

Survival condition for low-frequency quasi-one-dimensional breathers in a two-dimensional strongly anisotropic crystal

A. V. Savin, E. A. Zubova, and L. I. Manevitch

Institute of Chemical Physics RAS, 4 Kosygin str., Moscow 119991, Russia

(Received 29 December 2004; revised manuscript received 21 March 2005; published 21 June 2005)

We investigate a two-dimensional (2D) strongly anisotropic crystal (2D SAC) on substrate: 2D system of coupled linear chains of particles with strong intrachain and weak interchain interactions, each chain being subjected to the sine background potential. Nonlinear dynamics of one of these chains when the rest of them are fixed is reduced to the well known Frenkel-Kontorova (FK) model. Depending on strength of the substrate, the 2D SAC models a variety of physical systems: polymer crystals with identical chains having light side groups, an array of inductively coupled long Josephson junctions, anisotropic crystals having light and heavy sublattices. Continuum limit of the FK model, the sine-Gordon (sG) equation, allows two types of soliton solutions: topological solitons and breathers. It is known that the quasi-one-dimensional topological solitons can propagate also in a chain of 2D system of coupled chains and even in a helix chain in a three-dimensional model of polymer crystal. In contrast to this, numerical simulation shows that the long-living breathers inherent to the FK model do not exist in the 2D SAC with weak background potential. The effect changes scenario of kink-antikink collision with small relative velocity: at weak background potential the collision always results only in intensive phonon radiation while kink-antikink recombination in the FK model results in long-living low-frequency sG breather creation. We found the survival condition for breathers in the 2D SAC on substrate depending on breather frequency and strength of the background potential. The survival condition bears no relation to resonances between breather frequency and frequencies of phonon band—contrary to the case of the FK model.

DOI: 10.1103/PhysRevB.71.224303

PACS number(s): 63.20.Ry, 05.45.-a, 63.20.Dj

I. INTRODUCTION

The Frenkel-Kontorova (FK) model (a linear chain of harmonically coupled particles on the sine background potential)¹ is the most commonly used and comprehensively investigated (see monographs)^{2,3} one-dimensional (1D) model of a crystal. In the case of weak background potential (weakly discrete system) it seems to be especially appropriate for polymer crystals: quasi-1D topological solitonlike excitations predicted by its continuum limit, the sine-Gordon (sG) equation, can propagate in a chain of a two-dimensional (2D) system of coupled chains^{4,5} and even in a helix chain in a three-dimensional (3D) model of polymer crystal (see, for example, Ref. 6). The sG equation is the only nonlinear wave equation of type

$$u_{tt} - u_{xx} + g(u) = 0 \quad (1)$$

which possesses also one-parametric family of exact solutions in the form of low-frequency breathers.⁷ Frequencies of the breathers fill the gap between zero and the minimal frequency in phonon spectrum ω_{FK} . If the breather frequency approaches ω_{FK} , the breather amplitude tends to zero, and the breather width—to infinity (“phonon” limit). If the breather frequency tends to zero, the breather approaches a full kink-antikink profile.

Although exact time-periodic space-localized solutions are absent in the FK model,⁸ numerical simulations^{9,10} show that in the FK model the sG breathers survive, and, although lose energy due to resonances of odd multiples to the breather frequency with phonon frequencies, have their lifetime long enough even in the case of strong discreteness

(10^4 – 10^5 periods when the third harmonic to its frequency is greater than the upper phonon band edge).⁹ In the case of weak discreteness the losses of energy are hardly perceptible.¹⁰

In connection with studying real physical quasi-1D systems such as long Josephson junctions and quasi-1D ferromagnets there emerged many works treating behavior of sG breathers under action of perturbations breaking exact integrability: dissipative and diverse conservative terms (see Ref. 11–13, and references therein). Analytical treatment of the problem is possible if one considers the corresponding perturbation in the inverse scattering transform¹¹ or if one obtains the multiple-scale asymptotic expansion¹² in the limit of high breather frequencies. It is also possible to derive some estimates in general case.¹³ As one can easily predict, the breather lifetime proved to be long if perturbation is small. In nonintegrable models with background potentials sufficiently different from the sine function breatherlike long-living nonlinear excitations are observed numerically (the ϕ^4 model—Ref. 14, the double sG, the square well potential—Ref. 15). For the ϕ^4 model it is shown¹⁶ that the radiation rate of a small-amplitude “breather” lies beyond all orders in asymptotic expansion.

All this allows one to look on such breathers as being “elementary excitations” in a crystal, together with kinks and antikinks (topological solitons) and phonons. This implies that the breathers can noticeably contribute to thermodynamic properties of a crystal¹⁷ and even must be used in phenomenological approaches to the sG thermodynamics instead of phonons.^{18,19}

But a real crystal (for example, a polymer one with identical chains having light side groups as polyethylene) con-

sists of all mobile chains, the moving neighbors being creating the background potential for every chain. It is interesting to investigate whether the low-frequency breathers could survive by such an extension of the FK model. The simplest generalization enough for this purpose is a 2D array of parallel linear coupled chains (intrachain interactions are much stronger than interchain ones):⁴ 2D strongly anisotropic crystal (2D SAC). Two neighboring moving chains create the background potential for every chain, and the system possesses translational invariance exactly as a genuine 3D crystal.

Considering other physical situations which allow use of the FK model, one can find it useful to extend the model by imposition of the sine background potential on every chain of the array. A manifest example is an array of inductively coupled long Josephson junctions (see, for instance, review).²⁰ One can also have in mind a crystal including chains of strongly interacting light atomic groups coupled to nearly immobile heavy clusters of atoms creating a background potential (an instance is 4-methyl-pyridine crystal which includes chains of pairs of rotating methyl groups attached to heavy pyridine rings—see, for example, article).²¹ To take into account similar situations we have extended our model imposing the background sine potential on every chain (2D SAC on substrate).

The paper is organized as follows. In Sec. II we introduce the model of a 2D SAC: free and on substrate (with background potential imposed on every chain). In Sec. III we obtain phonon spectrum of the model presented. In Sec. IV we describe a low-frequency breather degradation in the free crystal. Section V is devoted to investigation of the survival condition for low-frequency breathers in the crystal on substrate. Section V contains conclusions of the investigation.

