Supersonic and multiple topological excitations in the driven Frenkel-Kontorova model with exponential interaction

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The criteria for the existence of supersonic and multiple topological excitations (kinks) in the driven Frenkel-Kontorova model (a chain of atoms placed into an external periodic potential) with anharmonic (exponential) interatomic interactions are studied.

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I. INTRODUCTION

Topological excitations play a very important role in system dynamics, because they are responsible for mass and charge transport in solids and on crystal surfaces. As classical examples, one can mention dislocations described by the Frenkel-Kontorova (FK) model [1], where the topological excitations correspond to kinks that describe local compression or expansion of a commensurate structure. The FK model has numerous applications in superionic conductivity, surface physics, hydrogen-bonded chains, Josephson junctions, tribology, etc. (e.g., see [2] and references therein).

In the continuum limit approximation, the equation of motion of the FK model reduces to the exactly integrable sine-Gordon (SG) equation. But in continuum models, even in a model with anharmonic (but local) interaction, the topological excitations are always subsonic, the kink cannot propagate with a velocity v larger than the sound speed c because of Lorentz contraction of kink's width. Moreover, in the classical FK model, the kinks of the same topological charge repel from one another and, therefore, they cannot carry a multiple topological charge.

However, simulation demonstrates that supersonic kinks as well as multiple kinks do exist. For example, Fig. 1 shows the propagation of supersonic single and double kinks in the FK model with exponential interatomic interaction. The motion of topological solitons with *supersonic* velocities was firstly predicted, to the best of our knowledge, analytically by Kosevich and Kovalev [3] in the FK model with some specific interatomic interaction in the continuum limit approximation. Later, supersonic topological solitons were observed by Bishop *et al.* [4] in molecular dynamics study of polyacetylene. Then the supersonic kinks were studied numerically in the discrete FK model with anharmonic interaction by Savin [5]. It was shown that for certain supersonic kink velocities, when its width coincides with that of the corresponding Toda soliton [6], the kink propagates almost without energy losses. *Multiple* fast (but subsonic) kinks were firstly observed numerically by Peyrard and Kruskal [7] in the classical highly discrete FK model. Alfimov *et al.* [8] have shown that multiple kinks exist also in continuum systems with *nonlocal* interaction. The bounded states of kinks (subsonic as well as supersonic) in the case of anharmonic interaction were also studied numerically by Zolotaryuk *et al.* [9]. It was found that these multiple kinks are asymptotically unstable. The dynamics of the generalized FK chain *driven* by a dc external force was studied numerically in [10,11], where we observed the existence of supersonic kinks and multiple (double and triple at least) kinks. Recently, the existence of multiple kinks for certain kink velocities in the *discrete* FK-type model was proven rigorously [12].

The aim of the present paper is to find the criteria for the existence of supersonic and multiple topological excitations in the FK-type models. We will show that, first, the model must be *discrete* as was already mentioned above. Second, because kink's motion in a discrete chain is damped due to radiation of phonons, we must apply *a driving force* to support the motion (this point was lost in the previous studies [3–5,7–9]). Third, the interatomic interaction must be *anharmonic*. Under these three conditions, the model admits both *supersonic kinks* and *multiple kinks*.

The paper is organized as follows. The model is introduced in Sec. II. Then in Sec. III the problem is studied with

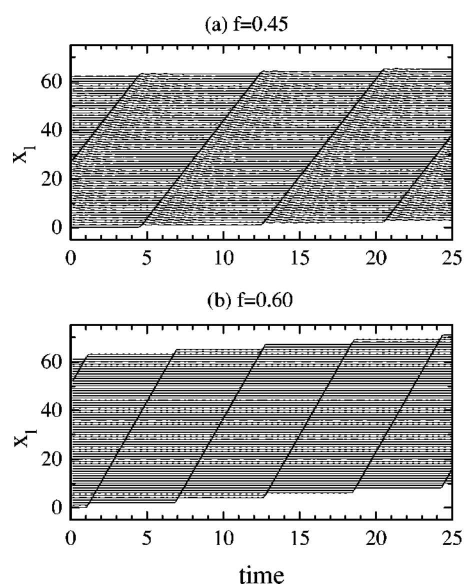

FIG. 1. Atomic trajectories of the FK model with exponential interaction for $\beta = 1/\pi$, $g = 1$, and $\eta = 0.05$. (a) The single supersonic kink, $f = 0.45$, $v_k/c \approx 1.28$, and (b) the double kink, $f = 0.60$, $v_k/c \approx 1.75$.

