Nonlinear dynamics of the Frenkel-Kontorova model with impurities

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The nonlinear dynamics of the Frenkel-Kontorova (FK) model with local impurities is considered analytically. Impurity modes, i.e., nonlinear oscillations localized near the impurity, are studied. We show that the low-frequency impurity mode can be regarded as a breather trapped by the impurity, and a similar approach is possible for the high-frequency mode. The stability of the nonlinear modes is investigated, and laws of their decay caused by nonintegrability of the system are determined. Considering a single kink in the FK chain, we derive the effective equation of motion for its collective coordinate, which takes into account inhomogeneities and the discreteness of the model. The adiabatic interaction of the kink with an impurity is analyzed. We show that the chain's discreteness plays an important role in the kink scattering. In particular, the reflection of the kink by a heavy-mass impurity is stipulated by the Peierls-Nabarro (PN) potential arising from the lattice discreteness, so that the reflection does not occur in the continuum model. The threshold velocity (or the threshold impurity mass) for kink reflection is determined by the amplitude of the PN potential. We also demonstrate that local impurities modify transport properties of one-dimensional systems, and the change of the kink diffusion coefficient depends on the character of the kink interaction with a separate impurity (repulsion or attraction).

I. INTRODUCTION

The study of nonlinear phenomena in inhomogeneous and disordered systems is of a great interest[1] to understand whether or not nonlinearity qualitatively modifies the effects of disorder on transport properties, and, vice versa, whether or not disorder modifies the remarkable solitonic properties of nonlinear systems. To understand the behavior of nonlinear excitations in disordered systems, it is important to investigate their interaction with separate impurities (see, e.g., Refs. 2–6).

In the linear case, impurities generate a number of features in the dynamics of a system under consideration. Firstly, as was shown by Anderson[7] (see also Ref. 8), the transmission coefficient $T(L)$ of the linear wave propagating through a disordered system of width L behaves like $T(L)=\exp(-L/\lambda)$, where λ is the localization length. Secondly, separate impurities in a harmonic lattice generate a new type of excitations, the so-called impurity modes, i.e., local oscillations around the impurity atoms (see the pioneer work,[9] and also, e.g., Refs. 10–13). The impurity modes have frequencies lying outside the frequency zone of the ideal lattice and make significant contributions into various characteristics of crystals with impurities.

As is well known, homogeneous nonlinear systems support the undistorted propagation of localized waves, the so-called solitons. Both of the above mentioned effects are strongly modified in the nonlinear case. For example, the soliton scattering by impurities leads to a new mechanism of the transport properties in disordered systems (see Refs. 4, 5, and 14–16). Namely, it was demonstrated in numerical simulations[16] that, due to modulation instability, a nonlinear periodic wave generates, in a focusing nonlinear medium, a number of solitons which have a little scattering by impurities.[4,5] The dynamics of solitons is mainly determined by their nature. Nontopological (dynamical) solitons may be trapped by impurities to form a nonlinear oscillating mode (see, e.g., Refs. 17 and 18) which fade due to discreteness effects. Otherwise, the topological soliton (kink) behaves like a particle in effective impurity potential (see survey[19] and references therein). In the last case the soliton propagation through a disordered system is defined mostly by the dynamics of the soliton near separate local impurity.[5]

Many effects in nonlinear systems of the condensed matter physics may be considered in the framework of the Frenkel-Kontorova (FK) model[20], which describes the behavior of a harmonic chain of atoms in a periodic external potential. This model was proposed to describe the mobility of dislocations in solids.[20–23] Then it was successfully employed to investigate the dynamics of crystal growth (e.g., Refs. 24–27) and the behavior of adsorbed layers (e.g., Refs. 28–32). Namely, the layer of atoms adsorbed on stepped or furrowed crystal surfaces may be treated as a quasi-one-dimensional system where adsorbed atoms (adatoms) situated in one "furrow" of the substrate can be approximately regarded as a quasi-independent chain of atoms, the periodic external potential being the substrate potential. In a long-wavelength limit, excitations of the FK model are described by a nonlinear differential equation, the sine-Gordon (SG) equation (see, e.g., Ref. 23). Note that a number of physical objects allowing a model description with the help of the

SG equation is known: domain walls in magnetic materials (see, e.g., Ref. 32), fluxons in long Josephson junctions (e.g., Ref. 35), charge-density waves in quasi-one-dimensional conductors,[33] etc.

The exactly integrable SG system has the following important property: any nonlinear excitation can be presented as a set (but not a superposition) of noninteracting quasiparticles; phonons (quasilinear waves), breathers (dynamical solitons), and kinks (topological solitons). This is a result of the inverse scattering transform applied to the SG equation (see, e.g., Ref. 34). Within the scope of the SG model, excitations move freely and their collisions are "elastic."[34] For real physical systems, the dynamics may be described in terms of the same quasiparticles which, however, now interact with one another or with impurities. The interaction of nonlinear excitations with impurities plays an especially important role in transport properties of one-dimensional systems because the kinks and breathers may be trapped or reflected by the local inhomogeneities. Note that the breather captured by an impurity may be regarded as a *nonlinear impurity mode.*

There are a number of papers considering the interaction of solitons with impurities in the framework of the SG model (see, e.g., Refs. 35–38 and also references in the review paper[19]). Most of the studies are related to the fluxon scattering by local inhomogeneities in long Josephson junctions (JJ),[35,36,38] where the inhomogeneities are installed into the junctions during their fabrication (see, e.g., Ref. 39).

For the FK model, a homogeneous vacuum solution of the SG equation corresponds to a commensurate structure when all atoms lie in the minima of the substrate potential while a kink (antikink) is an excessive atom (atom vacancy) in the commensurate structure (see, e.g., Ref. 32). The motion of such excessive atoms along the chain is described by the motion of kinks and, therefore, the analysis of the kink dynamics is important to clarify, for example, the surface diffusion and drift of adatoms.[31] From this point of view, it is an important problem to study extended versions of the FK model which take into account a more complex character of atomic interactions in the chain, e.g., local anharmonic,[26,27] long-range exponential,[40,41] or power[42] interactions between atoms, as well as the interaction between separate chains.[43,44]

In the framework of the FK model, two new features in the soliton-impurity interaction arise. Firstly, in the discrete atomic chain, a free motion of a kink corresponding to a continuum SG model is substituted by its motion in a periodic Peierls-Nabarro (PN) potential whose amplitude is always less than the amplitude of the substrate potential (see, e.g., Ref. 23). Parameters of a kink moving in the PN potential are changed periodically, which results in radiation of phonons leading to the kink pinning (e.g., Refs. 45–49). As a result, the discreteness effects which are absent in long JJ's may significantly modify the dynamics of kink scattering by impurities. The second feature of a discrete chain with impurities is the excitation of nonlinear impurity modes during soliton-impurity scattering.

The present paper aims to consider the dynamics of kinks and nonlinear impurity modes in the FK model with impurities. We demonstrate that the nonlinear mode may be regarded as a breather localized on an impurity. The first papers devoted to this problem[50,51] indicated that nonlinearity may produce a new effect: impurity modes may exist with frequencies close to the lower edge of the linear spectrum for both signs of the impurity mass changes. However, we show that the low-frequency impurity mode near the light mass is unstable, and therefore it cannot exist even if nonlinearity is included in the consideration. Due to the nonintegrability of the system, the impurity modes slowly fade, emitting phonons (e.g., Ref. 11); thus, decay laws should be determined. For the kink we derive the effective equation of motion for its center in the discrete chain with an impurity. The discreteness effects may drastically modify the kink scattering by impurities. In particular, the mass impurity in the continuous SG system cannot reflect the kink. However, this effect is possible in the discrete chain, and the amplitude of the PN potential plays a dominant role in the threshold velocity (or the threshold impurity mass) allowing the reflection. We also demonstrate that impurities change the transport properties of the one-dimensional systems. In particular, the change of the diffusion coefficient of the kink sufficiently depends on the character of the kink interaction with impurities (attraction or repulsion).

The paper is organized as follows. In Sec. II we describe the FK model with local impurities which change the atomic mass in the lattice, strength between neighboring atoms in the chain, and the substrate potential. Considering a discrete chain in the harmonic approximation, we briefly observe results related to impurity modes (Sec. III). Nonlinear impurity modes are investigated in Sec. IV, and their decay is studied in Sec. V. Considering a single SG kink in Sec. VI, we derive the effective equation of motion for the kink collective coordinate taking into account the lattice spacing and inhomogeneities. Analysis of this equation is also presented in Sec. VI. Section VII discusses the influence of impurities on the kink diffusion coefficient. Last, Sec. VIII contains a summary and concluding remarks.