II. THE 2D STRONGLY ANISOTROPIC CRYSTAL: FREE AND ON SUBSTRATE

Let us first take a 2D array of parallel linear coupled chains (intrachain interactions are much stronger than interchain ones) of (classical) particles (Fig. 1): a free 2D SAC. To catch the main physical meaning of the model it is enough to allow interchain interactions only between particles of the nearest neighboring chains. Then Hamiltonian of the system is written as

$$H_0 = \sum_{m,n} \left\{ \frac{1}{2} \dot{u}_{m,n}^2 + \frac{1}{2} (u_{m,n+1} - u_{m,n} + c - c_0)^2 + \sum_{j=-\infty}^{+\infty} U(r_{m,n;j}) \right\}, \quad (2)$$

where the dot denotes time derivative, c_0 is the period of a separate chain, c —the longitudinal period of the crystal, $u_{m,n}$ is longitudinal deviation of the particle (m, n) from its equilibrium position (shown in Fig. 1) in the crystal (we keep transversal deviation $y_{m,n}=0$), the potential $U(r_{m,n;j})$ describes interaction of the n th particle in the m th chain with the $(n+j)$ th particle in the $(m+1)$ th chain, $r_{m,n;j}$ being the distance between the particles

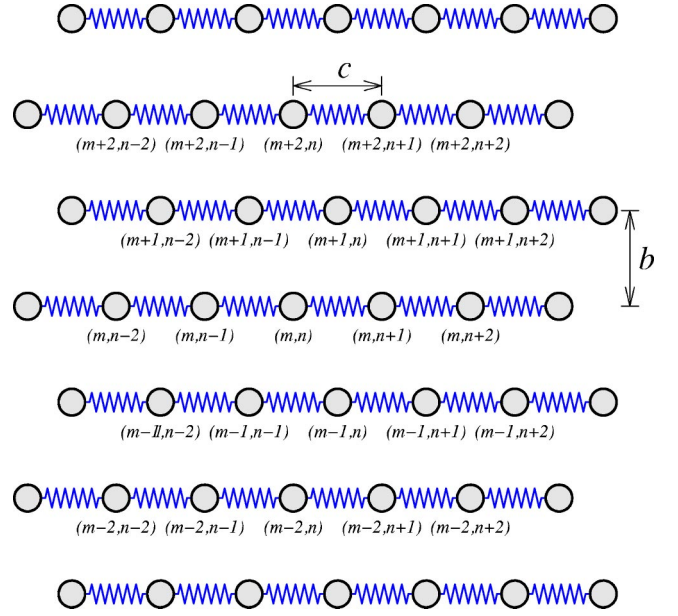


FIG. 1. The 2D strongly anisotropic crystal: 2D array of weakly coupled chains: intrachain interactions are much stronger than interchain ones (weak discreteness limit). We choose unit length so that $c=1$ in the equilibrium ground state of the free crystal. In the 2D SAC on substrate the sine potential is imposed on every chain of the free crystal so that minima of the potential coincide with equilibrium positions of the particles.

$$r_{m,n;j} = \{[(j - (-1)^m/2)c + u_{m+1,n+j} - u_{m,n}]^2 + b^2\}^{1/2}.$$

The ground state of the system ($u_{m,n} = \dot{u}_{m,n} = 0$) has the energy per particle

$$E(b, c, c_0) = \frac{1}{2} (c - c_0)^2 + \sum_{j=-\infty}^{+\infty} U(R_j),$$

where $R_j = [b^2 + c^2(j+1/2)^2]^{1/2}$ is the distance between the n th and the $(n+j)$ th particles of the m th (m is odd) and $(m+1)$ th chains. Equilibrium values of b and c minimize the expression at given c_0 . Equivalently, if one chooses c as unit length, one can find equilibrium values of c_0 and b . Hereafter we imply that the crystal is initially in its equilibrium ground state with $c=1$.

The present 2D model was first introduced in Ref. 4. One can take into account also transversal displacements of particles.⁵ The model allows existence and propagation of quasi-1D topological solitonlike excitations. The authors of the articles^{4,5} used the Morse potential for interactions between particles $U(r_{m,n;j})$ as very suitable for numerical calculations. Here we exploit the more physical Lennard-Jones potential (truncated)

$$U(r) = \varepsilon \left(\frac{r_0}{r} \right)^6 \left[\left(\frac{r_0}{r} \right)^6 - 2 \right] f(r), \quad (3)$$

where the truncation function $f(r) = \{1 - \tanh[\mu(r - d_0)]\}/2$ ($\mu \sim 1$, $d_0 \gg r_0$) is introduced for convenience of numerical calculations. It allows one to avoid taking into

TABLE I. Dependence of longitudinal s_x and transversal s_y sound velocities, characteristic frequencies ω_{\max} and ω_{FK} in the free SAC on the value of the parameter ε .

ε	s_x	s_y/b	ω_{\max}	ω_{FK}
0.07	0.7530	0.4916	2.1174	0.6952
0.007	0.9781	0.1555	2.0120	0.2197
0.0007	0.9978	0.0492	2.0012	0.0694

account interactions of the particles placed one from another farther than $r \approx d_0$.

It is known²² that if the equilibrium distance between particles r_0 falls into the interval $0.91 < r_0 < \infty$ the shape of the background potential generated by neighboring chains is close to the sine function. We have chosen $r_0 = 1.67(d_0 = 20, \mu = 2)$ because it corresponds to model of polyethylene crystal with “united atoms.”^{6,23} At this value of r_0 the background potential generated by immobile neighbors

$$V(u) = 2 \sum_{j=-\infty}^{+\infty} \{U[r_j(u)] - U(R_j)\}, \quad (4)$$

where $r_j(u) = [b^2 + (u + j + 1/2)^2]^{1/2}$ [note that $R_j = r_j(0)$], is the sine function accurate within 0.1%: $V(u) \approx \epsilon[1 - \cos(2\pi u)]$, where background potential amplitude $\epsilon = 0.1757\varepsilon$. So dynamics of one chain when the rest of them are fixed is reduced to the FK model

$$H_0^{(FK)} = \sum_n \left\{ \frac{1}{2} \dot{u}_n^2 + \frac{1}{2} (u_{n+1} - u_n)^2 + V(u_n) \right\}. \quad (5)$$

The width of a static kink of tension in the model of polyethylene crystal with united atoms (about 30 periods) coincides with the width of a static kink in our model of coupled linear chains if the intensity of interchain interactions $\varepsilon = 0.0007$. We have also considered the cases of stronger interactions $\varepsilon = 0.007, 0.07$. The first two cases correspond to limit of weak discreteness. In the last case the sound velocity in transversal direction is equal to one in longitudinal direction (see Table I). When the chains are assembled into the crystal the transversal equilibrium period appears to be $b = 1.5666$ independent on ε . Only c_0 is ε dependent.