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the help of the continuum limit approximation. We show that if the discreteness effects are properly taken into account, the model formally allows both supersonic kinks and multiple kinks. Moreover, we prove that for a given set of parameters the model admits either the single-kink solution or the double-kink solution, but not both solutions simultaneously. Numerical solution of the corresponding ordinary differential equation, which can be obtained with any desired accuracy, does show the existence of supersonic and multiple kinks. In Secs. IV and V we develop an approximate variational approach that helps to find the conditions for existence of supersonic and multiple kinks. We show that supersonic kinks may exist in the model with anharmonic interaction only, and the multiple kinks may be stable for supersonic velocities only. These conclusions are confirmed by simulation. Finally, Sec. VI concludes the paper with the comment that supersonic kinks and multiple kinks may be considered as ''disturbed'' Toda solitons.

II. MODEL

We consider the chain of atoms placed into the sinusoidal substrate potential and driven by a dc force f applied to all atoms, so that the equation of motion is

$$\ddot{x}_l(t)+\eta\dot{x}_l(t)+\frac{\partial}{\partial x_l}[V(x_{l+1}-x_l)+V(x_l-x_{l-1})]+\sin x_l(t)-f=0, \tag{1}$$

where x_l is the coordinate of the lth atom, η is the external viscous damping coefficient introduced to compensate the driving force, and

$$V(x)=V_0\exp(-\beta x) \tag{2}$$

describes the exponential repulsion between nearest neighboring atoms. We assume periodic boundary conditions with the number of atoms $N=N_s+p$, where N_s is the number of wells of the periodic potential, so we have one multiple p kink (p excessive atoms) inserted into the commensurate structure. Similarly, to the Toda model [6], one may add also an attractive linear interaction, so that the interaction reduces to the harmonic one in the limit $\beta\rightarrow 0$ (the classical FK model) and to the hard-core interaction in the opposite limit $\beta\rightarrow\infty$. Throughout the paper, we use the dimensionless system of units, where the atomic mass is $m=1$, the period of the external potential is $a=2\pi$ and its amplitude is $\varepsilon=2$. In these units, a characteristic frequency of atomic vibration at a minimum of the external potential is $\omega_0=1$, a characteristic time scale is $\tau_0=2\pi$, and the maximum value of the external dc force, when the minima of the sinusoidal substrate potential disappear and the topological excitations cannot exist anymore, is $f=1$.

III. CONTINUUM APPROXIMATION

The systematic procedure to derive the equation of motion in the continuum limit starting from the discrete lattice was proposed by Rosenau [13]. For the anharmonic FK model (1) it leads, in the first order of the discreteness parameter, to the equation

$$\ddot{u}+\eta\dot{u}-d^2u''(1-\alpha du')+\sin u-f-h^2[\ddot{u}''+(u')^2\sin u-u''\cos u]=0, \tag{3}$$

where $d=a\sqrt{g}$ is the width of the static kink, g is the elastic constant defined as $g=V''(a)=V_0\beta^2\exp(-\beta a)$, the anharmonicity parameter α is defined as

$$\alpha=-\frac{a}{d}\frac{V'''(a)}{V''(a)}=\frac{\beta}{\sqrt{g}}, \tag{4}$$

and the parameter $h^2=a^2/12=\pi^2/3$ describes the discreteness effects. Looking for a traveling-wave solution of Eq. (3) in the form $u(x,t)=u_{\rm k}(x-vt)\equiv u_{\rm k}(z)$, we obtain the equation

$$h^2v^2u_{\rm k}''''+(c^2-v^2-h^2\cos u_{\rm k})u_{\rm k}''+h^2(u_{\rm k}')^2\sin u_{\rm k}-\alpha d^3u_{\rm k}''u_{\rm k}'+\eta vu_{\rm k}'-\sin u_{\rm k}+f=0, \tag{5}$$

where $c=2\pi\sqrt{g}$ is the sound speed (in our system of units $c=d$).

