frac{\mathrm{d}v}{\mathrm{d}\zeta}\right)^2 + v + v^3 = 0. \tag{11}$$

For Eq.(11), the formal solution obtained by using the Jacobi elliptic function expansion method can also be written as expression (8). Similarly, the expansion coefficients can be determined, and nonlinear periodic wave for Eq.(1) can be obtained as

$$u(x,t) = 2\arctan[m\mathrm{sn}[k_{\mathrm{wave}}(x - v_{\mathrm{wave}}t), m]], \tag{12}$$

where $k_{\mathrm{wave}} = \dfrac{k^2 - k^2m^2 - 1}{2k(1-m^2)}$ and $v_{\mathrm{wave}} = \dfrac{k^2 - k^2m^2 + 1}{k^2 - k^2m^2 - 1}$ are wave number and wave speed respectively. sn is the Jacobi elliptic sine function and m is its modulus.

3. Dynamic characters of excitations in 1D FK model

We consider the damped FK model with a peculiar anharmonic interatomic interaction and a sinusoidal substrate potential at zero temperature. So the motion equation takes the following form:

$$\begin{aligned} &\ddot{u}_i + \gamma\dot{u}_i + \sin u_i \\ &= K(u_{i+1} - 2u_i + u_{i-1}) \\ &\quad + K'\left[(u_{i+1} - u_i)^2 - (u_i - u_{i-1})^2\right], \end{aligned} \tag{13}$$

where u_i denotes the position of the ith element in the chain, γ is the coefficient of the external viscous damping, K is the elastic constant of harmonic interaction between the nearest-neighbouring atoms and K' is the anharmonicity parameter of interaction between the nearest-neighbouring atoms. Throughout the paper we use a dimensionless system of units and assume that the atomic mass $m_{\mathrm{a}} = 1$. For such a complex system we cannot obtain the exact solutions from this model, so we use a numerical method to obtain the approximate solutions for the given boundary condition and the initial condition. Here we follow the method given by Currie *et al*,[28] therefore we take an excitation of SG model with some initial speed as an initial configuration to obtain the approximate solution for the FK model. The forth-order Runge–Kutta integration algorithm is implemented to solve the equations of motion and the time steps are adjusted according to the numerical accuracy.

3.1. Subsonic kink (antikink)

First, we study the standard FK model. For this model, a free moving subsonic kink (antikink) will turn immediately into a moving localized kink (LK) due to emission of phonon wave packets with loss of its energy for dissipation. For a moving LK, due to the competition between the coupling and the periodic potential, the array oscillates during its drift on the substrate, leading to continuous emission of phonon wave packets. Under certain conditions, the kink motion and emitted phonon wave packets may become phase-locked, forming quantized speeds. Then, due to loss of more energy caused by phonon emission, the kink will be pinned by the Peierls–Nabarro (PN) potential and becomes an LK. In Fig.1(a), we give the evolution of the average kinetic energy $\varepsilon_{\mathrm{p}}(t) = \dfrac{1}{N}\sum_{i=1}^{N}(v_i^2/2)$ of the moving subsonic kink of expression (2) with an initial speed (v_0) of $0.8c$ in the FK chain when $K = 0.5625$, $\gamma = 0$ and $K' = 0$. As can be seen from Fig.1(a), for $t < t_1$, the average kinetic energy loses at a very high rate, so