Now let us introduce the SAC on substrate. The substrate is the sine background potential V_s imposed on every chain of the free crystal. The Hamiltonian of the system becomes

$$H = H_0 + \sum_{m,n} V_s(u_{m,n}), \quad V_s(u) = \epsilon_s [1 - \cos(2\pi u)]. \quad (6)$$

When we fix all the chains in the model except one, we get the FK model with more strong background potential

$$\begin{aligned} H^{(FK)} &= H_0^{(FK)} + \sum_n V_s(u_n) \\ &= \sum_n \left\{ \frac{1}{2} \dot{u}_n^2 + \frac{1}{2} (u_{n+1} - u_n)^2 + E [1 - \cos(2\pi u_n)] \right\}, \end{aligned} \quad (7)$$

where $E = \epsilon + \epsilon_s$. Let us introduce the parameter of “fasten-

ing” $\alpha = \epsilon_s/E$ ($0 \leq \alpha \leq 1$). In the crystal with all mobile chains on substrate the value α is the imposed part of the background potential for a chain and the value $(1 - \alpha)$ is the part created by mobile neighboring chains.

The system of equations of motion for the SAC on substrate takes the form

$$\ddot{u}_{m,n} = - \frac{\partial H}{\partial u_{m,n}},$$

$$n = 0, \pm 1, \pm 2, \dots, \quad m = 0, \pm 1, \pm 2, \dots \quad (8)$$

with the Hamiltonian (6). In numerical simulations we considered the dynamics of a bounded rectangular fragment of the crystal ($1 \leq n \leq N, 1 \leq m \leq M$) with fixed boundary conditions in both directions.

III. PHONON SPECTRUM OF THE SAC ON SUBSTRATE

As we have chosen particles numeration not coinciding with one based on translation of the crystal cell, phonon modes have the more complicated form

$$u_{2m,n} = A \exp i[q_1 n + q_2 2m - \omega t],$$

$$u_{2m+1,n} = A \exp i[q_1(n - 1/2) + q_2(2m + 1) - \omega t],$$

$$n = 0, \pm 1, \pm 2, \dots, \quad m = 0, \pm 1, \pm 2, \dots \quad (9)$$

where $A \ll 1$. Substituting the ansatz (9) into the linearized system of Eqs. (8) with imposed periodic boundary conditions in both directions one can obtain the dispersion equation

$$\begin{aligned} \Omega(q_1, q_2) &= \left(4\pi^2 \epsilon_s + 2(1 - \cos q_1) \right. \\ &\quad \left. + 4 \sum_{j=0}^{+\infty} K_j \{1 - \cos[(j + 1/2)q_1] \cos q_2\} \right)^{1/2}, \end{aligned} \quad (10)$$

where rigidities are $K_j = U'''(R_j)(j + 1/2)^2/R_j^2 + U'(R_j)b^2/R_j^3$. Values of the rigidities are in direct proportion to the parameter of interchain interaction ε ; for $\varepsilon = 0.07$ they are $K_0 = 0.199, K_1 = -0.061, K_2 = -0.014, K_3 = -0.002$.

Dispersion Eq. (10) gives the minimal

$$\omega_{\min} = \Omega(0, 0) = 2\pi\sqrt{\epsilon_s} \quad (11)$$

and the maximal

$$\omega_{\max} \triangleq \Omega(\pi, q_2) = \left(4\pi^2 \epsilon_s + 4 + 4 \sum_{j=0}^{+\infty} K_j \right)^{1/2} = (4\pi^2 E + 4)^{1/2} \quad (12)$$

possible frequencies. In the crystal without substrate ($\epsilon_s = 0$) the minimal frequency is zero (there is no lower gap in the spectrum) because in this case the crystal possesses translational invariance and there appear acoustic phonons in the spectrum. The cut of the dispersion surface (10) at $q_2 = \pi/2$

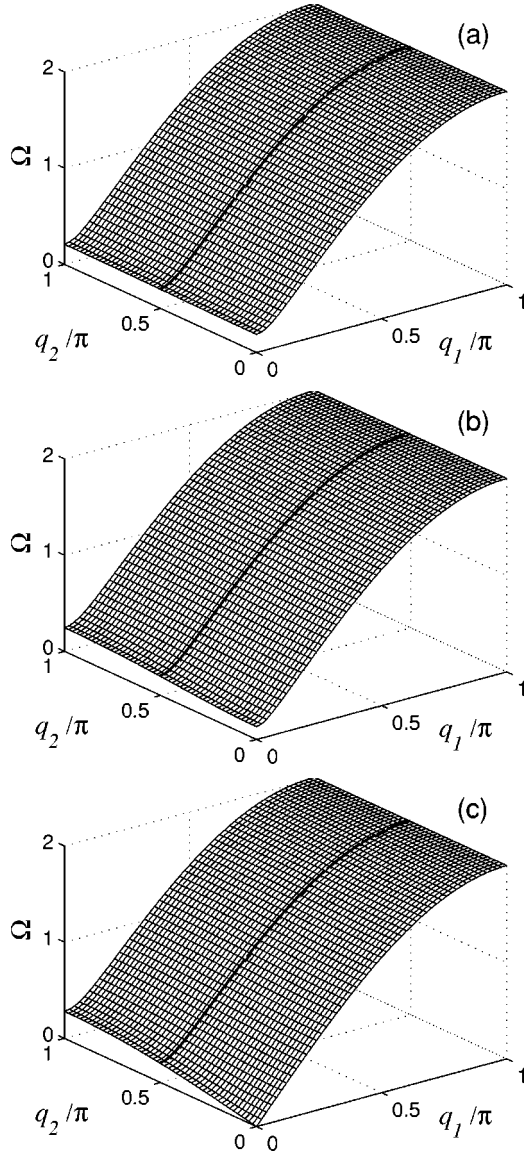


FIG. 2. Dispersion surface $\omega = \Omega(q_1, q_2)$ for the 2D SAC. The model parameters $r_0 = 1.67$, $E = 0.001$. We show the surface for three descending values of fastening parameter α : $\alpha = 0.9$ (a), $\alpha = 0.45$ (b), $\alpha = 0$ —the free crystal (c). The curve on the surface is the dispersion curve for the corresponding FK model (approximation of immobile chains) $\omega = \Omega(q_1, \pi/2)$.