II. MODEL

We start from the FK Hamiltonian

$$H=\sum_j \left\{ \frac{1}{2} m_j \left[\frac{dx_j}{dt} \right]^2 + \tfrac{1}{2} g_j (x_{j+1}-x_j-b)^2 + \tfrac{1}{2} \varepsilon_j \left[1-\cos\left[\frac{2\pi x_j}{a} \right] \right] + v(x_j) \right\}, \quad (2.1)$$

where x_j is the position of the jth atom. The first term in Eq. (2.1) is the kinetic energy of the atomic chain, while the last three terms describe the potential energy which consists of the energy of a pairwise interaction of atoms between themselves, the energy of atom interaction with the substrate, and the external potential $v(x)$. Here we consider only the case of $b=a$ when the commensurate structure of atoms is the ground state of the system. Then, the atomic coordinates x_j can be represented as

$$x_j = ja + u_j \ . \tag{2.2}$$

The equation of motion corresponding to the Hamiltonian (2.1) has the form

$$m_j \frac{d^2 u_j}{dt^2} + m_j \eta \frac{du_j}{dt} + g_j(u_j - u_{j+1}) + g_{j-1}(u_j - u_{j-1}) + \tfrac{1}{2}\varepsilon_j \sin u_j - f_j = 0 \ , \tag{2.3}$$

where $f_j = -\partial v(ja + u_j)/\partial u_j$, and we have taken into account dissipative losses due to the energy exchange between the chain and the substrate [the second term in Eq. (2.3)].

The standard FK model assumes homogeneous parameters: $m_j = m$, $\eta_j = \eta$, $g_j = g$, $\varepsilon_j = \varepsilon$, and $v(x) \equiv 0$. For a homogeneous chain it is convenient to use the normalized units when $m = 1$, $\varepsilon = 2$, and $a = 2\pi$, so that the Hamiltonian (2.1) takes the form

$$H_0 = \sum_j \left[\frac{1}{2} \left[\frac{du_j}{dt} \right]^2 + \tfrac{1}{2} g (u_{j+1} - u_j)^2 + (1 - \cos u_j) \right] . \tag{2.4}$$

The harmonic approximation for the interparticle interactions [second term in Eq. (2.1)] is valid if the interatomic interactions are much stronger than their interaction with the substrate, i.e., if $g \gtrsim 1$. In another case we have to improve the model (see, e.g., Ref. 42). In the case $g \gg 1$, we may use the continuum approximation substituting into Eq. (2.1) the following expressions: $j \to y = ja$, $u_j \to u(y)$, $\sum_j \to \int dy/a$. Using the transformation $y \to x = y + u(y)$ so that $dy = dx[1 - u_x(x)]$, the Hamiltonian (2.1) may be transformed into the following one:

$$H = a^{-1} \int dx \left[\tfrac{1}{2} m(x) u_t^2 + \tfrac{1}{2} g(x) a^2 u_x^2 - v(x) u_x + \tfrac{1}{2} \varepsilon(x)(1 - \cos u) \right] , \tag{2.5}$$

where the subscripts "x" and "t" stand for partial derivatives in the space and time variables, respectively. The third term in Eq. (2.5) describes the action of the slowly varying external potential $v(x)$ on "excessive" atoms in the chain; the latter is characterized by the density $\rho(x) = -u_x/2\pi$. This effect is well studied (see, e.g., Refs. 45 and 52) and we will not consider it in the present study.

In this paper we investigate only local impurities in the FK chain; when one of the atoms in the chain, say $j = 0$, has parameters which are different from the atoms of the lattice, it is characterized by (i) the change of interaction with the substrate,

$$\varepsilon_0 = 2 + \Delta\varepsilon \ , \tag{2.6a}$$

(ii) another mass,

$$m_0 = 1 + \Delta m \ , \tag{2.6b}$$

(iii) the change of the interaction with its neighbors,

$$g_0 = g_{-1} = g + \Delta g \ , \tag{2.6c}$$

and (iv) the change dissipative loss,

$$\eta_0 = \eta + \Delta\eta \ . \tag{2.6d}$$

The total Hamiltonian of the system in that case may be presented as follows:

$$H = H_0 + \delta H \ , \tag{2.7}$$

where H_0 is defined in Eq. (2.4), and

$$\delta H = \tfrac{1}{2} m \left[\frac{du_0}{dt} \right]^2 + \tfrac{1}{2} \Delta g [(u_1 - u_0)^2 + (u_0 - u_{-1})^2] + \tfrac{1}{2} \Delta\varepsilon (1 - \cos u_0) \ . \tag{2.8}$$

In the continuum approximation we have to put, in Eq. (2.5), the following functions:

$$\varepsilon(x) = 2 + \Delta\varepsilon a \delta(x) \ , \tag{2.9a}$$

$$m(x) = 1 + \Delta m a \delta(x) \ , \tag{2.9b}$$

$$g(x) = g + \Delta g a \delta(x) \ . \tag{2.9c}$$

III. IMPURITY MODES IN THE HARMONIC APPROXIMATION

To study the linear excitations of the FK model, we will consider small oscillations of atoms near their equilibrium positions $|u_j| \ll 2\pi$ and put

$$\cos u_j \simeq 1 - \tfrac{1}{2} u_j^2 \ . \tag{3.1}$$

In this approximation, the FK chain without impurities supports the linear waves,

$$u_j(t) = u_j(0) \exp[i\omega(k)t - ikaj] \ , \tag{3.2}$$

where the frequency $\omega(k)$ and the wave number k are connected by the dispersion relation ($a = 2\pi$)

$$\omega^2(k) = 1 + 4g \sin^2(\pi k), \quad |k| < \tfrac{1}{2} \ . \tag{3.3}$$

In the inhomogeneous FK chain, impurities generate the co-called impurity modes, the local oscillations of atoms near the impurities.[9–13] The frequency of the impurity modes lies outside the frequency zone of the linear spectrum (3.3). The analytical investigation of the impurity mode may be carried out with the help of the Green-function technique (see, e.g., Refs. 11 and 23). We briefly present the results.

Let us introduce the Green function $\tilde{G}(t)$ and its Fourier transformation $G(\omega)$, defined in the usual way:

$$\tilde{G}(t; j_1, j_2) = -i(m_{j_1} m_{j_2})^{1/2} \langle \hat{T} \hat{u}_{j_1}(t) \hat{u}_{j_2}(0) \rangle \ ,$$
$$\hat{G}(\omega; j_1, j_2) = \lim_{\delta \to 0} \int_{-\infty}^{+\infty} dt \exp(i\omega t - \delta|t|) \tilde{G}(t; j_1, j_2) \ , \tag{3.4}$$

where $\hat{T}$ is the time-ordering operator and $\hat{u}_j(t)$ is the displacement operator in the Heisenberg representation. The function $\hat{G}(\omega)$ satisfies the matrix equation

$$(\omega^2 - \hat{B})\hat{G} = 1 \ , \tag{3.5}$$

where the matrix $\hat{B}$ has the elements

$$B(j_1, j_2) = (m_{j_1} m_{j_2})^{-1/2} \frac{\partial^2 H}{\partial u_{j_1} \partial u_{j_2}} \ . \tag{3.6}$$

For the homogeneous FK model with the Hamiltonian H_0, the nonzero elements are

$$B_0(j,j)=1+2g, \quad B_0(j,j\pm1)=-g \ , \tag{3.7}$$

where we have used the index "0" to note the homogeneous case. In this case, the matrix equation (3.5) produces the chain of equations for the function

$$G_0(j_1,j_2)=G_0(|j_1-j_2|) \ ,$$

e.g.,

$$\begin{aligned}&(\omega^2-1-2g)G_0(0)=1-2gG_0(1) \ ,\\ &(\omega^2-1-2g)G_0(1)=-g[G_0(0)+G_0(2)] \ ,\\ &\cdots \ .\end{aligned} \tag{3.8}$$

It is easy to show that the solution of Eqs. (3.8) has the form

$$G_0(j)=Ay^{|j|} \ , \tag{3.9a}$$

where

$$y=-x+i(1-x^2)^{1/2} \ , \tag{3.9b}$$

$$A=-i/[2g(1-x^2)^{1/2}] \ , \tag{3.9c}$$

$$x=(\omega^2-1-2g)/2g \ , \tag{3.10a}$$

and, in the case of $|x|>1$, the square root in Eqs. (3.9) should be taken as

$$(1-x^2)^{1/2}=-i\,\mathrm{sgn}(x)(x^2-1)^{1/2} \ . \tag{3.10b}$$

When $-1<x<1$, the frequency ω lies in the region $\omega_{\min}<\omega<\omega_{\max}$, where $\omega_{\min}=1$ and $\omega_{\max}=(1+4g)^{1/2}$ [see Eq. (3.3)]. Note that the following expressions are valid:

$$\begin{aligned}&G_0(0)G_0(2)=G_0^2(1) \ ,\\ &g[G_0^2(1)-G_0^2(0)]=G_0(1) \ .\end{aligned} \tag{3.11}$$

When the local impurity is inserted into the chain, so that the expressions (2.6) are valid, the matrix $\hat{B}$ may be presented in the form $\hat{B}=\hat{B}_0+\delta\hat{B}$, where

$$\delta B(1,1)=\delta B(-1,-1)=\Delta g \ , \tag{3.12a}$$

$$\delta B(0,\pm1)=g[1-(1+\Delta m)^{-1/2}]-\Delta g(1+\Delta m)^{-1/2} \ , \tag{3.12b}$$

$$\delta B(0,0)=[\tfrac{1}{2}\Delta\varepsilon+2\Delta g-(1+2g)\Delta m](1+\Delta m)^{-1} \ . \tag{3.12c}$$

The Green function of the chain with impurity satisfies the Dyson equation

$$\hat{G}=\hat{G}_0+\hat{G}_0\delta\hat{B}\hat{G} \ . \tag{3.13}$$

The solution of Eqs. (3.12) and (3.13) has the form

$$G(0,0)=Z^{-1}\{G_0(0)+\delta B(1,1)[G_0^2(1)-G_0^2(0)]\} \ , \tag{3.14a}$$

where

$$\begin{aligned}Z=&1-\delta B(0,0)G_0(0)-4\delta B(0,1)G_0(1)\\ &-\delta B(1,1)[G_0(0)+G_0(2)]\\ &+[2\delta B^2(0,1)-\delta B(0,0)\delta B(1,1)]\\ &\times[G_0^2(1)-G_0^2(0)] \ .\end{aligned} \tag{3.14b}$$

As is well known, zeroes of the function $Z(\omega)$ determine the spectrum of the FK chain with an impurity. In particular, solutions with $|x|>1$, i.e., for $0<\omega<\omega_{\min}$ or $\omega>\omega_{\max}$, describe the local impurity modes. To analyze the modes, let us consider the partial cases.

