Interaction of a kink soliton with a breather in a Fermi-Pasta-Ulam chain

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The collision process between a breather and moving kink soliton is investigated both analytically and numerically in Fermi-Pasta-Ulam (FPU) chains. As it is shown by both analytical and numerical consideration low amplitude breathers and soft kinks retain their shapes after interaction. Low amplitude breather only changes the location after collision and remains static. As the numerical simulations show, the shift of its position is proportional to the stiffness of the kink soliton, what is in accordance with the analytical predictions made in this paper. The numerical experiments are also carried out for large amplitude breathers and some interesting effects are observed: The odd parity large amplitude breather does not change position when colliding with a widely separated soft kink-antikink pair, while in the case of a closely placed kink-antikink pair the breather transforms into the moving one. Therefore it is suggested that the "harmless" objects similar to the kink solitons in FPU chains could be used in order to displace or move the strongly localized structures in realistic physical systems. In particular, the analogies with quasi-one-dimensional easy-plane-type spin structures are discussed.

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I. INTRODUCTION

Chains of classical anharmonic oscillators can serve as models for more complex physical systems which under definite conditions could be treated as one-dimensional objects, e.g., optical fibers, magnetic film waveguides, quasi-one-dimensional spin systems, DNA, ionic crystals, etc. By modeling various physical processes one can directly see consequences using computer simulations and compare them with the established analytical schemes. In the present paper we propose to model different nonlinear processes in chains of coupled oscillators making simultaneous interpretations and predictions concerning real physical systems.

The one-dimensional chain of equal-mass oscillators, already the simplest model exhibits the following nontrivial phenomena such as: energy equipartition [1,2], appearance of various patterns [3] and localizations [4] (either moving [5] or static [6,7]), different regimes of chaotic dynamics [8,9], etc. Therefore these classical systems could serve as tools for better understanding of nonlinear phenomena in completely different (on first sight) many-body systems. For instance, invariance under the simple symmetry transformation $u_n \rightarrow u_n + \mathrm{const}$ (u_n is a displacement of nth oscillator) relates the Fermi-Pasta-Ulam (FPU) chain [10] (interparticle forces are functions of only relative displacements) with a wide class of systems with continuous symmetries [11], e.g., quasi-one-dimensional easy-plane ferromagnets and antiferromagnets [12], ferrimagnetic spiral structures [13], and even quantum Hall double layer (pseudo-) ferromagnets [14]. Such systems are characterized by the infinitely degenerated energy ground state. Spontaneous breakdown of the symmetry (by choosing a definite ground state) leads to the appearance of the gapless Goldstone mode forming the kink solitons in a low energy limit. These localized solutions are well known for easy-plane magnetic structures [13,15] and demonstrate similar properties as in the case of FPU chains [16,17].

The main difference between Goldstone mode kink solitons and ordinary kinks of models related to the sine-Gordon equation (particularly, its discrete analogy-Frenkel-Kantorova model [18,19]) is that the former do not carry a topological charge. Besides that, the kinks are believed to be the exact solutions [20] in the FPU chain. Because of these circumstances it is expected that they should not decay by themselves and do not destruct other localizations during the scattering process as long as no energy redistribution is required. In this connection it should be mentioned that the FPU chain, the linear spectrum of which is bounded from above, exhibits another nontrivial solution in high energy limit. This solution represents the intrinsic localized mode (discrete breather) [21,22], which in a low amplitude limit could be considered as the particular case of semidiscrete envelope soliton [23,24]. Let us note a direct analogy of the above with quasi-one-dimensional magnetic systems where similar localizations have recently been discovered [25,26] or predicted [27].

As it follows from the analytical and numerical considerations made in the present paper the kink solitons are indeed "harmless:" after interaction the shapes of both kink and breather remain unchanged. The collision only causes the shift of the position of spatially localized breather or its transformation into the slowly moving one. In this connection let us make a comparison with the strongly inelastic scattering process between kinks and breathers of the sine-Gordon equation [28,29], although it should be mentioned that in the latter case the nonlinear objects are solutions of continuous equation unlike the discrete FPU model considered in the present paper.

For analytical consideration in weakly nonlinear limit the

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multiple scale analysis will be used in order to present the quantitative picture for kink-breather collision. But first, well known solutions for kink and breather will be briefly rederived in order to introduce the method of calculations [30,31].