produces the dispersion curve for the corresponding FK model (the crystal with only one chain mobile):

$$\begin{aligned} \Omega_{FK}(q) &= \Omega(q, \pi/2) = \left\{ 4\pi^2 \epsilon_s + 2[1 - \cos(q)] + 4 \sum_{j=-\infty}^{+\infty} K_j \right\}^{1/2} \\ &= \{4\pi^2 E + 2[1 - \cos(q)]\}^{1/2}. \end{aligned}$$

The minimal frequency for the FK model is nonzero at any value of ϵ_s :

$$\omega_{FK} = 2\pi\sqrt{E}. \quad (13)$$

We have presented the plot of the dispersion surface for $E = 0.001$ and different values of α in Fig. 2 together with the

dispersion curve for the corresponding FK model.

In the free crystal ($\epsilon_s = 0$) the velocity of longitudinal long phonons s_x and the velocity of transversal long phonons s_y equal to

$$s_x = \lim_{q_1 \rightarrow 0} \Omega(q_1, 0)/q_1 = \left[1 + \sum_{j=-\infty}^{+\infty} (j+1/2)^2 K_j \right]^{1/2},$$

$$s_y = b \lim_{q_2 \rightarrow 0} \Omega(0, q_2)/q_2 = b \left(\sum_{j=-\infty}^{+\infty} K_j \right)^{1/2}.$$

Dependence of some quantities characterizing the free crystal on the parameter of interchain interactions ϵ is presented in the Table I.

IV. LOW-FREQUENCY QUASI-1D BREATHER DEGRADATION IN THE FREE 2D SAC

We carried out all the simulations in finite crystal containing 51 chains of 400 particles each. We have imposed damping on all the boundary particles (utmost particles of every chain and all the particles of two utmost chains) so to secure absorption of phonons radiated by the breather. We chose zero initial conditions for all the chains except the central one where we started with the profile in accord with the breather solution of the sine-Gordon equation

$$u_n(t) = \frac{2}{\pi} \arctan \left\{ \frac{\sqrt{1-\nu^2}}{\nu} \frac{\sin(\nu\omega_{FK}t)}{\cosh(n\omega_{FK}\sqrt{1-\nu^2})} \right\} \quad (14)$$

($0 \leq \nu \leq 1$) because in all simulations we deal with the case of weak discreteness and we seek for stable (though may be slowly damped) solutions similar to the sG breathers, localized mainly on one chain. So we expect that if there is such a solution, and it is a stable one, it will be formed from the initial sG profile, some radiation being emitted in the act of forming and adsorbed at the utmost particles of the crystal.

Let us first compare behavior of a sG breather in the FK model [all the chains are kept immobile except one—with number $m = (M+1)/2$ —containing the breather] and in the model of crystal (all the chains are mobile) without imposed background potential. To cover situations from very weak to moderate interchain interactions we performed numerical simulations at three values of the parameter $\epsilon = 0.07, 0.007, 0.0007$.

Numerical simulation with the initial conditions according with the analytical form of the sG breather (14) showed that the sG breather in the FK model enjoys regular stable oscillations for a very long time. Figure 3(a) shows an example for the breather with frequency $\omega_b = 0.07\omega_{FK} = 0.0157$ ($\epsilon = 0.007$). We have observed at least 10^4 oscillations without visible decrease in amplitude. Analysis of the work done by the frictional force applied to the two utmost particles of the chain and the Fourier analysis of particles' oscillations showed that the breather very slowly emits phonons having