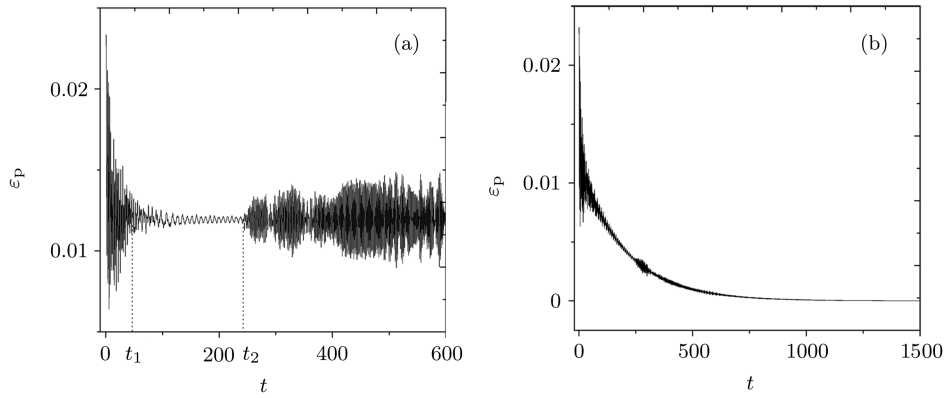


Fig.1. The evolution of the average kinetic energy $\varepsilon_p(t)$ of the moving subsonic kink of expression (2) at an initial speed (v_0) of $0.8c$ in the FK chain, with $K = 0.5625$, $\gamma = 0$ and $K' = 0$ and the evolution of the average kinetic energy $\varepsilon_p(t)$ of the moving subsonic kink of expression (2) at an initial speed (v_0) of $0.8c$ in the FK chain (b), with $K = 0.5625$, $\gamma = 0.005$ and $K' = 0$.

that this condition does explain phonon emission from the moving kink. However, at the moment t_1 the first-order resonance disappears and the emission-induced damping is now caused by the second-order resonance, so that the value of the effective friction is abruptly lowered. Correspondingly, the kink radiation becomes drastically smaller, and the average kinetic energy decreases now much more slowly. Then the free kink becomes a moving LK. At the moment t_2, the second-order resonance condition becomes invalid, and for $t > t_2$ emission of phonons by the kink should increase, so subsequently the kink will be trapped by the PN potential and becomes an LK. In Ref.[17], the motion of subsonic kink in a standard map was illuminated by the evolution of the kink speed, here our interpretation is similar to that in Ref.[17].

Second, we study the standard damped FK model. The evolution of the average kinetic energy of the kink of expression (2) in the damped standard FK model ($K = 0.5625$, $\gamma = 0.005$ and $K' = 0$) is shown in Fig.1(b). Obviously $\varepsilon_p(t)$ decays to zero. It means that due to the damp, the moving kink immediately reduces its speed down to zero and reaches a stationary state without any phonon emission.

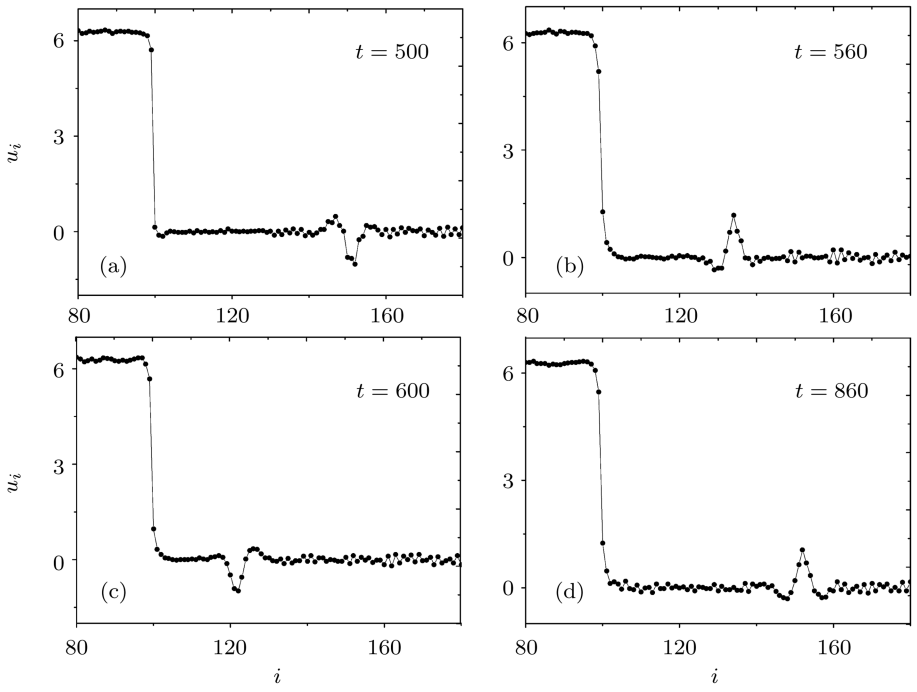


Fig.2. Shapes of the moving localized antikink of expression (2) with an initial speed (v_0) of $0.8c$ in the FK chain at different time moments for $K = 0.5625$, $\gamma = 0$ and $K' = 0.075$.