(a) $\Delta\varepsilon\neq0$, $\Delta g=\Delta m=0$. Then, $\delta B(0,0)=\frac{1}{2}\Delta\varepsilon$, and equation

$$Z\equiv1-G_0(0)\delta B(0,0)=0$$

leads to the result that the impurity mode exists in the region $\omega>\omega_{\max}$ if $\Delta\varepsilon>0$ (deep well), and it exists in the region $0<\omega<\omega_{\min}$ if $\Delta\varepsilon<0$ (shallow well). The frequency of the impurity mode ω_l is determined by the equation

$$\mathrm{sgn}(x)(x^2-1)^{1/2}=\Delta\varepsilon/4g \ , \tag{3.15}$$

which has a solution

$$\omega_l^2=1+2g\pm(4g^2+\Delta\varepsilon^2/4)^{1/2}, \quad \Delta\varepsilon\gtrless0 \ . \tag{3.16}$$

(b) $\Delta m\neq0$, $\Delta g=\Delta\varepsilon=0$. In this case,

$$\begin{aligned}&\delta B(0,0)=-(1+2g)\Delta m/(1+\Delta m) \ ,\\ &\delta B(0,1)=g[1-(1+\Delta m)^{-1/2}] \ ,\end{aligned}$$

and

$$Z=(1+\Delta m)^{-1}[1+\Delta m\omega^2G_0(0)] \ .$$

The local mode exists for $\Delta m>0$ (heavy mass) in the region $0<\omega<\omega_{\min}$, and, for $-1<\Delta m<0$ (light mass), it exists at $\omega>\omega_{\max}$ and its frequency is defined by the equation

$$\mathrm{sgn}(x)(x^2-1)^{1/2}=-\Delta m(x+1+1/2g) \ . \tag{3.17}$$

The solution is

$$\omega_l^2=\frac{1+2g\mp[4g^2+\Delta m^2(1+4g)]^{1/2}}{1-\Delta m^2}, \quad \Delta m\gtrless0 \ . \tag{3.18}$$

(c) $\Delta g\neq0$, $\Delta m=\Delta\varepsilon=0$. Then, $\delta B(1,1)=\Delta g$, $\delta B(0,1)=-\Delta g$, $\delta B(0,0)=2\Delta g$, and

$$Z=1+\Delta g[-3G_0(0)+4G_0(1)-G_0(2)] \ .$$

The local mode exists *only for* $\Delta g>0$ (more strong interactions with neighbors) and its frequency ω_l ($\omega_l>\omega_{\max}$) is a solution of the equation ($x>1$)

$$[1+(\Delta g/g)(2+x)](x^2-1)^{1/2}=(\Delta g/g)(x+1)^2 \ . \tag{3.19}$$

IV. NONLINEAR IMPURITY MODES

A. Low-frequency modes

We will study the low-frequency impurity modes for a nonlinear lattice in the long-wavelength limit when the

motion equations of the FK model may be transformed to the SG equation

$$u_{tt}-u_{zz}+\sin u=0 \ . \tag{4.1a}$$

Here, as usual, we introduce the dimensionless variable

$$z=x/l, \ l=ag^{1/2} \ , \tag{4.1b}$$

l being the kink width.

As is well known, the SG equation is the exactly integrable one[34] and it has three types of nonlinear excitations: phonons, kinks, and breathers. The latter is the nonlinear localized oscillations of the form

$$u_{\rm br}(z,t) = 4\tan^{-1}\left\{\frac{(1-\Omega^2)^{1/2}}{\Omega}\frac{\sin(\Omega t)}{\cosh[(1-\Omega^2)^{1/2}z]}\right\} \ . \tag{4.2}$$

The breather frequency Ω lies in the bottom gap of the linear spectrum $0<\Omega<\omega_{\rm min}=1$. For a small amplitude of oscillations i.e., in the case of $\beta\equiv(1-\Omega^2)^{1/2}\ll 1$, the breather (4.2) may be transformed to the following form:

$$u_{\rm br}(z,t)\simeq 4\beta\sin[(1-\beta^2/2)t]\,\mathrm{sech}(\beta z) \ . \tag{4.3}$$

The frequency $\Omega=1-\beta^2/2$ of localized oscillations is close to the boundary frequency $\omega_{\rm min}=1$. Thus, nonlinearity leads to the appearance of local oscillations in the chain which are similar to the linear impurity modes in the sense that their frequencies lie outside the linear spectrum.

To analyze the influence of nonlinearities on the impurity mode, or, vise versa, the influence of an impurity on the breather oscillations, let us consider the FK model with an impurity in the continuum approximation when the system is described by the inhomogeneous SG equation:

$$\tilde{m}(z)u_{tt}-[\tilde{g}(z)u_z]_z+\tilde{\varepsilon}(z)\sin u=0 \ , \tag{4.4a}$$

where, according to Eqs. (2.9) and (4.1b),

$$\begin{aligned}&\tilde{\varepsilon}(z)=1+\epsilon_1\delta(z), \quad \epsilon_1=\Delta\varepsilon/2\sqrt{g} \ ,\\ &\tilde{m}(z)=1+\epsilon_2\delta(z), \quad \epsilon_2=\Delta m/\sqrt{g} \ ,\\ &\tilde{g}(z)=1+\epsilon_3\delta(z), \quad \epsilon_3=\Delta g/g\sqrt{g} \ .\end{aligned} \tag{4.4b}$$

For simplicity, we will only consider the case $\epsilon_1\equiv\epsilon\neq 0$, $\epsilon_2=\epsilon_3=0$, so that Eqs. (4.4) reduce to

$$u_{tt}-u_{zz}+\sin u=-\epsilon\delta(z)\sin u \ . \tag{4.5}$$

In the linear approximation, when $\sin u\simeq u$, the impurity mode is the solution of the linear equation

$$\begin{aligned}&u_{tt}-u_{zz}+u=-\epsilon\delta(z)u \ ,\\ &u=A\exp(-q|z|)\cos(\omega_l t) \ ,\end{aligned} \tag{4.6}$$

where the frequency ω_l is defined by the relation

$$(1-\omega_l^2)^{1/2}=-\epsilon/2 \ . \tag{4.7}$$

Thus, it follows that, in the long-wavelength limit the impurity mode exists only for $\epsilon<0$. For $|\epsilon|\ll 1$, Eqs. (4.7) and (4.46) lead to the previously obtained Eq. (3.16).

To study the impurity mode in the nonlinear case it is convenient to consider, instead of Eq. (4.5), the equivalent equations

$$u_{tt}-u_{zz}+\sin u=0 \ , \tag{4.8a}$$

$$u_z|_{0+}-u_z|_{0-}=\epsilon\sin u(0) \ . \tag{4.8b}$$

Taking into account the small nonlinearity only, we put $\sin u\simeq u-u^3/6$ and make the substitution

$$u=\Psi e^{it}+\Psi^* e^{-it} \tag{4.9}$$

(the asterisk stands for the complex conjunction) in Eqs. (4.8) to obtain an equation for the complex envelope $\Psi(z,t)$,

$$2i\Psi_t-\Psi_{zz}-\tfrac{1}{2}|\Psi|^2\Psi=0 \ , \tag{4.10a}$$

with the matching condition at $z=0$

$$\Psi_z|_{0+}-\Psi_z|_{0-}=\epsilon\Psi(0) \ . \tag{4.10b}$$

Having derived Eq. (4.10a), the condition $\Psi_{tt}\ll\Psi_t$ was supposed to be held. Equation (4.10a) has the form of the nonlinear Schrödinger (NLS) equation. Its soliton solution at rest has the form

$$\Psi(z,t)=2\beta\exp(-i\beta^2 t/2)\,\mathrm{sech}[\beta(z-z_0)] \ , \tag{4.11}$$

z_0 being an arbitrary parameter. Note that solutions (4.11) and (4.9) coincide with the small-amplitude breather (4.3).