Although the traveling-wave ansatz may be too crude due to radiation of phonons by the moving kink [e.g., see Fig. 1(a)], Kink's asymptotic can be found with the help of Eq. (5) rigorously, because the radiation has to decay due to nonzero damping coefficient η in the model under consideration. At $z\rightarrow\infty$, substituting $u_{\rm k}(z)-u_f\propto\exp(-z/d_1)$ into Eq. (5), we obtain for the kink width $d_1(v)$ the equation

$$d_1^4\cos u_f+d_1^3\eta v-d_1^2(c^2-v^2-h^2\cos u_f)=(hv)^2, \tag{6}$$

where $\cos u_f=(1-f^2)^{1/2}$. Similarly, we can find the tail asymptotic behind the kink, $u_{\rm k}(z)-(u_f+2\pi p)\propto\exp(z/d_2)$ at $z\rightarrow-\infty$; the width $d_2(v)$ has to satisfy the same equation (6) but with $v\rightarrow -v$. One can see that at low velocities, $|v|\ll c$, the discreteness effects lead to a decrease of the kink width in agreement with theory [2]. However, now Eq. (6) has a solution for *any* kink velocity v. Thus, the discreteness effects remove the restriction $|v|<c$ of SG-type equations. Now even for the classical FK model with harmonic interaction the kink may move with any velocity v.

A kink solution corresponds to a separatrix of the continuum limit equation. To find the separatrix of Eq. (5), let us normalize the coordinate $\tilde{z}=z/d$, the velocity $\tilde{v}=v/c$, and define the dimensionless discreteness parameter $\tilde{h}=h/d=1/\sqrt{12g}$. Introducing the new variable $\xi=u_{\rm k}(\tilde{z})$ and the function $w(\xi)=u_{\rm k}'(\tilde{z})$, Eq. (5) can be rewritten as

$$\{\tilde{h}^2\tilde{v}^2[w'''(\xi)w^2(\xi)+4w''(\xi)w'(\xi)w(\xi)+[w'(\xi)]^3]-\alpha w'(\xi)w(\xi)+(1-\tilde{v}^2-\tilde{h}^2\cos\xi)w'(\xi)+(\tilde{h}^2\sin\xi)w(\xi)+\eta\tilde{v}\}w(\xi)-\sin\xi+f=0. \tag{7}$$

A (multiple) kink solution has to satisfy the boundary conditions $u_{\rm k}(-\infty)=u_f+2\pi p$, $u_{\rm k}(+\infty)=u_f$, $u_{\rm k}'(\pm\infty)=0$, or

$$w(u_f+2\pi p)=w(u_f)=0. \quad (8)$$

For example, if $w(\xi)$ is a separatrix for the double kink ($p=2$), it has to connect the points $(\xi=u_f+4\pi, w=0)$ and $(\xi=u_f, w=0)$. However, due to periodicity of the substrate potential, the function $w(\xi+2\pi)$ must correspond to the separatrix solution as well. Thus, on the (ξ,w) plane the separatrices of the multiple ($p\geqslant 2$) kinks must intersect at some point with $w\neq 0$. One can show that in the model without the discreteness effects, $h=0$, when the phase space of Eq. (7) is two-dimensional, such intersections are forbidden [14]. Thus, Eq. (7) with $h=0$ allows neither supersonic kinks nor multiple kinks. On the contrary, at $h\neq 0$ the phase space of Eq. (7) is four-dimensional, thus the separatrices corresponded to multiple kinks may not intersect, and multiple kinks are allowed in principle [12]. Thus, *the discrete model formally allows both supersonic and multiple topological excitations*.