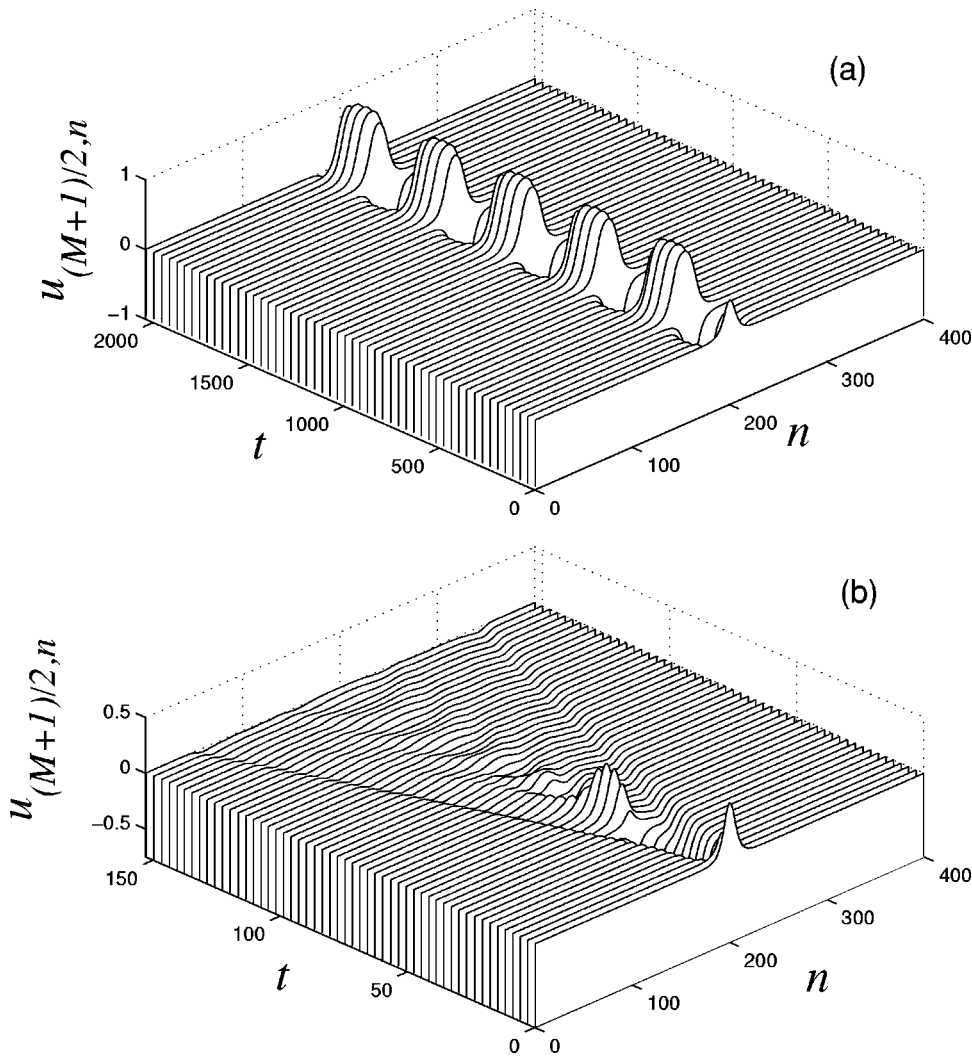


FIG. 3. Low-frequency sG breather in the free 2D SAC ($\alpha=0$, $\epsilon=0.007$, $M=51$, $N=400$): oscillations in the FK model (the case of immobile neighboring chains) (a) and degradation in the crystal with all mobile chains (b). We show the displacements $u_{26,n}$ of the 26th chain containing the breather in successive time moments t . Breather frequency is $\omega_b = 0.0157$.

frequency equal to threefold frequency of the breather. The emission is much less than one which was observed in work⁹ because we deal with the case of weak discreteness.

Then we tried to find similar quasi-1D breatherlike excitation in the crystal with all the chains mobile. We started with the same initial conditions according with (14) as in the

FK model. The simulation showed that so excited breather quickly comes to ruin. Its lifetime is less than two its periods [Fig. 3(b)]. The destruction results from the intensive emission of phonons into the neighboring chains (see Fig. 4). Energy of the excitation spreads to all the particles. So one can conclude that the low-frequency quasi-1D breathers

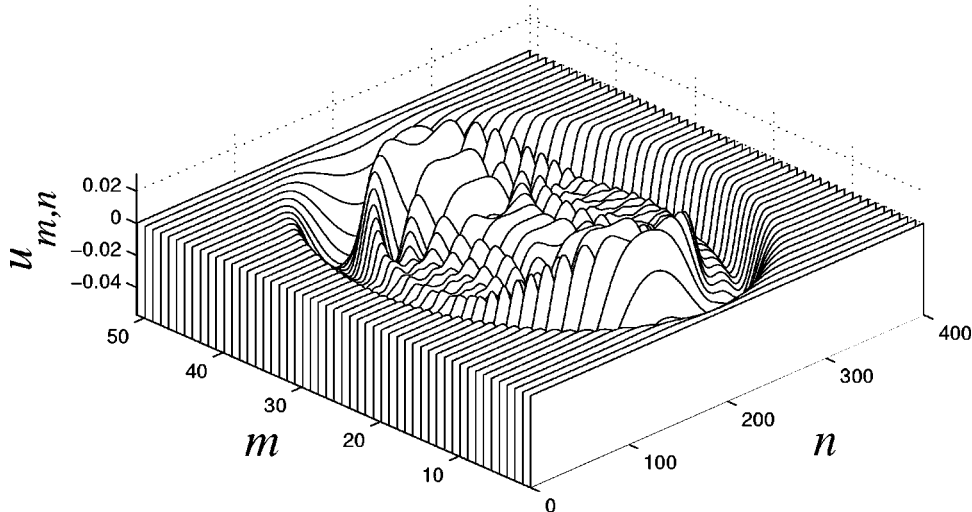


FIG. 4. State of the free 2D crystal ($\alpha=0$, $\epsilon=0.007$, $M=51$, $N=400$) resulting from destruction of a low-frequency ($\omega_b = 0.0157$) sG breather placed onto the 26th chain. The displacements $u_{m,n}$ are shown at time moment $t = 150$.