Looking for a solution of the inhomogeneous system in the form

$$\Psi(z,t)=2\beta\exp(-i\beta^2 t/2)\,\mathrm{sech}[\beta(|z|+z_0)] \ , \tag{4.12}$$

from the matching condition (4.10b), we obtain an equation for the parameter z_0:

$$\tanh(\beta z_0)=-\epsilon/2\beta \ . \tag{4.13}$$

Equations (4.12) and (4.9) yield the solution for atomic displacements

$$\begin{aligned}&u(z,t)=4\beta\,\mathrm{sech}[\beta(|z|+z_0)]\cos(\Omega_l t),\\ &\Omega_l=1-\beta^2/2 \ .\end{aligned} \tag{4.14}$$

The solutions (4.13) and (4.14) describe the *nonlinear impurity mode*. It has different shapes for $\epsilon<0$ and $\epsilon>0$ (see Fig. 1). For $\epsilon<0$, Eq. (4.13) yields $z_0>0$, and the impurity mode has a shape similar to the harmonic case [Fig. 1(a)], and, in the limit $z_0\to\infty$, this mode coincides with the harmonic one. The frequency Ω_l of the nonlinear mode is determined by Eq. (4.13) and, contrary to the harmonic approximation, now it depends on the amplitude of oscillations, which is characterized by the parameter z_0. According to Eq. (4.13), the solution of Eq. (4.14) exists provided $\beta\geq\frac{1}{2}|\epsilon|$ or $\Omega_l\leq\omega_l$.

In the case of $\epsilon>0$, Eq. (4.13) leads to $z_0<0$, and the impurity mode (4.14) has two maxima [Fig. 1(b)]. However, as will be shown in Sec. IV C, this mode is unstable. Note that the solutions similar to those presented above were first obtained in Ref. 51 (see also Ref. 18).

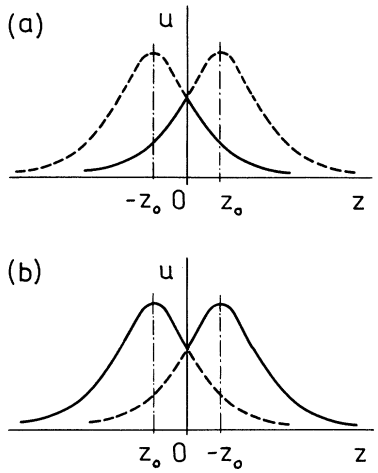

FIG. 1. The shape of the low-frequency nonlinear impurity mode for (a) $\epsilon<0$ and (b) $\epsilon>0$.

B. High-frequency mode

We now study the nonlinear oscillating mode localized near the impurity with frequencies close to the maximum frequency of the harmonic chain $\omega_{\max}=(1+4g)^{1/2}$.

Let us consider the FK model defined by the Hamiltonian (2.4) and (2.6)–(2.8) for the case of $\Delta\varepsilon\neq 0$, $\Delta m=\Delta g=0$:

$$\frac{d^2u_j}{dt^2}+g(2u_j-u_{j+1}-u_{j-1})+(1+\tfrac{1}{2}\Delta\varepsilon\delta_{j0})\sin u_j=0 \ . \tag{4.15}$$

Since we are interested in frequencies close to $\omega_{\max}$, for which neighboring atoms oscillate in almost opposite phases (i.e., short-wavelength limit), it is natural to introduce the quantities v_j defined as

$$u_j=(-1)^j v_j \ . \tag{4.16}$$

Because v_j is a slowly varying function of the number j, we can use the continuum approximation and transform the difference equations (4.15) to the following differential equation ($a=2\pi$)

$$v_{tt}+ga^2v_{xx}+4gv+\sin v=0 \tag{4.17}$$

with the condition, at $x=0$,

$$ga(v_x|_{0+}-v_x|_{0-})=-\tfrac{1}{2}\Delta\varepsilon\sin v(0) \ . \tag{4.18}$$

To study small-amplitude oscillations, $|v|\ll 1$, we put $\sin v\simeq v-v^3/6$, so that Eq. (17) takes the form

$$v_{tt}+ga^2v_{xx}+\omega_{\max}^2v-\tfrac{1}{6}v^3=0 \ . \tag{4.19}$$

In the linear approximation, the solution of Eqs. (4.18) and (4.19) has the form ($z=x/a\sqrt{g}$)

$$v(z,t)=A\exp(-\kappa|z|)\cos(\omega_l t) \ , \tag{4.20a}$$

where $\kappa=\omega_l^2-\omega_{\max}^2>0$. The frequency ω_l is defined by the relation

$$(\omega_l^2-\omega_{\max}^2)^{1/2}=\Delta\varepsilon/4\sqrt{g} \ , \tag{4.20b}$$

so that the solution exists only for $\Delta\varepsilon>0$.

In the nonlinear case, we look for a solution in the form

$$v(z,t)=\Psi(z,t)\exp(i\omega_{\max}t)+\Psi^*(z,t)\exp(-i\omega_{\max}t) \ , \tag{4.21}$$

where $\Psi(z,t)$ is a slowly varying function. Substituting Eq. (4.21) into Eq. (4.18), we may obtain the resultant nonlinear equation for the envelope function $\Psi(z,t)$,

$$2i\omega_{\max}\Psi_t+\Psi_{zz}-\tfrac{1}{2}|\Psi|^2\Psi=0 \tag{4.22}$$

with the matching condition

$$\Psi_z|_{0+}-\Psi_z|_{0-}=-\epsilon\Psi(0) \ , \tag{4.23}$$

where, according to Eqs. (2.9a) and (4.4b), $\epsilon=\Delta\varepsilon/2\sqrt{2}$.

Equation (4.22) is the NLS equation with different signs of dispersive and nonlinear terms. As is shown, this equation has no localized solutions similar to Eqs. (4.10) and (4.11), and, as a result, the solution shown in Fig. 1(b), is not possible. However, there is another solution of the equation,

$$\Psi(z,t)=2\beta\frac{\exp[i(\beta^2/2\omega_{\max})t]}{\sinh[\beta(z-z_0)]} \ ,$$

which has a singularity at $z=z_0$. Using the matching condition (4.23), we look for the impurity mode in the form

$$\Psi(z,t)=2\beta\exp[i(\beta^2/2\omega_{\max})t]\operatorname{cosech}[\beta(|z|+z_0)] \ , \tag{4.24}$$

z_0 being a positive parameter which should be defined. Substituting Eq. (4.24) into Eq. (4.23), we obtain the relation

$$\coth(\beta z_0)=\epsilon/2\beta \ . \tag{4.25}$$

Equations (4.21) and (4.25) yield the high-frequency *nonlinear impurity mode* ($\beta\ll 1$) (see Fig. 2)

$$v(z,t)=4\beta\operatorname{cosech}[\beta(|z|+z_0)]\cos(\Omega_l t) \ , \qquad \Omega_l=\omega_{\max}+\beta^2/2\omega_{\max} \ . \tag{4.26}$$

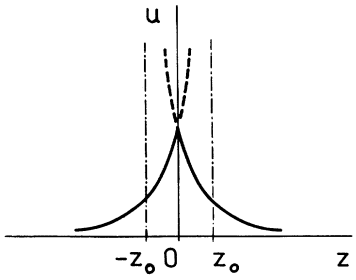

FIG. 2. The shape of the high-frequency nonlinear impurity mode for $\epsilon>0$.

The linear approximation (4.21) corresponds to the limit $z_0 \to \infty$, when the amplitude of oscillations tends to zero. However, for the finite amplitude of oscillations ($0 < z_0 < \infty$), the frequency Ω_l depends on the amplitude, so that $\omega_{\max} < \Omega_l < \omega_l$.

C. Stability of impurity modes

In previous subsections we dealt with the quiescent impurity modes. However, in the limit case described, for example, by Eq. (4.14), the NLS approach developed above can be generalized to describe small oscillations of the impurity mode near the inhomogeneity. These oscillations will be called external to distinguish them from the internal oscillations of the impurity mode with the frequency $\Omega_l \simeq 1-\beta^2/2$. The approach presented below allows us to analyze the stability of nonlinear impurity modes.

Let us look for a solution $u(z,t)$ of Eq. (4.8) in the form [cf. (4.14)]

$$u(z,t)=4\beta_j \operatorname{sech}(\beta_j|z|+\phi_j)\cos(\Omega_l t) , \tag{4.27}$$

where $j=1$ for $z<0$ and $j=2$ for $z>0$. Inserting Eq. (4.27) into the boundary condition (4.8b), we readily obtain the equations

$$\beta_1 \operatorname{sech}\phi_1=\beta_2 \operatorname{sech}\phi_2 , \tag{4.28a}$$

$$\beta_1 \tanh\phi_1+\beta_2 \tanh\phi_2=-\epsilon , \tag{4.28b}$$

where we have set $\sin u(0) \simeq u(0)$. The system of two linear equations (4.28) for β_j yields

$$\beta_j=-\epsilon \cosh\phi_j/(\sinh\phi_1+\sinh\phi_2) . \tag{4.29}$$

Small external oscillations of the impurity mode can be described by setting $\phi_{1,2}=\phi\pm\psi(t)$, $\psi \ll \phi$, where $\phi=\beta z_0$ is a constant and ψ is a slowly varying function in time. Inserting these expressions into Eq. (4.29), we obtain the values of $\beta_{1,2}$:

$$\beta_{1,2}=-\tfrac{1}{2}\epsilon \mp \tfrac{1}{2}\epsilon \tanh\psi-\epsilon(1\mp\psi)e^{-2\phi}+O(\psi^3 e^{-2\phi}) \tag{4.30}$$

[recall that $\exp(-2\phi)=-(\beta-\frac{1}{2}\epsilon)/\epsilon$ is a small quantity].