Third, we study the anharmonic FK model. In the generalized FK model, where the interatomic interaction is anharmonic, some new features may appear. Recall that the main effect of anharmonicity gives rise to the violation of the kink–antikink symmetry, then we will find that when $K' > 0$, the antikink of expression (2) moves more slowly than the kink of expression (2). So in the anharmonic FK model, the motion of subsonic antikink is similar to that described above in the standard FK model, but it is trapped by the PN potential much earlier. Moveover, under some certain conditions, additional excitations with frequencies outside the phonon spectrum can appear for the antikink of expression (2) due to anharmonicity of the intertomic interaction. For example, the moving localized antikink can excite a moving long-living breather mode at its head when its motion and its emission becomes phase-locked (see Fig.2). However, for the kink of expression (2), we find that at the beginning the pure phononic (nonlocalized) mode emerges in its tail, but the degree of the phonon localization increases with its propagation. So the oscillation in the kink tail becomes more and more irregular, and finally this localization leads the system to sharply turn into a running state.

3.2. Supersonic kink (antikink)

In fact, the additional shape modes may appear due to the deviation of substrate potential from the sinusoidal form, due to anharmonicity of the interatomic interaction, and even solely due to discreteness effects. Moveover, the additional shape modes are excited by phonons either simultaneously or separately. It should be noted that the kink shape will strongly affect the final results as can be seen below.

First, in the standard FK model, if we start from the supersonic kink (antikink) of expression (9) with an initial speed, such a kink can propagate through the chain without any emission for some time, then a discrete breather will appear at the tail of it. This breather does not move with the kink, but its amplitude increases (see Fig.3(a)). At a high amplitude of its vibration it may decay into a kink–antikink pair, then the subsequent collision between newly created kink and antikink leads to a sharp transition to a running state. Figure 3(b) shows the evolution of the average kinetic energy $\varepsilon_{\rm p}(t)$ of the fast moving kink of expression (9) in the standard FK chain when $K = 2$. For $t < t_1$, the kink propagates through the chain without any emission, so its average kinetic energy keeps constant; At the moment t_1, the kink begins to excite the discrete breather at its tail. And when $t_1 < t < t_2$, the amplitude of the breather increases immediately, so the average kinetic energy of the kink increases at a very high rate. At the moment t_2, the breather decays into a kink–antikink pair, and for $t > t_2$, the system turns into a running state. Correspondingly, the evolution of the average kinetic energy becomes irregular.

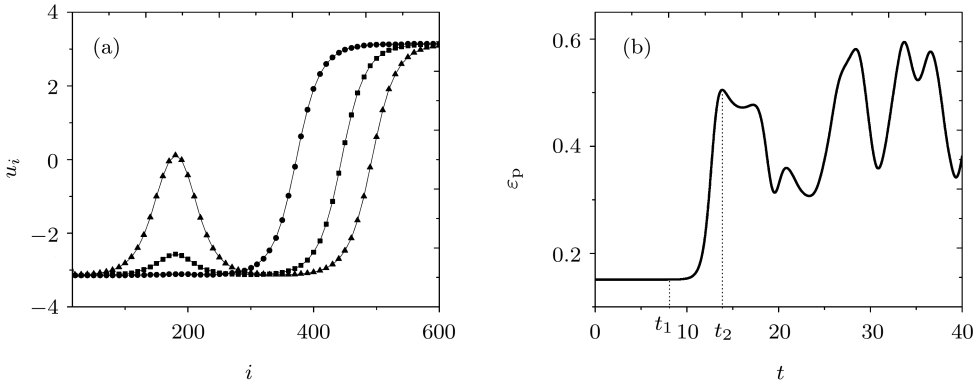


Fig.3. (a) Shapes of the fast moving kink of expression (9) in the standard FK chain at different time moments for $K = 2$, where circled, squared and triangled lines denote the time moments being 8, 11 and 13 respectively, and (b) the evolution of the average kinetic energy of the kink in Fig.3(a).