Although we cannot find the separatrix solution analytically, the ordinary differential equation (7) can be solved numerically with any desired accuracy. Thus, if one could find a separatrix solution corresponded to supersonic or multiple kink, this will prove their existence. Indeed, looking for a separatrix solution numerically for the $\beta=1/\pi$ and $\eta=0.05$ case, we found that at small discreteness, $g=10$, so that $\tilde{h}\approx 0.09$ and $\alpha\approx 0.1$, the separatrix solution corresponds to the 2π kink at forces as large as $f=0.9$, when the kink is supersonic, $v_{\mathrm{k}}/c\approx 1.13$. On the other hand, for higher discreteness, $g=1$ so that $\tilde{h}\approx 0.29$, we saw the 2π kink at $f\leqslant 0.2$ when $v_{\mathrm{k}}/c\lesssim 1$, and the 4π-kink at $f\geqslant 0.6$ when $v_{\mathrm{k}}/c>1.3$. *Thus, both supersonic kinks and multiple kinks do exist*, at least for some particular choices of model parameters.

Near kink's tails, $z\rightarrow\pm\infty$, e.g., for $\xi=u_f+2\pi n+\epsilon$, where $|\epsilon|\ll 1$, we can use the expansion

$$w(\xi)=a_1\epsilon+\frac{1}{2}a_2\epsilon^2+\frac{1}{6}a_3\epsilon^3+\cdots, \quad (9)$$

where $a_1\equiv w'(u_f)$, $a_2\equiv w''(u_f)$, etc. Substituting this expansion into Eq. (7) and grouping together the terms of the same power of ϵ, we obtain the following equation for a_1 [cf. with Eq. (6)],

$$\tilde{h}^2\tilde{v}^2a_1^4+(1-\tilde{v}^2-\tilde{h}^2\cos u_f)a_1^2+\eta\tilde{v}a_1-\cos u_f=0, \quad (10)$$

which always has two roots, one positive and one negative, for any kink velocity v. Then, equating the terms for higher powers of ϵ, we obtain the relations that uniquely determine the coefficients a_2, a_3, etc. Thus, the separatrix solution of Eq. (7) is *unique*, i.e., for a given set of system parameters *the model has either the single-kink solution or the double-kink one*, but never both solutions simultaneously.

Thus, we have demonstrated the existence of supersonic and multiple kinks in the driven discrete FK model with anharmonic interaction (note that the discreteness of the model and the anharmonicity of the interaction are the necessary conditions). But to find the parameter range for their existence (the sufficient conditions), we have to study numerically either the continuum-limit equation (7) or, better, the original discrete model (1). The approximate variational approach described below essentially simplifies this task.

IV. SUPERSONIC KINKS

It is easy to show that in the case of $f=\eta=h=0$, Eq. (5) corresponds to an extremum of the following energy functional [15],

$$E[u(z)]=\int dz\left[\frac{c^2-v^2}{2}(u')^2-\frac{\alpha d^3}{6}(u')^3-\cos u\right]. \quad (11)$$

Substituting a simple SG-type ansatz

$$u_{\mathrm{SG}}(z)=4\tan^{-1}\exp(-z/d_{\mathrm{eff}}) \quad (12)$$

into Eq. (11), we obtain

$$E(d_{\mathrm{eff}})=4\frac{c^2-v^2}{d_{\mathrm{eff}}}+\frac{2\pi}{3}\alpha\frac{c^3}{d_{\mathrm{eff}}^2}+4d_{\mathrm{eff}}. \quad (13)$$

Although the variational approach does not describe rigorously the kink tails because of neglecting the discreteness effects, it allows us to find analytically the shape of the kink's core and, therefore, to calculate approximately the kink velocity for the model with anharmonic interaction. Indeed, looking for extrema of the function $E(d_{\mathrm{eff}})$, we come to the equation $E'(d_{\mathrm{eff}})=0$, or

$$\kappa^3=\left[1-\left(\frac{v}{c}\right)^2\right]\kappa+\frac{\pi}{3}\alpha, \quad (14)$$

where we introduced the new variable $\kappa=d_{\mathrm{eff}}/d$. For the harmonic interaction, $\alpha=0$, Eq. (14) has a solution for $|v|<c$ only, which describes relativistic narrowing of the SG kink, $\kappa=[1-(v/c)^2]^{1/2}$. But for the anharmonic interaction, $\alpha>0$, Eq. (14) has a solution for *any* kink velocity v, including supersonic velocities $|v|>c$. We emphasize that *supersonic excitations are possible for kinks (local compressions) only*.