The underlying SG equation (4.5) for small u corresponds to the following Lagrangian expanded in powers of the wave field up to u^4 terms:

$$L=\tfrac{1}{2}\int_{-\infty}^{+\infty} dz[u_t^2-u_z^2-u^2+\tfrac{1}{12}u^4-\epsilon u^2\delta(z)] . \tag{4.31}$$

Inserting (4.27) and (4.30) into (4.31), in the first approximation we may obtain the effective Lagrangian averaged in the fast internal oscillations,

$$L=T-U=-4\epsilon\left[\frac{d\psi}{dt}\right]^2 e^{-2\phi}-12\epsilon^3\psi^2 e^{-4\phi} . \tag{4.32}$$

In the lowest approximation we have used

$$\frac{d\beta}{dt} \simeq -\frac{\epsilon}{2}\frac{d\psi}{dt} .$$

As a result, we immediately find the frequency ω of the small external oscillations

$$\omega^2=-3\epsilon(\beta+\tfrac{1}{2}\epsilon) , \tag{4.33}$$

where we have substituted

$$\exp(-2\phi)=-(\beta+\tfrac{1}{2}\epsilon)/\epsilon .$$

The result (4.33) is valid provided $\omega^2 \ll \epsilon^2$ (cf. Ref. 18).

Clearly, the small external oscillations of the nonlinear impurity mode are stable only for $\epsilon<0$ [Fig. 1(a)]. In the opposite case, $\epsilon>0$ [Fig. 1(b)], in contrast to predictions of Refs. 50 and 51, the nonlinear impurity mode is unstable and it will decay into two independent SG breathers.

In a general case $\epsilon_1 \neq 0$, $\epsilon_2 \neq 0$, $\epsilon_3 \neq 0$, the nonlinear impurity modes can be constructed in a similar way. The low-frequency mode has the form given by Eq. (4.14), and the high-frequency mode is described by Eqs. (4.16) and (4.26). It may be proved that the nonlinear modes with $z_0>0$ [see Fig. 1(a)] are stable whenever the modes similar to those shown in Fig. 1(b) ($z_0<0$) are unstable in respect to small shifts of their maxima away from the impurity. Thus, the nonlinearity does not change the conditions for the appearance of impurity modes established in Sec. III, but it reduces the frequency of local oscillations with the increasing of their amplitude.

V. DAMPING OF IMPURITY MODES

In this section we briefly discuss the lifetime of the localized vibrational excitations. Evidently, those in the exactly integrable systems local excitations, such as breathers in the SG system or impurity modes in the harmonic chain, have an infinite lifetime. However, in the nonintegrable systems, the lifetime should be finite due to the energy exchange between different degrees of freedom caused by their nonlinear coupling.

Firstly, let us consider the low-frequency impurity mode. According to Sec. IV A, in the long-wavelength approximation this mode can be considered as a breather pinned by the impurity. Therefore, it is useful to discuss briefly the breather stability in the nonintegrable systems. As is well known (see, e.g., Ref. 34), the existence of exact regular time-periodic solutions is a remarkable property of exactly integrable nonlinear systems. While the existence of stationary one-soliton solutions (e.g., kinks in the FK chain) does not purport exact integrability, it is usually believed that only integrable systems possess exact oscillating states (breathers) which lose no energy through radiation. (Some discussions of the point and efforts to construct periodic breatherlike solutions in a more general Klein-Gordon equation may be found in Ref. 53.) However, in many problems, physically important equations are not exactly integrable, and breathers slowly fade due to energy emission even if dissipative losses are absent. The emission rate due to the nonintegrability is usually exponentially small in the case of small-amplitude breathers (see, e.g., Refs. 53–57). For example, in the so-called double SG equation

$$u_{tt}-u_{xx}+\sin u=\epsilon \sin 2u ,$$

the energy emission rate W for the small-amplitude breather (4.3) is[57]

$$W=\frac{36\sqrt{2}}{5}\pi^2\epsilon^2\exp(-2\sqrt{2}\pi/\beta) .$$

Analogous results may be obtained for other perturbed terms.[53-57] Therefore, the small-amplitude breather in nonintegrable homogeneous systems is a long-lived oscillating object.

The situation is drastically changed for the inhomogeneous systems[37] when the breather interacts with an impurity. In the above-mentioned case, the exponentially small factor in W is $\exp(-\pi k/\beta)$, k being the radiation wave number, and k/β is proportional to the ratio of the breather's size $\sim\beta^{-1}$ [see Eq. (4.3)] to the radiation wavelength $\lambda=2\pi/k$. If a perturbation contains its own length scale L, the mentioned ratio changes into L/λ, and, in particular, if $L\lesssim 1$, the energy emission rate is not exponentially small, i.e., a breather is not very long lived. This is valid for the breather pinned by an impurity too.

Let us consider again the case $\Delta\varepsilon\neq 0$, $\Delta m=\Delta g=0$, which is described by Eq. (4.5). All necessary calculations for this case have been made by Kivshar and Malomed.[37,56] Here we briefly describe the results from the viewpoint of the dynamics of the nonlinear impurity modes. The large-amplitude SG breather (4.2) with $\beta\lesssim 1$, which can be considered as the coupled kink-antikink pair oscillated near the impurity, emits radiation very fast to be transformed into a small-amplitude breather (4.3) with $\beta\ll 1$. The evolution of the breather's frequency Ω is governed by the equation[37]

$$\Omega(t)=\Omega(0)+C\epsilon^2 t, \quad C\approx 0.014 . \tag{5.1}$$

The law (5.1) is valid provided $t\lesssim t^*\sim\epsilon^{-2}$. For $t>t^*$, the breather becomes a small-amplitude one, and its energy emission rate takes the form[18,37]

$$W=\frac{1875}{8\sqrt{2}}\epsilon^2[\beta'(\beta'-\epsilon)]^3 , \tag{5.2}$$

where $\beta'=\beta+\frac{1}{2}\epsilon$ is the breather amplitude defined at $z=0$ [see Eqs. (4.13) and (4.14)]. According to the equation

$$\frac{dE_{\rm br}}{dt}\equiv 16\frac{d\beta'}{dt}=-W ,$$

$E_{\rm br}$ being the breather energy, at the final stage of the breather evolution ($0<\beta'\ll\epsilon$), its amplitude evolves as

$$\beta'\simeq \text{const}/(|\epsilon|^5 t)^{1/2} , \tag{5.3}$$

so that the breather decays according to the power law (5.3). Of course, the same is true for the nonlinear low-frequency impurity mode (4.14).

To consider the high-frequency impurity mode (Fig. 2), the discreteness of the FK chain should be taken into account from the very beginning. In this case, calculations of the lifetime may be carried out by the diagram perturbation theory (see, e.g., Ref. 58). The amplitude of the impurity mode decreases exponentially,

$$A(t)=A(0)\exp(-\eta_s t/2) , \tag{5.4}$$

where η_s is the sum of different contributions. For example, we may include the anharmonicity of the interaction

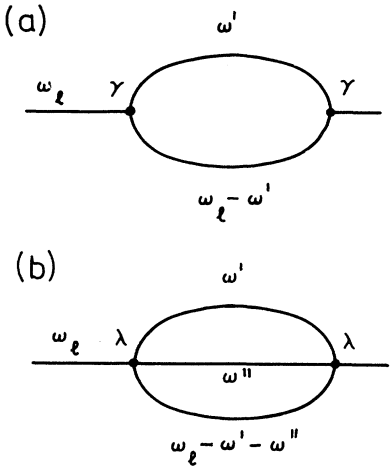

FIG. 3. Diagrams for decay of the impurity mode excitation.

potential of the nearest-neighboring atoms,

$$\tfrac{1}{2}gx^2\rightarrow\tfrac{1}{2}gx^2(1+\gamma x) ,$$

that leads to the contribution

$$\eta'\sim\gamma^2\int d\omega' G(\omega')G(\omega_l-\omega') \tag{5.5}$$

and corresponds to the decay of the impurity excitation into two phonons [Fig. 3(a)]. Besides, the anharmonicity of the substrate potential

$$1-\cos u\simeq\tfrac{1}{2}u^2-\lambda u^4, \quad \lambda\equiv\tfrac{1}{24} ,$$

causes the decay into three phonons [Fig. 3(b)] and leads to the contribution

$$\eta''\sim\lambda^2\int d\omega'\int d\omega'' G(\omega')G(\omega'')G(\omega_l-\omega'-\omega'') . \tag{5.6}$$

We have no aim to present the results in their exact form for the FK chain because they have a cumbersome form and were obtained for the three-dimensional lattice (see, e.g., Refs. 11 and 59–61). Note only that the contribution (5.5) is nonzero if $2\omega_{\min}<\omega_l<2\omega_{\max}$ (analogously, $\eta''\neq 0$ if $3\omega_{\min}<\omega_l<3\omega_{\max}$). Unlike the harmonic lattice with acoustic spectrum, the FK chain has the optical spectrum ($\omega_{\min}\neq 0$). Therefore, in the case of $\omega_{\max}<2\omega_{\min}$, or $g<3/4$, there exists the forbidden gap so that $\eta'=0$ for impurity mode frequencies satisfy the inequality $\omega_{\max}<\omega_l<2\omega_{\min}$. Analogously, $\eta''=0$ if $g<2$ and $\omega_{\max}<\omega_l<3\omega_{\min}$. In these cases the impurity mode, possibly, decays by the power law similar to the low-frequency case.