Second, if we consider the effect of external viscous damping, the shape of the kink of expression (9) in this FK chain is essentially changed compared with that in the standard FK model. As can be seen from Fig.4(a), the breather appears in the middle of the kink but not at the tail of it. Moveover, as shown in Fig.3(b), the time for the kink moving without any emission and the time before the system turning into

a running stat are shorter than those in the standard FK model. Owing to damping, the average kinetic energy decreases when the kink moves without any emission, therefore it will decay to zero when $t \to \infty$.

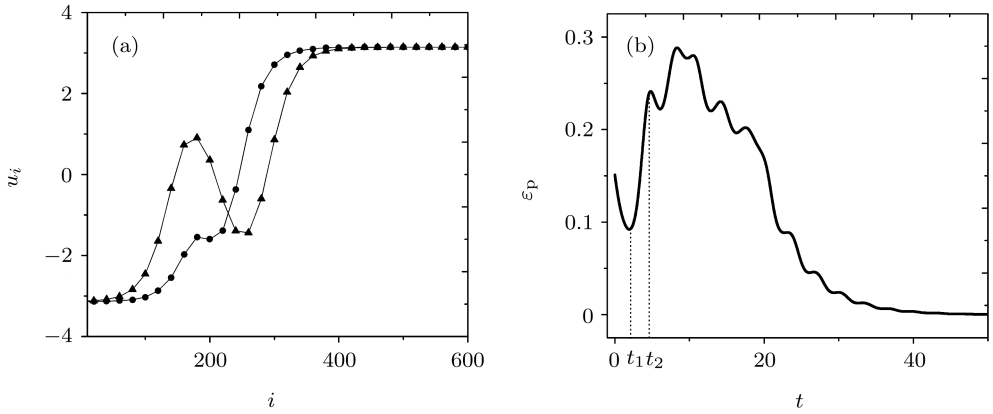


Fig.4. (a) Shapes of the fast moving kink of expression (9) in the standard damped FK chain at different time moments for $K = 2$ and $\gamma = 0.2$, where for circled and triangled lines denote the time moments being 3 and 5 respectively, and (b) the evolution of the average kinetic energy of the kink in Fig.4(a).

Third, we find that in the anharmonic FK model, the shape of the kink is similar to that in the standard FK chain. But the creation and the destruction of the breather are much earlier than that in the standard FK chain due to the effect of anharmonicity.

3.3. Nonlinear periodic wave

We have discussed the single kink in the FK model above. Now we focus on a train of equidistant kinks (nonlinear periodic wave) in the FK model. First, in the standard FK model, as seen in Fig.5, the shape of the periodic wave of expression (12) is modified by the lattice discreteness, and the wave will decay slowly. Second, in the standard damped FK chain, the periodic wave of expression (12) can keep its shape, but its amplitude will become smaller and smaller. (see Fig.6). Third, in the anharmonic FK model, the propagation behaviour of the periodic wave is the same as that of standard chain, but the anharmonicity may speed up the destruction of a kink.