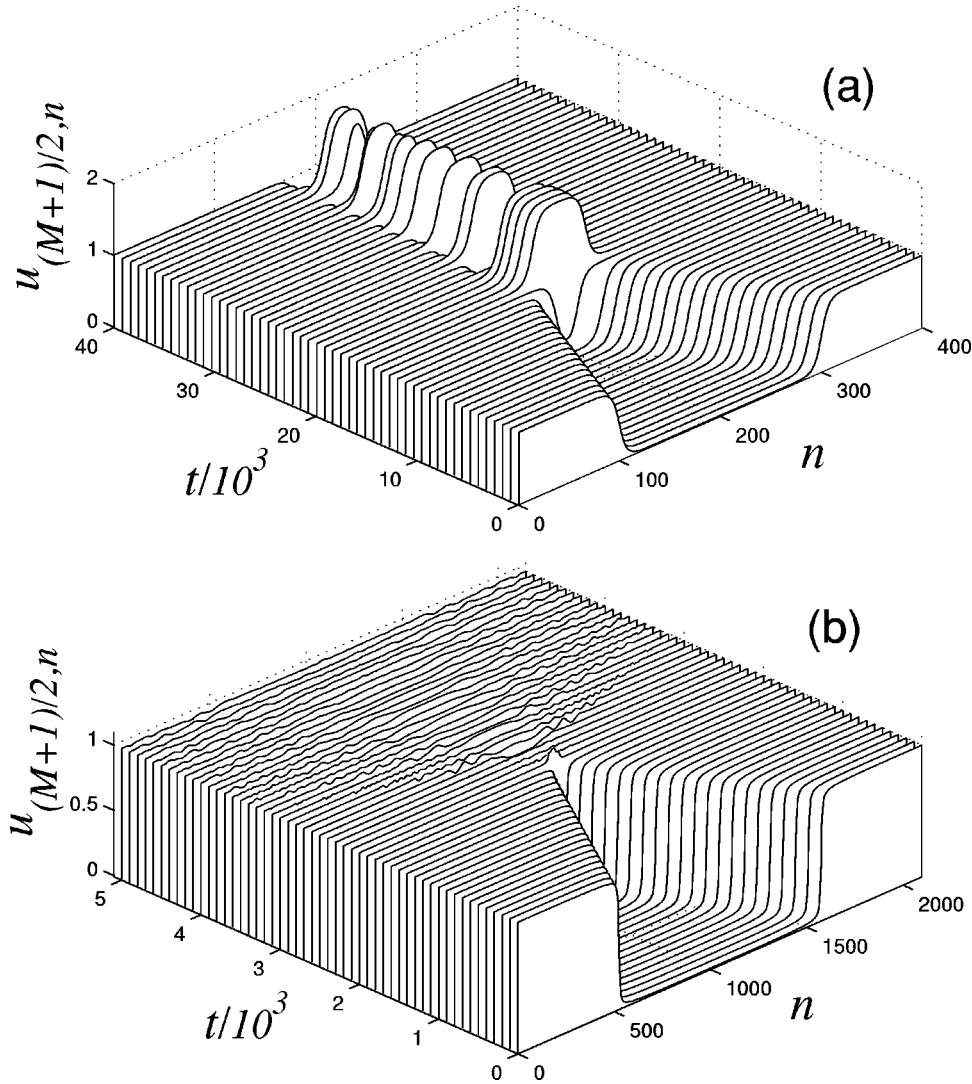


FIG. 5. Kink-antikink recombination in a chain having immobile (a) and mobile (b) neighboring chains. Collision of solitons in the FK model (soliton velocity $s = 0.005$) results in creation of a low-frequency sG breather. Collision of solitons in a chain of the free 2D SAC (soliton velocity $s = 0.25$) results in intensive radiation of phonons. Crystal parameters are $\varepsilon = 0.007$, $\alpha = 0$.

similar to the sG ones are absent in the model of free 2D crystal.

This conclusion accords with the observed difference between the two models under study in scenario of kink-antikink recombination when they collide with small relative velocity. Indeed, in the FK model (with the sine potential as well as with the double sine or the square well ones) kink and antikink can form oscillating breatherlike state, their energy remaining for a long time localized¹⁵—see Fig. 5(a), while in the model of free crystal the energy of colliding solitons scatters at once with phonons—see Fig. 5(b).

This result seems to be trivial because our free 2D SAC possesses translational invariance like a genuine one, so its phonon spectrum has not the lower gap in phonon spectrum [see Fig. 2(c)] and all the breather's frequencies fall into phonon band. Therefore the resonance interaction between a breather and a corresponding phonon must take place and the breather energy is to be transmitted to the phonons, resulting in quick breather degradation.

But situation turns out to be not so simple as that. Indeed, let us now impose the sine background potential on every chain in the array. There appears the lower gap in the phonon spectrum. Considering like before, we may suppose that the

breather with the frequency below the lower bound of the phonon spectrum will survive, while the one above it will be ruined through interaction with phonons. Let us check on this supposition.

V. LOW-FREQUENCY QUASI-1D BREATHER SURVIVAL CONDITION IN THE SAC ON SUBSTRATE

Now we exploit the full model (6). Let us choose an example $E = 0.001$. So we fix the full background potential generated by both the substrate and the mobile neighboring chains ($E = \varepsilon_s + \varepsilon$). If the neighboring chains are fixed too, we obtain the FK model where the breather form is well approximated by the sG breather (14) because $E = 0.001$ corresponds to the case of weak discreteness. If we keep the value of E , the dispersion curve of this FK model does not change. Its minimal and maximal frequencies are from (12) and (13) $\omega_{FK} = 2\pi\sqrt{E} = 0.1987$ and $\omega_{\max} = (4\pi^2 E + 4)^{1/2} = 2.01$. As we have seen in the previous section, the sG breathers with frequencies $\omega_b = \nu\omega_{FK}$ ($0 \leq \nu \leq 1$) survive in such a model.

Let us now investigate the survival of such breathers by continually changing the part of imposed background potential $\alpha = \varepsilon_s/E$ over the range $0 \leq \alpha \leq 1$. Fixed value of E conserves

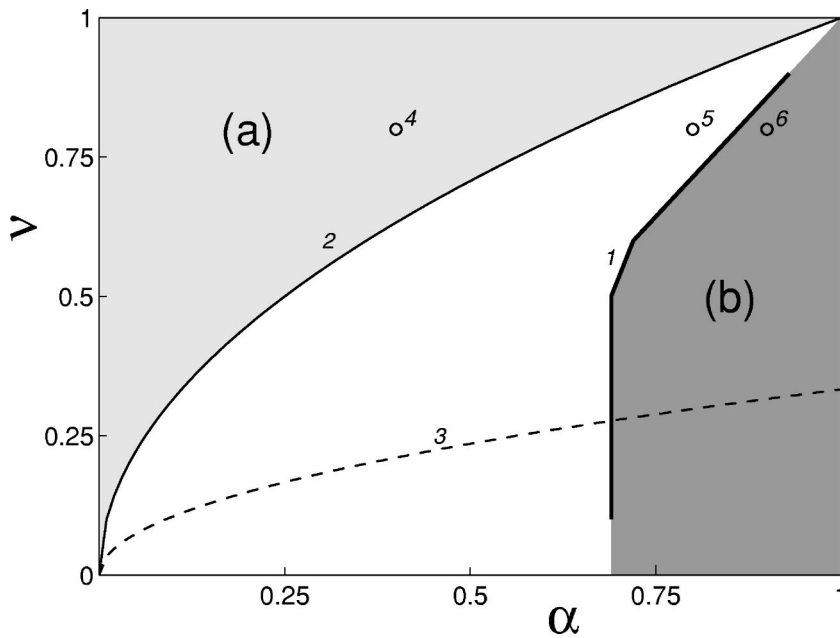


FIG. 6. Survival condition for the quasi-1D breather with the frequency $\omega_b = \nu\omega_{FK}$ in the 2D SAC on substrate ($E=0.001$) having the fastening parameter α . Curve 1 is the boundary between stable and damped breathers. It is the result of numerical experiments. The taupe area (b) is the survival zone of stable breathers. Curve 2 shows the lower frequency (divided by the frequency ω_{FK}) of phonon band in the crystal $\nu = \sqrt{\alpha}$, curve 3 is one third of the value of the curve 2. The grey area (a) is the lower part of phonon band. Points 4, 5, and 6 mark the breathers which behavior is represented in Fig. 8.

the dispersion curve of the corresponding FK model and corresponding sG breather solutions (14) which are used as initial conditions, while decreasing value of α lowers the lower bound of the phonon spectrum $\omega_{\min} = \sqrt{\alpha}\omega_{FK}$. So one should expect that the breather with frequency parameter ν in the crystal with parameter of “fastening” α will survive if $\nu \leq \sqrt{\alpha}$: if breather frequency falls into the lower gap of the phonon spectrum.