Considering the kink as a rigid quasiparticle, the kink effective mass can be introduced as (e.g., see [2])

$$m_{\mathrm{k}}=\frac{1}{a}\int_{-\infty}^{+\infty}dz[u'(z)]^2=\frac{4}{\pi d_{\mathrm{eff}}}. \quad (15)$$

Then, assuming that kink's parameters at nonzero f and η are the same as those for the $f=\eta=0$ case, the steady-state kink velocity can be found approximately from the equation

$$v_{\mathrm{k}}=f/m_{\mathrm{k}}\eta=\pi cf\kappa(v_{\mathrm{k}})/4\eta. \quad (16)$$

Using Eq. (16), Eq. (14) can be rewritten in the form

$$\left[1+\left(\frac{\pi f}{4\eta}\right)^2\right]\kappa^3=\kappa+\frac{\pi}{3}\alpha. \quad (17)$$

Numerical solution of Eq. (17) allows us to find the function $v_{\mathrm{k}}^{(\mathrm{var})}(f)$ that is shown by the dashed curve in Fig. 2 together

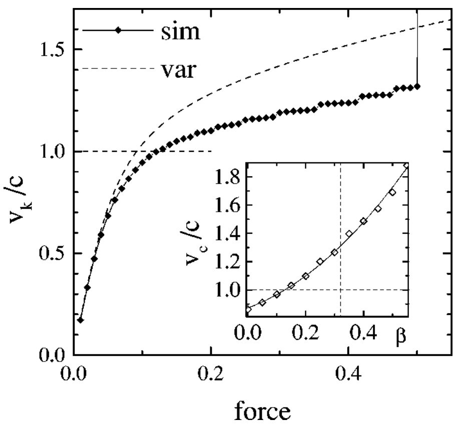

FIG. 2. The velocity v_{k} of the single kink versus the force for $\beta=1/\pi$, $g=1$, and $\eta=0.05$. The solid curve is for simulation results, and the dashed curve, for variational approximation. Inset: the critical kink velocity $v_{\mathrm{c}}(\beta)$ at the fixed force $f=0.5$.

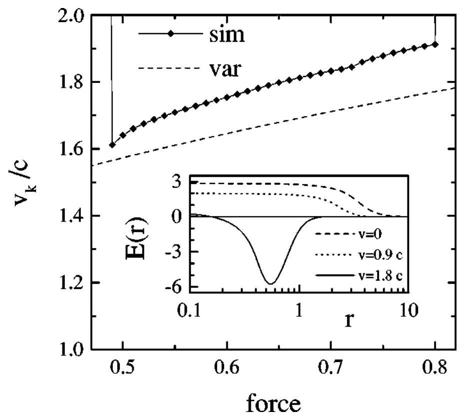

FIG. 3. The same as in Fig. 2 for the double kink. Inset: the effective energy $E(r)$ of the double kink as function of subkink's separation r for fixed kink velocities $v_{\mathrm{k}}=0$, 0.9 c and 1.8 c.

with the dependence $v_{\mathrm{k}}(f)$ obtained by solution of the discrete equation of motion (1). One can see that in the anharmonic model we always have $v_{\mathrm{k}}^{(\mathrm{var})}>c$ at $f\rightarrow 1$, and although the simulation velocity is lower than $v_{\mathrm{k}}^{(\mathrm{var})}$ due to additional damping of the moving kink because of phonon radiation, the discrete kink still may reach a supersonic velocity. Thus, the variational approach predicts that the supersonic kinks may be expected in the *anharmonic* FK model only.