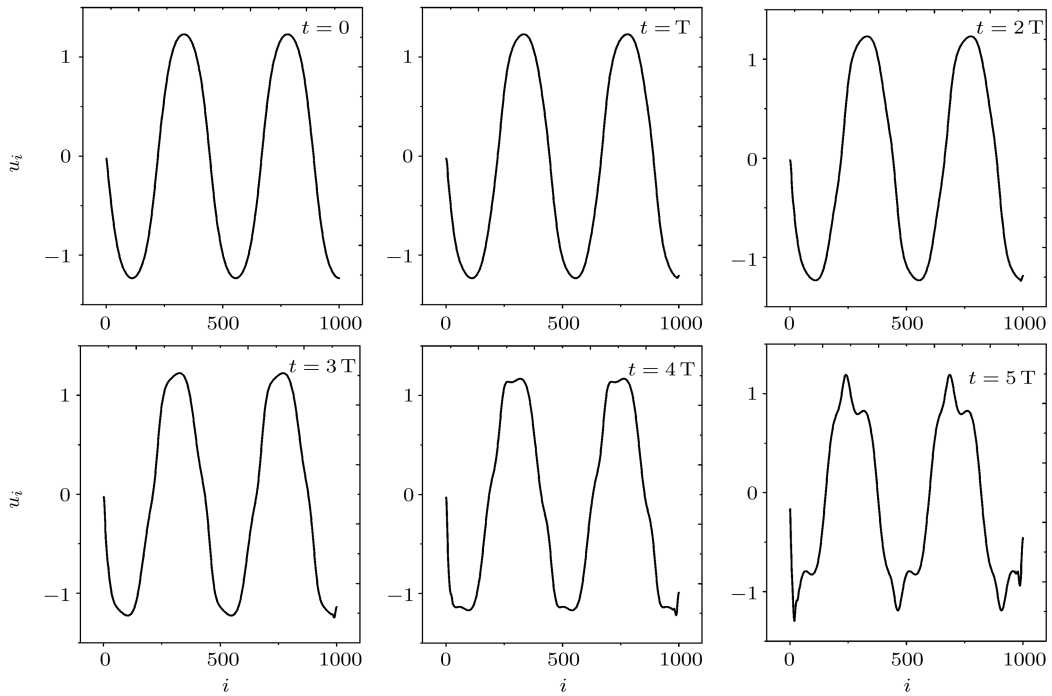


Fig.5. Shapes of the nonlinear periodic wave of expression (12) in the standard FK chain at different time moments for $K = 2$.

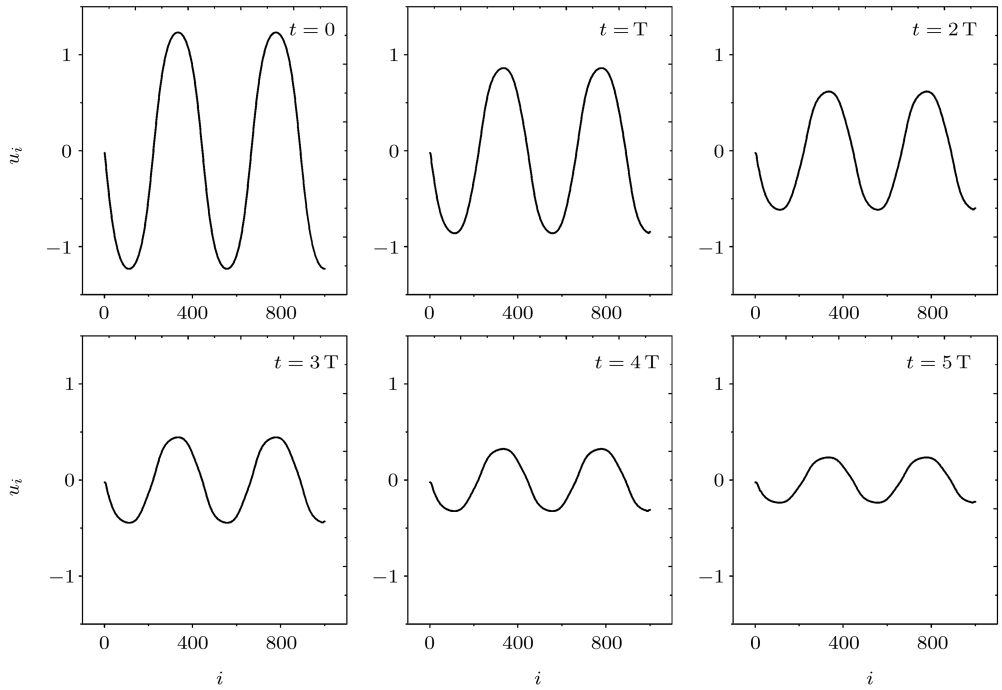


Fig.6. Shapes of the nonlinear periodic wave of expression (12) in the standard damped FK chain at different time moments for $K = 2$ and $\gamma = 0.1$.