Above we have supposed that the system is in its ground state and only one localized mode is excited, i.e., that the system temperature T is equal to zero. However, the rate of phonon damping η_s essentially depends on T, and the value of η_s increases with temperature (for details see, e.g., Refs. 60 and 61). Moreover, at $T\neq 0$, the diagrams in Fig. 3 lead to the nonzero contributions for the low-frequency modes as well as for the high-frequency modes with frequencies lying in the forbidden zone.

Thus, the power law (5.3) for $T=0$ must be changed to the exponential law (5.4) at $T>0$.

Finally, we have to note that there always exists the energy exchange between the FK chain and the substrate. This exchange may be described by some friction coefficient η [see Eq. (2.3)], and it leads to the additional contribution to the total rate η_s in Eq. (5.4), i.e., $\eta_s=\eta+\eta'+\eta''$. In particular, for the FK chain of adsorbed atoms, the contribution η is the main one.[60] Thus, usually in real physical systems, the amplitude of the impurity mode decays by the exponential law (5.4) with typical rates $\eta_s \sim 10^{-1}-10^{-3}$ (see Refs. 59–61).

VI. KINK SCATTERING BY IMPURITIES IN A DISCRETE CHAIN

A. Effective equation of motion for the kink center

To derive an effective equation for the dynamics of the SG kink center, it is convenient to use the effective Lagrangian approach (see, e.g. Refs. 6 and 62). Let us start from the Lagrangian of the inhomogeneous FK model:

$$L=\sum_j \left[\frac{1}{2} m_j \left[\frac{du_j}{dt} \right]^2 - \tfrac{1}{2} g_j (u_{j+1}-u_j)^2 - \tfrac{1}{2}\varepsilon_j \left[1-\cos\frac{2\pi u_j}{a} \right] \right] . \tag{6.1}$$

Considering a single-point impurity, we put

$$\varepsilon_j=\varepsilon+\Delta\varepsilon\delta_{j0}, \quad \Delta\varepsilon=E-\varepsilon , \tag{6.2a}$$

$$m_j=m+\Delta m\delta_{j0}, \quad \Delta m=M-m , \tag{6.2b}$$

$$g_j=g+\Delta g\delta_{j0}, \quad \Delta g=G-g , \tag{6.2c}$$

where the parameters E, M, and G are those related to the impurity.

Introducing the dimensionless variables,

$$\tau=(c/a)t, \quad \phi_j=(2\pi/a)u_j \tag{6.3}$$

and setting

$$\mu=a/l , \quad l=c/\omega_0 , \quad c^2=ga^2/m , \quad \omega_0^2=2\pi^2\varepsilon/ma^2 , \tag{6.4}$$

the Lagrangian (6.1) becomes

$$L=A\sum_j \left[\frac{1}{2} \left[\frac{d\phi}{d\tau} j \right]^2 \left[1+\frac{\Delta m}{m}\delta_{j0} \right] - \frac{1}{2} \left[1+\frac{\Delta g}{g}\delta_{j0} \right] (\phi_{j+1}-\phi_j)^2 - \mu^2 \left[1+\frac{\Delta\varepsilon}{\varepsilon}\delta_{j0} \right] (1-\cos\phi_j) \right] , \tag{6.5}$$

where $A=m(c/2\pi)^2$. In the notations (6.4), the parameter μ has the sense of a ratio of the lattice spacing a to the kink width l, and c is the sound velocity. We now assume that the coupling constant μ^2 between the lattice and the periodic potential is a small parameter. With this assumption, the distorted kink can reasonably be approximated by the ansatz (see, e.g., Refs. 6, 49, and 62)

$$\phi_j(\tau)=4\tan^{-1}(\exp\mu\xi_j) , \tag{6.6}$$

where

$$\xi_j=j-Y(\tau) . \tag{6.7}$$

The ansatz (6.6) is based on the well-known exact kink solution of the SG equation in the "nonrelativistic" limit (see, e.g., Ref. 34). Our aim is to derive an effective equation of motion for the kink coordinate $Y(\tau)$. Assuming the existence of the function $\phi_j(\tau)$ of the discrete variable j in the form (5.6), we can rewrite the Lagrangian (6.5) in the form

$$L/A=2\mu^2 \left[\left[\frac{dY}{d\tau} \right]^2 - 2 \right] \sum_n \cosh^{-2}(\mu\xi_n) + \frac{2\mu^2}{\cosh^2(\mu Y)} \left[\left[\frac{\Delta m}{m} \right] \left[\frac{dY}{d\tau} \right]^2 - \left[\frac{\Delta g}{g}+\frac{\Delta\varepsilon}{\varepsilon} \right] \right] , \tag{6.8}$$

where we have used the following relationships:

$$\frac{d\phi_j}{d\tau}=-\frac{2\mu}{\cosh\mu\xi_j}\frac{dY}{d\tau} , \quad 1-\cos\phi_j=2/\cosh^2\mu\xi_j , \quad \phi_{j+1}-\phi_j=4\tan^{-1}\frac{\sinh(\mu/2)}{\cosh(\mu\xi_j+\mu/2)} \simeq \frac{2\mu}{\cosh\mu\xi_j} . \tag{6.9}$$

Using the Poisson sum formula,

$$\sum_{n=-\infty}^{\infty} f(nh)h=\int_{-\infty}^{+\infty} dx\, f(x) \left[1+2\sum_{s=1}^{\infty}\cos\left[\frac{2\pi sx}{h} \right] \right] , \tag{6.10}$$

and keeping only the first-order term in Eq. (6.10) ($s=1$), we can rewrite the effective Lagrangian (6.8) in the following reduced form:

$$L/A=4\mu \left[\left[\frac{dY}{d\tau} \right]^2 - \frac{4\pi^2}{\sinh(\pi^2/\mu)}\cos(2\pi Y) \right] + \left[\left[\frac{\Delta m}{m} \right] \left[\frac{dY}{d\tau} \right]^2 - \left[\frac{\Delta g}{g}+\frac{\Delta\varepsilon}{\varepsilon} \right] \right] \times \frac{2\mu^2}{\cosh^2(\mu Y)} . \tag{6.11}$$

In the presence of dissipation and driving force, i.e., the terms $m\eta\dot{u}_j-f_j$ in the left-hand side (lhs) of Eq. (2.3), the variational principle must include the generalized force associated with the damping and driving (see details, e.g., in Ref. 62). As a result, the variational principle associated with the kink center Y leads to the generalized equation of motion

$$\frac{d^2X}{d\tau^2}=\frac{4\pi^3}{\sinh(\pi^2/\mu)}\sin\left[\frac{2\pi X}{\mu}\right]+\frac{\mu}{2\pi}F-\Gamma\frac{dX}{d\tau}+\frac{\mu}{2}\frac{\sinh X}{\cosh^3 X}\left[\left[\frac{\Delta m}{m}\right]\left[\frac{dX}{d\tau}\right]^2+\mu^2\left[\frac{\Delta g}{g}+\frac{\Delta\varepsilon}{\varepsilon}\right]\right], \quad (6.12)$$

where

$$X\equiv\mu Y\ , \quad (6.13a)$$

and the dimensionless driving force and friction coefficient are defined as

$$F=2\pi f/ga\ , \quad (6.13b)$$

$$\Gamma=\mu\eta/\omega_0\ . \quad (6.13c)$$

The value defined by the first term in the rhs of Eq. (6.12), i.e.,

$$\omega_p^2=\frac{8\pi^4}{\mu\sinh(\pi^2/\mu)}\ , \quad (6.14)$$

has the sense of the frequency of vibrations in the Peierls-Nabarro (PN) potential, the term $\omega_p^2\sin(2\pi X/\mu)$ being the PN periodic force generated by the discreteness of the chain. Note that a projection operator approach[49] using the bare ground state of the discrete SG lattice yields the similar result with the numerical coefficient 4 instead of $\pi^2/3\simeq 3.3$. Thus, the above approximation is quite good.

B. Adiabatic interaction of the kink with an impurity

First of all, it is pertinent to note that, in the absence of the discreteness effects [i.e., when the first term in the rhs of Eq. (6.12) is absent], the interaction of the SG kink with a local inhomogeneity was investigated in a number of works (see, e.g., Refs. 1, 18, 19, 38, and 56). The discreteness of the chain leads to the additional periodic potential so that the total effective potential for the kink motion may be presented as follows:

$$U_{\rm eff}(X)=U_p(X)+U_i(X)\ , \quad (6.15a)$$

$$U_p(X)=\frac{2\pi^2\mu}{\sinh(\pi^2/\mu)}\cos\left[\frac{2\pi X}{\mu}\right]\ , \quad (6.15b)$$

$$U_i(X)=\left[\frac{\Delta g}{g}+\frac{\Delta\varepsilon}{\varepsilon}\right]\frac{\mu^3}{4\cosh^2 X}\ , \quad (6.15c)$$

and the motion equation may be rewritten in the form ($F=\Gamma=0$)

$$\frac{d^2X}{d\tau^2}=-\frac{dU_{\rm eff}(X)}{dX}+\frac{\mu}{2}\left[\frac{\Delta m}{m}\right]\left[\frac{dX}{d\tau}\right]^2\frac{\sinh X}{\cosh^3 X}\ . \quad (6.16)$$

As follows from Eqs. (6.15c) and (6.16), the effect of two terms $\sim\Delta g$ and $\sim\Delta\varepsilon$ is the same, but the mass impurity gives an additional contribution to the effective equation (6.16) which cannot be included into the effective potential $U_{\rm eff}(X)$.