We have used the initial conditions in accord with the analytical form of the sG breather (14) (expecting, as in the previous section, that a stable quasi-1D breather will be formed from the initial sG profile) and watch the following behavior of the excitation in the same as in the previous section finite crystal having 51 chains of 400 particles each, the utmost particles of the crystal being subjected to damping force.

The result of the investigation is presented in Fig. 6. One can see that the area of parameters in which the stable quasi-1D breathers are formed, is sufficiently less than the lower gap in phonon spectrum. At weak substrate there are

no quasi-1D breathers at all, although the lower gap does exist. Comparing curves 1 and 3 one can also conclude that the position of the triple breather’s frequency relative to the phonon band has nothing to do with the survival condition as well—contrary to the case of the discrete FK model.^{9,10} One can suppose that there is another type of instability which destroys quasi-1D breathers in the crystal with interchain interactions much stronger than the substrate. In this area of parameters sufficiently 2D breathers may be stable ones instead of quasi-1D breathers which we are seeking for.

The form of the stable quasi-1D breather is shown in Fig. 7. The breather is mainly localized on one chain, only two chains next to this one have small perturbations. Fourier analysis of particles’ oscillations shows that the stable breather very slowly emits phonons having frequency equal to threefold frequency of the breather. In addition, in the frequency spectrum of the particles not belonging to the main chain the lower frequency of the phonon band is always present. The relative weight of this oscillations is the higher the father is the chain from the main one. The breath-

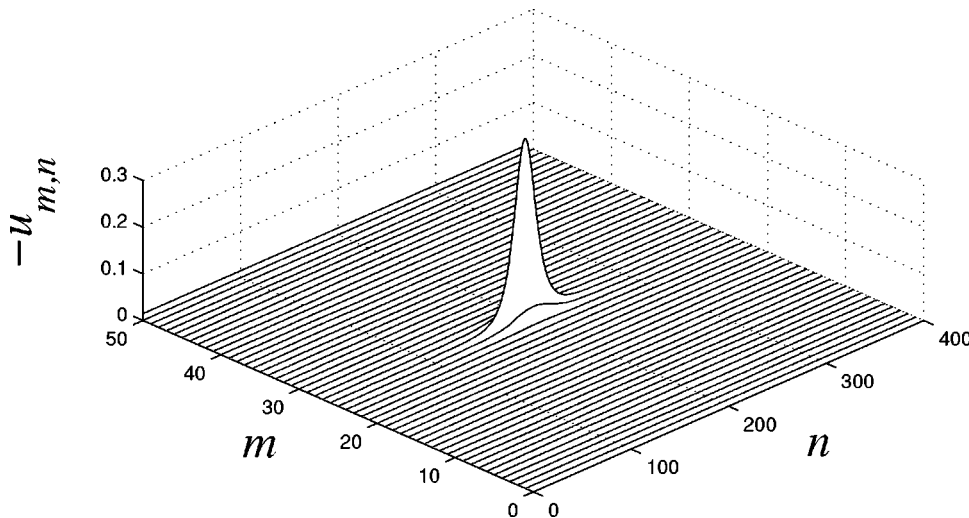


FIG. 7. Form of the stable quasi-1D breather with frequency $\omega_b = 0.8\omega_{FK}$ at time moment $t = 2640$ in the 2D SAC on substrate ($E=0.001$) having the fastening parameter $\alpha=0.9$.