3.4. Kink collision

In the preceding discussion, we considered the cases in which there was only one kink in the system. If the system contains several kinks (antikinks) simultaneously, they may collide with each other at some time. The SG equation is exactly integrable, i.e. it allows elastic interactions between all the excitations, and there appear only phase shifts for such collisions, so kinks can be treated as nonlinear quasi-particles in the SG model. However, in the FK model, due to the lattice discreteness, the interactions between excitations are not elastic, therefore some new features may appear, e.g. kink of expression (2) and antikink of expression (2) may collide inelastically, producing a long-lived breather mode, and the total topological charge of the system is conserved. This phenomenon has been mentioned in Ref.[17], and here we give a visual picture (see Fig.7). But if the effect of the model

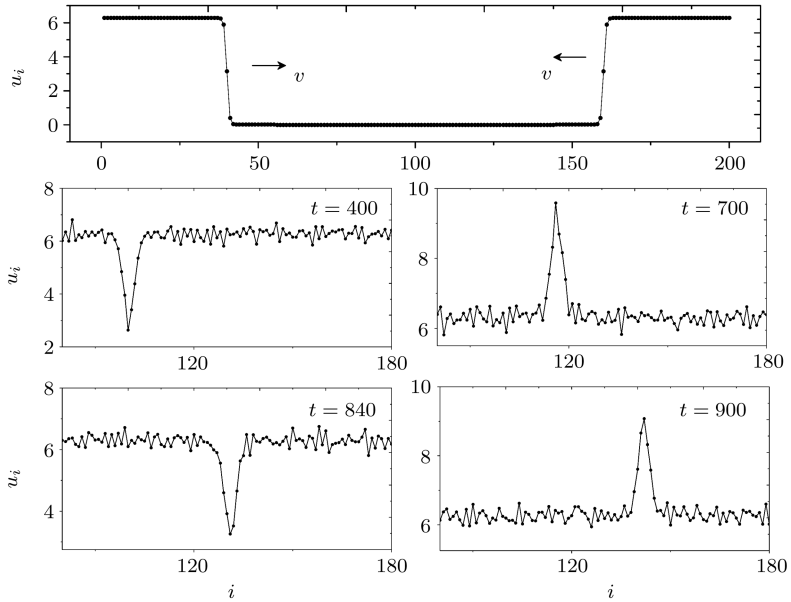


Fig.7. Shapes of the moving long-lived breather which is produced by the collision between kink of expression (2) and antikink of expression (2) in the standard FK chain at different time moments for $K = 1$.

discreteness is small, kinks can be treated as deformable quasi-particles, i.e. their shape is modified by the lattice discreteness and their motion can be described with the help of effective nonlinear quasi-particles approximately. For example, when the kink of expression (2) is reflected by the edge of the chain, it behaves like a particle (see Fig.8). However, in the anharmonic FK model, once the kink moves close to the boundary of the chain, the reaction between them may lead to a sharp transition to a running state.

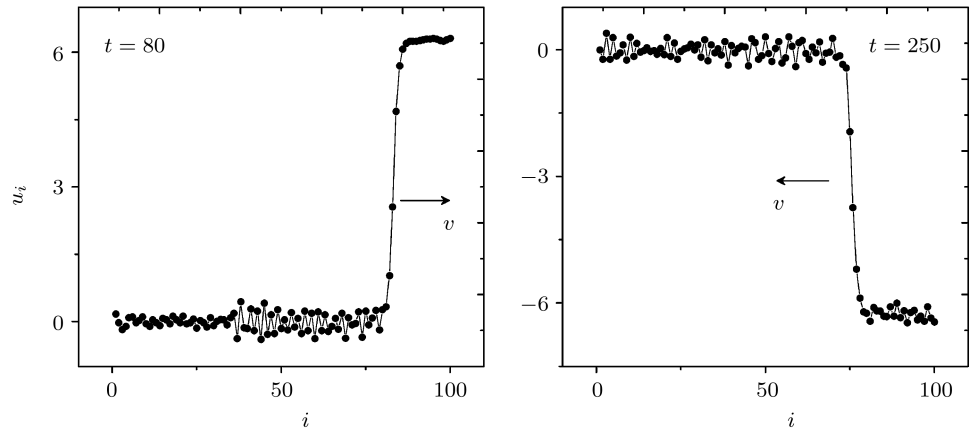


Fig.8. Shapes of the kink of expression (2) before and after it has been reflected by the edge of the chain in the standard FK chain for $K = 1$.