First, we will consider the case $\Delta g\neq 0$, $\Delta\varepsilon\neq 0$, $\Delta m=0$, when the kink dynamics is determined by the effective potential (6.15). In this case, Eq. (6.16) conserves the effective energy

$$E_k=\tfrac{1}{2}X_\tau^2+U_{\rm eff}(X)=\text{const}\ , X_\tau\equiv\frac{dX}{d\tau}\ , \quad (6.17)$$

and the system dynamics on the phase plane (X_τ, X) is determined by the dependence

$$X_\tau=\pm[2E_k-U_{\rm eff}(X)]^{1/2}\ ,$$

and it is shown in Fig. 4. The potential $U_{\rm eff}$ consists of the frequently oscillating PN potential U_p (with the period $\mu\ll 1$) and the slowly varying impurity potential U_i. Far from the impurity ($|X|\gg 1$), the kink velocity is modulated by the PN potential, and, at small velocities, the kink may be pinned by a PN well. The impurity potential U_i reaches its extremum at $X=0$,

$$U_i(0)=\tfrac{1}{4}\mu^3\left[\frac{\Delta g}{g}+\frac{\Delta\varepsilon}{\varepsilon}\right]\ . \quad (6.18)$$

Thus, in the case of

$$\Delta g/g+\Delta\varepsilon/\varepsilon>0\ , \quad (6.19a)$$

the impurity potential is repulsive [see Fig. 4(a)], and the kinks with small velocities are reflected by the impurity. Clearly, in this case, the small-velocity kinks are trapped in space between such impurities. Otherwise, if

$$\Delta g/g+\Delta\varepsilon/\varepsilon<0\ , \quad (6.19b)$$

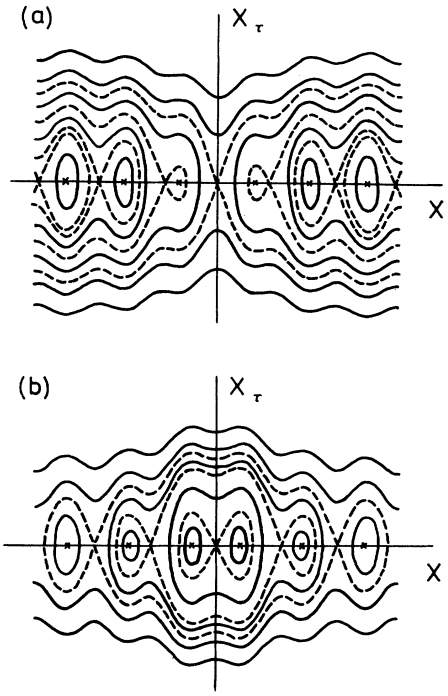

FIG. 4. The phase plane corresponding to Eq. (6.17) for (a) $(\Delta g/g+\Delta\varepsilon/\varepsilon)>0$ and (b) $(\Delta g/g+\Delta\varepsilon/\varepsilon)<0$. Separatrices are shown by dashed curves.

the impurity potential is attractive [see Fig. 4(b)], so that the kink may be pinned by the impurity and its frequency in the vicinity of the impurity is ($\mu \ll 1$)

$$\Omega^2=\left[\frac{d^2U_i}{dX^2}\right]_{X=0}=-\tfrac{1}{2}\mu^3\left[\frac{\Delta g}{g}+\frac{\Delta\varepsilon}{\varepsilon}\right] . \tag{6.20}$$

However, if the kink energy is so small that the kink is pinned by the PN well, then it oscillates with the frequency

$$\omega_j^2=\left[\frac{d^2U_{\text{eff}}}{dX^2}\right]_{X=X_j} =\omega_p^2-\tfrac{1}{2}\mu^3\left[\frac{\Delta g}{g}+\frac{\Delta\varepsilon}{\varepsilon}\right]\frac{1-2\sinh^2X_j}{\cosh^4X_j} , \tag{6.21}$$

where $X_j=\mu(j+\frac{1}{2})$, and ja is the distance from the impurity.

It is important to note that the local impurity potential U_i acts on kinks and antikinks in the same way, whenever the "external" impurity potential [see the last term in Eq. (2.3)] moves kinks and antikinks in the opposite directions.

Let us now consider the mass impurity. According to Eq. (6.16), at $\Delta g=\Delta\varepsilon=0$ the kink dynamics is described by the equation

$$\frac{d^2X}{d\tau^2}=\frac{4\pi^3}{\sinh(\pi^2/\mu)}\sin\left[\frac{2\pi X}{\mu}\right] +\frac{\mu}{2}\left[\frac{\Delta m}{m}\right]\left[\frac{dX}{d\tau}\right]^2\frac{\sinh X}{\cosh^3X} . \tag{6.22}$$

When the discreteness is absent, the kink coordinate $X(\tau)$ and its velocity $X_\tau(\tau)$ are connected by the relation

$$X_\tau(\tau)=X_\tau(0)\exp\left[-\frac{\mu}{4}\frac{\Delta m}{m}\operatorname{sech}^2X(\tau)\right] . \tag{6.23}$$

In the case of a heavy impurity ($\Delta m>0$), the kink decreases its velocity near the impurity; however, it cannot be reflected by it because of $X_\tau(\tau)\sim X_\tau(0)$ (see the phase plane shown in Fig. 5). The discreteness allows the kink to be reflected by the impurity. To analyze the kink dynamics in this case and calculate the threshold velocity, let us consider the function

$$y=X_\tau^2(\tau)\equiv y(X) . \tag{6.24}$$

Substituting Eq. (6.24) into Eq. (6.22) yields

$$y'\equiv\frac{dy}{dX}=2\epsilon_1\sin\kappa X+\epsilon_2 y\frac{\sinh X}{\cosh^3X} , \tag{6.25}$$

where we have introduced the notations

$$\epsilon_1=\frac{4\pi^3}{\sinh(\pi^2/\mu)}\equiv\frac{\mu\omega_p^2}{2\pi},\quad \epsilon_2=\mu\frac{\Delta m}{m},\quad \kappa=\frac{2\pi}{\mu} . \tag{6.26}$$

Equation (6.25) may be simply integrated to yield

$$y(X)=\exp\left[-\frac{\epsilon_2}{2\cosh^2X}\right] \left[C+2\epsilon_1\int_0^X dx'\sin(\kappa x')\exp\left[\frac{\epsilon_2}{2\cosh^2x'}\right]\right] , \tag{6.27}$$

C being an arbitrary constant. The dependence $y(X)$ is depicted in Fig. 6 for $\epsilon_2>0$. The curve at $C=0$ corresponds to the separatrix which divides two different types of the kink motion, namely, transmission ($C>0$) and reflection ($C<0$). To calculate the threshold velocity, we put $C=0$ and consider the asymptotic of Eq. (6.27) at $X\to\infty$,

$$y(X)\simeq\frac{2\epsilon_1}{\kappa}(1-\cos\kappa X)+\epsilon_1\epsilon_2\int_0^\infty dx\frac{\sin\kappa x}{\cosh^2x} . \tag{6.28}$$

The last term in Eq. (6.28) describes the shift of the phase curves due to the impurity. Using Eqs. (6.24) and (6.26), we obtain the threshold velocity for the kink reflection by

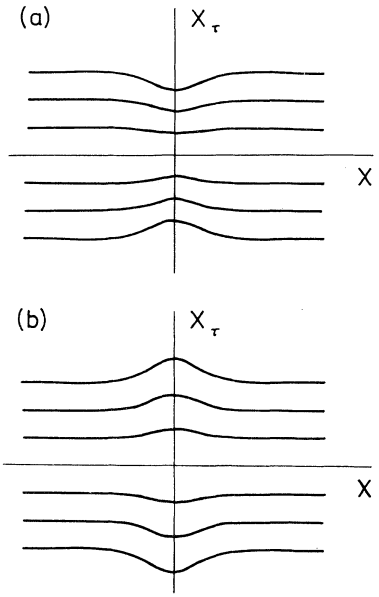

FIG. 5. The phase plane (X_τ, X) corresponding to the kink scattering by a mass impurity in the continuum approximation for (a) $\Delta m>0$ and (b) $\Delta m<0$.