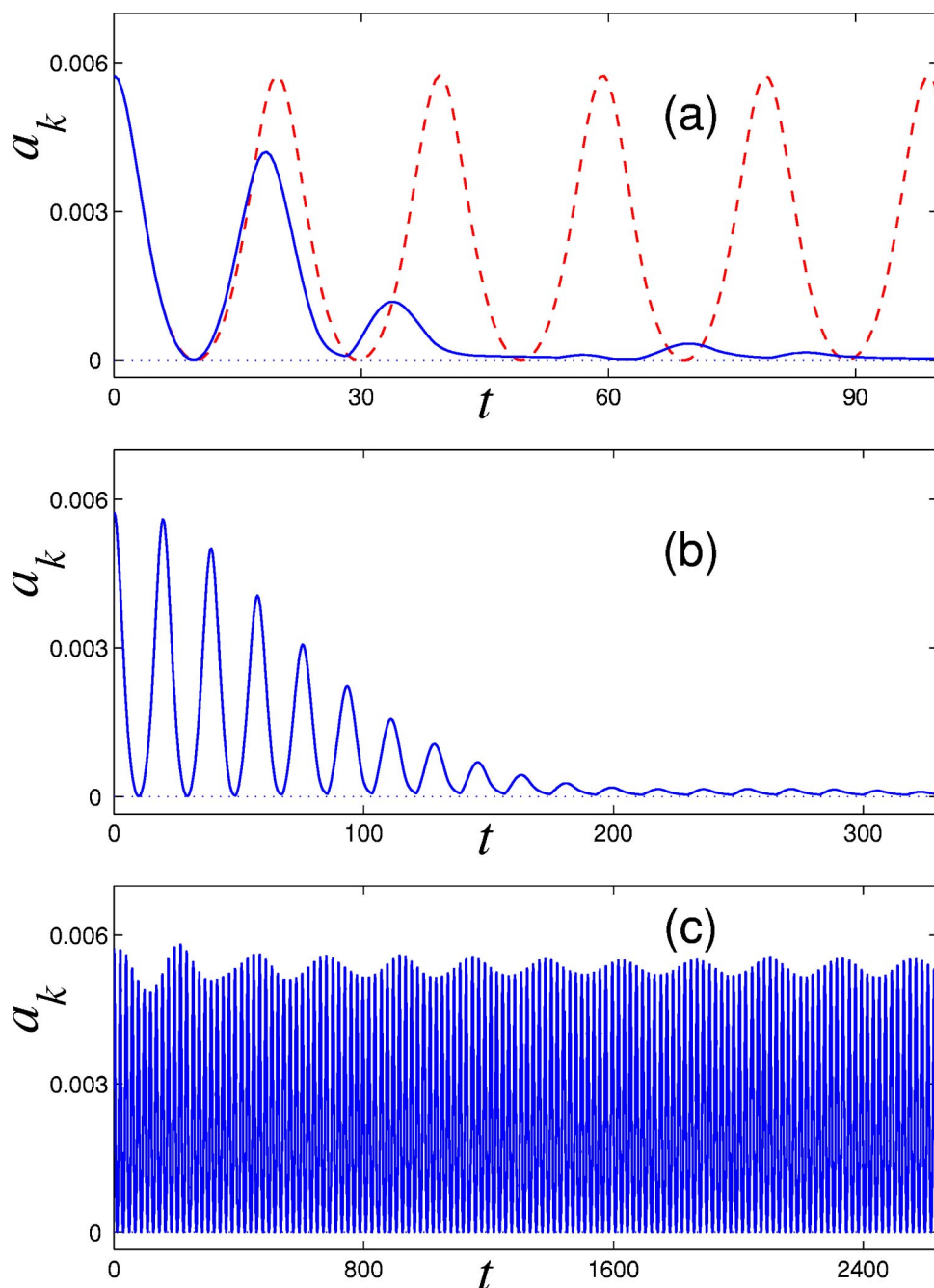


FIG. 8. Transition from the damped breather mode to the stable one in the 2D SAC on substrate ($E=0.001$). We show time dependence of function $a_k(t)=\max_n[u'_{M/2+1,n}(t)]^2$ —squared maximal velocity of particle in the chain $M/2+1$ containing breather with frequency $\omega_b=0.8\omega_{FK}$ for three values of fastening parameter α : $\alpha=0.4$ (dashed line represents the case of $\alpha=1$ for comparison) (a), $\alpha=0.8$ (b), $\alpha=0.9$ (c).

ers far away from the survival area have a finite short lifetime—see Fig. 8(a). Figures 8(a)–8(c) show a rather sharp transition from the damped mode to the stable one.

VI. CONCLUSIONS

So one can see that survival of quasi-1D low-frequency breather in 2D strongly anisotropic crystal on substrate depends mainly on the degree of fastening of the crystal. In weakly discrete case $E=0.001$ stable breather mode can exist only at strong fastening $\alpha>0.69$ for breathers with low frequencies. For breathers with higher frequencies the survival area is still more narrow. The survival condition bears no relation to resonances between breather frequency and fre-

quencies of phonon band—contrary to the case of the FK model. Low-frequency breathers can not exist as “elementary excitations” in free crystals (as crystalline polyethylene), while they can be present in crystals on substrate with strong external background potential (anisotropic crystals with heavy and light sublattices as 4-methyl-pyridine crystal).

ACKNOWLEDGMENTS

The authors thank the Russian Foundation for Basic Research (Award Nos. 04-02-17306 and 04-03-32119) for financial support. One of the authors (E.A.Z.) also acknowledges substantial help of the Russian Science Support Foundation.

- ¹T. A. Kontorova and Ya. I. Frenkel, *Zh. Eksp. Teor. Fiz.* **8**, 89 (1938) (in Russian); **8**, 1340 (1938) (in Russian).
- ²O. M. Braun and Yu. S. Kivshar, *Phys. Rep.* **306**, 1 (1998).
- ³O. M. Braun and Yu. S. Kivshar, *The Frenkel-Kontorova Model: Concepts, Methods, and Applications* (Springer-Verlag, Berlin, 2004).
- ⁴P. L. Christiansen, A. V. Savin, and A. V. Zolotaryuk, *Phys. Rev. B* **57**, 13564 (1998).
- ⁵A. V. Savin, J. M. Khalack, P. L. Christiansen, and A. V. Zolotaryuk, *Phys. Rev. B* **65**, 054106 (2002).
- ⁶E. A. Zubova, N. K. Balabaev, L. I. Manevitch, *Zh. Eksp. Teor. Fiz.* **115**, 1063 (1999) [*J. Exp. Theor. Phys.* **88**, 586 (1999)].
- ⁷S. Kitchenassamy, *Commun. Pure Appl. Math.* **44**, 789 (1991).
- ⁸J. Szeftel and G. Huang, *Eur. Phys. J. B* **27**, 329 (2002).
- ⁹R. Boesch and M. Peyrard, *Phys. Rev. B* **43**, 8491 (1991).
- ¹⁰S. V. Dmitriev, T. Shigenari, K. Abe, A. A. Vasiliev, and A. E. Miroshnichenko, *Comput. Mater. Sci.* **18**, 303 (2000).
- ¹¹A. C. Scott, *Phys. Scr.* **20**, 509 (1979).
- ¹²M. Remoissenet, *Phys. Rev. B* **33**, 2386 (1986).
- ¹³Y. S. Kivshar and B. A. Malomed, *Europhys. Lett.* **4**, 1215 (1987).
- ¹⁴A. E. Kudryavtsev, *JETP Lett.* **22**, 82 (1975).
- ¹⁵M. J. Ablowitz, M. D. Kruskal, and J. F. Ladik, *SIAM J. Appl. Math.* **36**, 428 (1979).
- ¹⁶H. Segur and M. D. Kruskal, *Phys. Rev. Lett.* **58**, 747 (1987).
- ¹⁷A. R. Bishop, *J. Phys. A* **14**, 1417 (1981).
- ¹⁸K. Sasaki, *Phys. Rev. B* **33**, 2214 (1986).
- ¹⁹S. G. Chung, *Int. J. Mod. Phys. B*, **8**, 2447 (1994).
- ²⁰A. V. Ustinov, *Physica D* **123**, 315 (1998).
- ²¹F. Fillaux and C. J. Carlile, *Phys. Rev. B* **42**, 5990 (1990).
- ²²E. A. Zubova, *Zh. Eksp. Teor. Fiz.* **120**, 1027 (2001) [*J. Exp. Theor. Phys.* **93**, 895 (2001)].
- ²³N. K. Balabaev, O. V. Gendelman, M. A. Mazo, and L. I. Manevitch, *Zh. Phys. Chim.* **69**, 24 (1995) (in Russian).