3.5. Breather

Finally, we discuss the dynamic features of the breather of expression (3) in the standard FK model. As shown in Fig.9, being the same as the kink of expression (2) in the FK model, the breather also emits phonon wave packets due to lattice discreteness which acts as an external perturbation and breaks the integrability of the SG model, and finally this emission leads the breather to decay. This result accords with the description in Ref.[17] well.

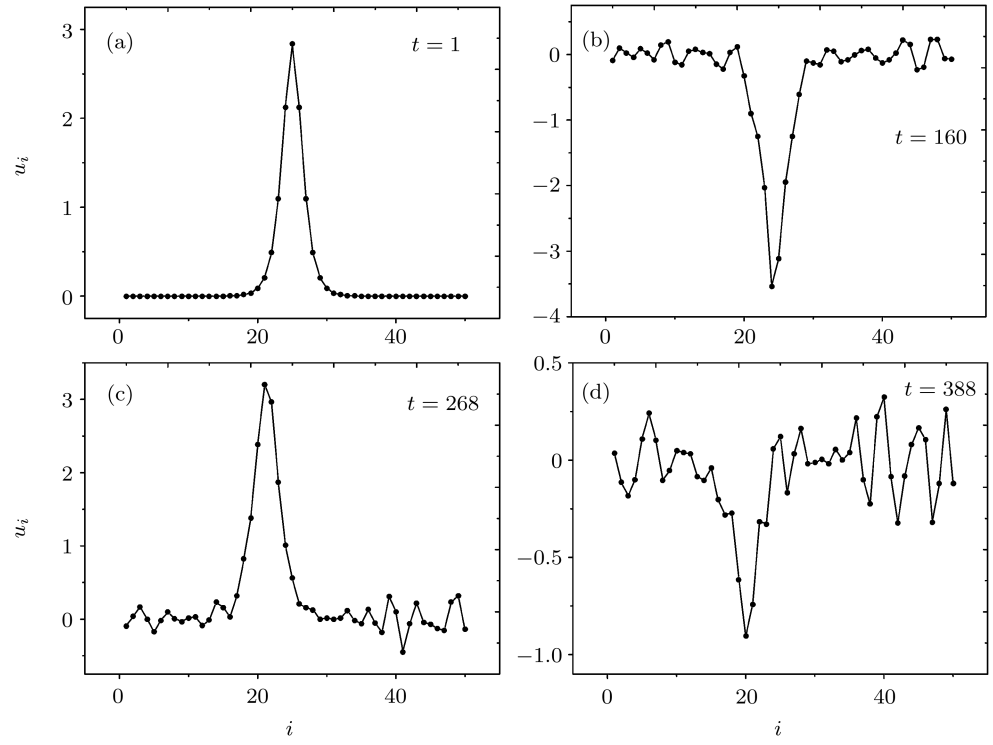


Fig.9. Shapes of the breather of expression (3) in the standard FK chain at different time moments for $K = 1$.

4. Conclusion

We have studied the dynamics of several excitations in three different FK models (standard, standard damped, and anharmonic FK models). We can know clearly that due to the discreteness effects, the dynamic characters of the excitations in the FK models differ essentially from those in the SG model. Compared with the SG model, the FK model has more interesting and important features. According to the discussion above, we can summarize as follows: when the model deviates from the exactly integrable one, the excitation shape deviates from the SG form. So the excitation emits phonon wave packets, even some excitations (e.g. kinks) may excite additional shape modes with frequencies outside the phonon spectrum. Moveover, damping and anharmonicity may greatly affect the characters of the excitations, even some new features may appear in the damped or anharmonic FK model.

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