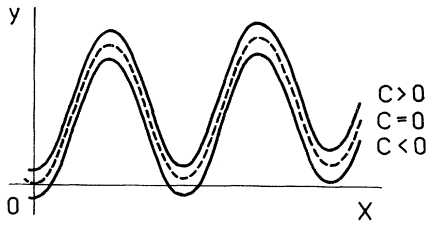

FIG. 6. The function $y=X_\tau^2$ at different values of the parameter C for $\epsilon_2>0$. The curve at $C=0$ (shown by dashed curve) is the separatrix corresponding to the threshold condition.

a heavy mass impurity

$$V_{\rm cr}=\frac{c}{\mu}\left[\frac{dX}{d\tau}\right]_{\rm cr}=\frac{c\omega_p}{\sqrt{2\pi}}\left[\frac{\Delta m}{m}\right]^{1/2} I\left[\frac{2\pi}{\mu}\right], \quad (6.29)$$

where

$$I^2(x)\equiv\int_0^\infty dy\,\sin(xy)/\cosh^2 y\ .$$

When the kink velocity V at infinity is fixed but the impurity mass is a parameter, the kink will be reflected provided

$$M>M_{\rm cr}=m+\frac{2\pi m}{\omega_p^2 I^2(2\pi/\mu)}\left[\frac{V}{c}\right]^2, \quad (6.30)$$

so that the critical mass is inversely proportional to the amplitude of the PN potential and directly proportional to the squared kink velocity.

When the dissipation and dc driving are present, the mean kink velocity is determined by the energy balance

$$V_0=cF/2\pi\Gamma=f/m\eta\ . \quad (6.31)$$

Substituting Eq. (6.31) into the threshold condition (6.29), we obtain the threshold value of the driving force allowing the kink transmission through the mass impurity

$$|f|>f_{\rm cr}=m\eta V_{\rm cr}\ , \quad (6.32)$$

$V_{\rm cr}$ being defined in Eq. (6.29).

It is interesting to note that the kink reflection by a mass impurity has been observed in numerical simulations performed for the discrete ϕ^4 system.[63] As was demonstrated in that paper, the critical mass $M_{\rm cr}$ for the kink reflection is much more than the mass of the lattice atoms and it depends on the kink velocity. According to our result (6.30), the effect is quite evident and it is determined by the discreteness effects in the nonlinear chain.

Finally, it is to be noted that the case of kink scattering by an impurity with changed dissipative losses, when $\eta_j=\eta+\Delta\eta\delta_{j0}$ in the motion equation (2.3), was considered in Ref. 38.

C. Radiative effects

Above we have used the so-called adiabatic approximation when radiative losses are neglected. However, during the scattering, the kink generates phonons, and this radiation may change the kink dynamics. The radiative effects are of three types.

The first type of radiation arises in the case when the kink propagates in a periodic external potential. The emission is caused by the discreteness effects and it is clearly absent when the PN potential vanishes. This emission was studied numerically and analytically in Refs. 47, 49, and 64. In particular, in the case of extreme discreteness ($g\lesssim 1$), the emission rate of the moving kink exhibits well-defined changes at some critical velocities.[64] The trapped kink oscillated in the nonlinear PN potential well emits large and sudden bursts of radiation when the frequency of oscillation reaches certain critical values corresponding to resonances with the linear spectrum.[49]

The second type of radiative effects is related to the kink scattering by an impurity. During the scattering the kink interacts with the impurity and generates phonons. As a result, its velocity is changed. This emission may be calculated in the lowest approximation as the kink emission in the continuum SG model with local inhomogeneities. A number of such problems was considered in the review paper.[19] The main result of such a scattering is the exponentially small emission of phonons in the limit $V\ll c$, V being the kink velocity (see details in Ref. 19).

At last, the third type of radiative effects is the excitation of an impurity mode by a scattering kink. The problem may be considered as radiative because it is stipulated by the kink energy lost due to excitation of the impurity mode oscillations. This effect was studied numerically for the ϕ^4 model.[63] Unlike the above two effects, the latter cannot be investigated in the framework of the lowest approximations of the perturbation theory.

VII. KINK DIFFUSION IN A CHAIN WITH IMPURITIES

For many applications of the FK model, for example, for surface physics, mass transport along the chain is a very important problem. As distinct from two- or three-dimensional systems, in the one-dimensional atomic chain impurities cannot be by-passed, and therefore impurities may drastically change the transport properties of the system.

In the FK model, the chemical diffusion along the chain is determined by the motion of kinks (see, e.g., Refs. 42, 65, and 66). For the temperature of the system T, which is lower then the amplitude of the PN potential E_p, the kink's motion has an activated character, so that, for the homogeneous FK chain, the kink diffusion coefficient is equal to[66]

$$D_0=Ra^2\ , \quad (7.1)$$

where a is the lattice constant, and the escape rate R is determined by the Kramers theory[67] as

$$R\simeq\frac{\omega_p}{2\pi}\exp(-E_p/kT)\ . \quad (7.2)$$

Note that here we have taken into account the energy exchange between the chain and the substrate, and suppose that the friction coefficient η has an intermediate value (see details in Refs. 42 and 60).

In the presence of impurities, the external potential for kink motion is changed. According to Eq. (6.15), the minima of the effective potential are equal to (we suppose $\Delta m=0$ for simplicity)

$$U_j=U_{\rm eff}(\mu j+\mu/2)\ , \quad (7.3)$$

and the maxima are determined by the expression

$$U_{j,j-1}=E_p+U_{\rm eff}(\mu j)\ . \quad (7.4)$$

Thus, the escape rate from the jth well to the $(j+1)$th one takes the form

$$R_{j+1,j}\simeq\frac{\omega_j}{2\pi}\exp(-E_{j+1,j}/kT)\ , \quad (7.5)$$

where the frequency ω_j is determined by Eq. (6.21), and the activation energy for the jump $j \to j+1$ is equal to

$$E_{j+1,j} = U_{j+1,j} - U_j \simeq E_p - \tfrac{1}{4}\mu^4 \left[\frac{\Delta g}{g} + \frac{\Delta \varepsilon}{\varepsilon} \right] \frac{\sinh(\mu j)}{\cosh^3(\mu j)} . \quad (7.6)$$

Let us suppose that the average distance between impurities is Na. Then the kink diffusion coefficient may be presented as

$$D = D_0 K , \quad (7.7)$$

where the value of K is determined by the escape rates (7.5) (see Ref. 68). The expression for K takes a simple form if all these minima of the external potential are equivalent, $U_j = 0$, so that

$$R_{j+1,j} = R_{j,j+1} \equiv R_j ,$$

or if all maxima of the effective potential have the same value $U_{j+1,j} = E_p$, so that

$$R_{j+1,j} = R_{j-1,j} \equiv R_j .$$

According to Ref. 69, in these cases

$$K = \langle R \rangle / R , \quad (7.8)$$

where

$$\frac{1}{\langle R \rangle} = \frac{1}{N} \sum_j^N \frac{1}{R_j} . \quad (7.9)$$

As follows from estimations[42,60] for adsystems, it is usually valid $g \sim 1$, so that the kink width $l \sim a$, and only one well or barrier, say $j = 0$, is changed significantly. In this case,

$$K = \frac{NR_0}{(N-1)R_0 + R} . \quad (7.10)$$

If $R_0 \simeq R$ or $N \gg 1$, then

$$K \simeq 1 - (R - R_0)/NR_0 .$$

For $R_0 \gg R$, we may obtain the result $K \simeq N/(N-1) \gtrsim 1$ and for $NR_0 \ll R$, $K \simeq NR_0/R \ll 1$. Therefore, the above estimations demonstrate that impurities may increase (if $R_0 \gg R$) or decrease (if $NR_0 < R$) the diffusion coefficient of the kink. Thus, the influence of impurities on transport properties of the kink-bearing systems is very important.

VIII. CONCLUDING REMARKS

We have considered the nonlinear dynamics of the FK chain with local impurities. In the linear limit, the most important dynamical effect in such an inhomogeneous chain is the appearance of impurity modes that contribute to the physical characteristics of the inhomogeneous system. The impurity modes have frequencies lying outside the spectrum zone, and they are, in fact, eigenstates of the system in the harmonic approximation. Nonlinearity leads to transformations of the impurity modes. The nonlinear impurity modes may be, in principle, constructed for various parameters of the chain, but they are stable only at the conditions when there are impurity modes in the harmonic system. Therefore, the conclusion of Refs. 50 and 51 that nonlinearity may strongly change the condition for creation of impurity modes is not valid. Note that the low-frequency modes may be considered as SG breathers pinned by inhomogeneities. The impurity modes have a long lifetime and, in principle, they may be observed in spectroscopic experiments.

The most important excitation of the FK chain is a kink, because kinks transfer a mass along the chain. For example, transport properties of stepped or furrowed crystal surfaces are mostly defined by the kink diffusion along special directions in adlayers. According to our results, the interaction of kinks with impurities may change the kink diffusion coefficient. It is interesting that the change (decreasing or increasing) depends on the total character of the kink-impurity interaction (repulsion or attraction). Note also that inhomogeneities may change the nucleation rate to create kink-antikink pairs from the vacuum (ground) state of the nonlinear chain. In such a case, the effect of repulsive impurities should be more efficient. These problems are now under consideration.

We have considered the FK chain, taking account of its applications to the system of one-dimensional atomic chains adsorbed on stepped or furrowed crystal surfaces. As was mentioned in the Introduction, the same model may be employed (in its discrete or continuum versions) to a number of various models of the condensed matter physics for which the FK model is applied. The results obtained for the dynamics of the inhomogeneous FK model may also be useful for those systems.

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