Returning back to the *discrete* model, note that in the classical FK model the driven kink cannot reach even the sound velocity, because it exists some critical kink velocity $v_{\mathrm{c}}<c$ above which the driven kink becomes unstable and the system goes to the ''running'' state, where all atoms move with the velocity $v\approx f/\eta$ [16]. However, in the anharmonic FK model, the critical kink velocity may exceed the sound speed as has been observed already in the simulation [10]. The dependence of v_{c} on the anharmonicity parameter β is shown as inset in Fig. 2. In this calculation we used the following algorithm [11]: for a fixed value of f (we took $f=0.5$), the friction was decreased starting from the overdamped case $\eta=1$ to the underdamped value $\eta=10^{-3}$ in 256 steps. At each step of η decreasing we waited until the steady state was reached and then checked if the transition to the running state took place.

V. MULTIPLE KINKS

To study multiple kinks with the help of a variational approach, let us consider the double kink as a sum of two single kinks separated by a distance r,

$$u_2(z)=u_{\mathrm{SG}}(z-r/2)+u_{\mathrm{SG}}(z+r/2). \tag{18}$$

Substituting the ansatz (18) into the functional (11), we obtain the effective energy $E(d_{\mathrm{eff}},r)$, which is now a function of two parameters d_{eff} and r. Looking for a minimum of $E(d_{\mathrm{eff}},r)$ over d_{eff} at r fixed, we found that for the classical FK model $\alpha=0$, the function $E(r)\equiv\min_{d_{\mathrm{eff}}}E(d_{\mathrm{eff}},r)$ is a monotonically decreasing function of r, i.e., the kinks are repelled from one another. On the other hand, for the anharmonic FK model the function $E(r)$ has a minimum at some $r=r_{\mathrm{min}}<\infty$, so two kinks attract one another and thus have to couple into a double kink. The ''dissociation'' energy of the double kink is very small at subsonic velocities, but becomes high enough at supersonic velocities (see inset in Fig. 3). The ''size'' r_{min} of the double kink decreases with $|v|$ increasing. Thus, although the variational approach with the SG-type ansatz is too crude, it nevertheless predicts that the multiple kinks could be stable for high (supersonic) kink velocities.

As is well known, the SG kinks of the same topological charge always repel from one another. The same is true for static ($v=0$) kinks of the discrete FK model, including the anharmonic ($\alpha\neq 0$) model [2] (contrary to the variational approximation that mistakenly predicted a weak attraction at $|v|<c$). Thus, there must exist a threshold kink velocity v_1 such that at small velocities $0\leqslant v<v_1$ the steady-state solution of the model corresponds to the 2π kink, while at high velocities $v>v_1$, it corresponds to the double (4π) kink (if v_1 is lower than the kink velocity at $f=1$, that is true at low enough values of η). Indeed, the simulation results presented in Fig. 3 demonstrate that the double kink is stable within the force interval $0.5<f<0.8$ but becomes unstable at higher as well as smaller forces, while the 2π kink is stable for $f<0.5$ only. Similarly, one could expect the existence of a second threshold velocity v_2 such that at $v>v_2$ the steady-state solution will correspond to the 6π kink, etc.

VI. CONCLUSION

Thus, we have shown that supersonic kinks as well as multiple kinks do exist in the driven discrete FK model, if the interatomic interaction is anharmonic. Note that both supersonic kinks and multiple kinks remain stable at nonzero system temperatures as well, at least for the time scale of our numerical simulation.

Notice also that at high forces the kink velocity is close to that of the Toda soliton [6]. Indeed, the Toda soliton is characterized by the ''jump'' $\Delta u=2\mu a/\beta$, where μ is the parameter coupled with the soliton velocity v by the relationship $v=c\sinh(\mu a)/\mu a$. In the presence of the external substrate potential due to boundary conditions the jump Δu

must be equal to $2\pi p$ for the p kink; thus we obtain $\mu a = \pi\beta p$, or $2\mu = p\beta$. In particular, for the anharmonicity parameter $\beta = 1/\pi$ used in the simulation, we have $v/c = (\sinh p)/p \approx 1.18$ for the 2π kink and $v/c \approx 1.81$ for the 4π kink, correspondingly. Thus, the supersonic and multiple kinks may be treated as Toda solitons ‘‘disturbed’’ by the external periodic potential.

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