II. ANALYTICAL SOLUTIONS FOR KINK SOLITON AND BREATHER IN WEAKLY NONLINEAR LIMIT

The equations of motion of the FPU oscillator chain are

$$\ddot{u}_n=(u_{n+1}-u_n)+(u_{n-1}-u_n)+(u_{n+1}-u_n)^3 +(u_{n-1}-u_n)^3, \tag{1}$$

where the dots over u_n express the time derivatives. Dimensionless units are used so that the masses, the linear and nonlinear force constants, and the lattice spacing are taken equal to unity. The real displacements are expressed from dimensionless ones (u_n) by dividing the latter on the coefficient $\sqrt{K_4/m}$, where m is a mass of particle and K_4 is a coefficient before the anharmonic quartic term. Thus if the nonlinear interaction is strong enough it is permissible to have large values of u_n (e.g., $u_n \gg 1$) and this does not cause the scattering of neighboring particles.

First let us derive the kink-soliton solution by assuming that u_n smoothly varies in space time. Then it is appropriate to introduce slow variables

$$\xi_1=\varepsilon(n-v_1 t), \quad \tau_1=\varepsilon^3 t \tag{2}$$

and denote

$$u_n=\varphi_1(\xi_1,\tau_1), \tag{3}$$

where ε is a formal small parameter indicating smallness or slowness of the variables before which it appears. Substituting Eq. (3) into the motion equation (1) and collecting the terms with the same order of ε it becomes possible to treat the problem perturbatively. In particular, the velocity v_1 is determined in the second approximation over ε:

$$v_1=\pm 1. \tag{4}$$

Without the restriction of generality let us further consider the solution with negative velocity $v_1=-1$. Other solutions will be recovered simply by changing the axis direction. Finally, in the forth approximation over ε the following nonlinear equation is obtained:

$$\frac{\partial^2\varphi_1}{\partial\xi_1\partial\tau_1}+\frac{1}{24}\frac{\partial^4\varphi_1}{\partial\xi_1^4}+\frac{3}{2}\left(\frac{\partial\varphi_1}{\partial\xi_1}\right)^2\frac{\partial^2\varphi_1}{\partial\xi_1^2}=0, \tag{5}$$

which is an exactly integrable modified Korteweg–de Vries equation [32] for the function $\partial\varphi_1/\partial\xi_1$. Equation (5) was derived for the FPU chain in Refs. [16,17] and finally leads to the kink-like solution for u_n:

$$u_n=\varphi_1=\sqrt{2/3}(\arctan[e^{A\sqrt{6}(n+t+(A/2)^2t)}]), \tag{6}$$

which has a similar form to the kinks for the sine-Gordon equation but note that although the tails of the kink solution Eq. (6) correspond to the different ground states ($u_n=0$ and $u_n=\pi/\sqrt{6}$ for $n\to-\infty$ and $n\to\infty$, respectively), these ground states carry the same energy because of the mentioned symmetry $u_n\to u_n+\text{const}$. These kinks do not carry topological charge and as far as they connect degenerate ground states they can be called Goldstone mode kinks. It should also be noted that in terms of relative displacements $v_n=u_{n+1}-u_n$ this object is a discretized version of the Korteweg-de Vries soliton and therefore the definition of kink soliton is usually used in literature for its identification. The similar localized objects could be created in magnetic structures with easy plane anisotropy where their appearance also is connected with the broken symmetry Goldstone mode. The transverse component of such magnetic localization (in-plane component) has a kink-like form, while out of the easy-plane component it represents the ordinary Korteweg-de Vries soliton [13,15].

The solution Eq. (6) is valid if one can neglect the higher derivatives. This could be achieved if the following condition is satisfied for the kink stiffness:

$$6A^2 \ll 1. \tag{7}$$

Afterwards let us rederive the breather solution using multiple scale analysis presenting u_n as the multiplication of harmonic oscillation and smooth envelope function

$$u_n=\frac{\varepsilon}{2}\varphi_2(\xi_2,\tau_2)e^{i(kn-\omega t)}+\text{c.c.}, \tag{8}$$

where c.c. denotes complex conjugation and new slow variables are defined as follows:

$$\xi_2=\varepsilon(n-v_2 t); \quad \tau_2=\varepsilon^2 t. \tag{9}$$

As far as only small displacements are considered it is natural to neglect the higher harmonics working in a rotating wave approximation. Carrying out the procedure similar to the previous case (collecting terms with the same harmonics and order of ε) in the first order over ε a well known dispersion relation for linear excitations in the FPU chain is obtained:

$$\omega=\omega_k\equiv\sqrt{2(1-\cos k)}. \tag{10}$$

In the second approximation the expression for group velocity is derived:

$$v_2=\frac{\sin k}{\omega_k}\equiv\frac{d\omega_k}{dk}, \tag{11}$$

and finally we get the nonlinear Schrödinger equation for the envelope function φ_2 in the third approximation over ε:

$$i\frac{\partial\varphi_2}{\partial\tau_2}-\frac{\omega_k}{8}\frac{\partial^2\varphi_2}{\partial\xi_2^2}-\frac{3}{8}\omega_k^3|\varphi_2|^2\varphi_2=0, \tag{12}$$

which permits bright soliton solution. Thus in terms of u_n the envelope soliton solution (moving with a group velocity v_2) is rederived (see e.g., Ref. [23]):

$$u_n=\frac{B\cos(nk-\tilde{\omega}_k t)}{\mathrm{ch}[\sqrt{3/2}B\omega_k(n-v_2t)]},$$

$$\tilde{\omega}_k=\omega_k(1+(3/16)\omega_k^2B^2),\quad B\ll 1. \tag{13}$$

The breather solution is obtained by setting $v_2=0$, therefore carrier wave number $k=\pi$ (thus $\omega=2$) should be considered according to relations (10) and (11). Thus we get the expression for the low amplitude breather solution:

$$u_n=\frac{B\cos(\pi n-2t-(3/2)B^2t)}{\mathrm{ch}(B\sqrt{6}n)},\quad B\ll 1, \tag{14}$$

which coincides with the corresponding breather solution obtained in Ref. [6].

III. INTERACTION BETWEEN KINK-SOLITON AND BREATHER

A. Analytical results in weakly nonlinear limit

Now let us start the main task of the paper: analytical description of kink-breather interaction. Keeping in mind that in the absence of either kink or breather one should come to the solutions (14) or (6), respectively, I am seeking the solution in the following form (using again the rotating wave approximation):

$$u_n=\varphi_1(\xi_1,\tau_1)+\frac{\varepsilon}{2}[\varphi_2(\xi_2,\tau_2)e^{i(\pi n-2t)+i\varepsilon\Omega(\xi_1,\tau_1)}+\text{c.c.}], \tag{15}$$

where the following choice for slow space-time variables is made:

$$\xi_1=\varepsilon(n+t)-\varepsilon^2\Psi_1(\xi_2,\tau_2),\quad \tau_1=\varepsilon^3t,$$

$$\xi_2=\varepsilon n-\varepsilon^2\Psi_2(\xi_1,\tau_1),\quad \tau_2=\varepsilon^2t. \tag{16}$$

Here the phase and argument shifts are introduced in order to decouple nonlinear equations. Substituting Eq. (15) into the initial equation of motion for the FPU chain Eq. (1) we get the following two nonlinear equations in the forth order over ε for zero harmonic and in the third order over ε for the first harmonic:

$$\frac{\partial^2\varphi_1}{\partial\xi_1\partial\tau_1}+\frac{1}{24}\frac{\partial^4\varphi_1}{\partial\xi_1^4}+\frac{3}{2}\left(\frac{\partial\varphi_1}{\partial\xi_1}\right)^2\frac{\partial^2\varphi_1}{\partial\xi_1^2}+\frac{1}{2}\left[\frac{\partial^2\varphi_1}{\partial\xi_1^2}+\frac{\partial\varphi_1}{\partial\xi_1}\frac{\partial}{\partial\xi_2}\right]\left[\frac{\partial\Psi_1}{\partial\xi_2}+6|\varphi_2|^2\right]=0, \tag{17}$$

$$i\frac{\partial\varphi_2}{\partial\tau_2}-\frac{1}{4}\frac{\partial^2\varphi_2}{\partial\xi_2^2}-3|\varphi_2|^2\varphi_2-\varphi_2\left[\frac{\partial\Omega}{\partial\xi_1}+3\left(\frac{\partial\varphi_1}{\partial\xi_1}\right)^2\right]=0. \tag{18}$$

The variables ξ_1 and ξ_2 in Exp. (16) are chosen such that group velocities for noninteracting kink soliton and breather (with carrier wave number equal to π) are $v_1=-1$ and $v_2=0$, which guarantees the satisfaction of the motion equation (1) in the lower orders over ε.

By letting

$$\frac{\partial\Psi_1}{\partial\xi_2}=-6|\varphi_2|^2,\quad \frac{\partial\Omega}{\partial\xi_1}=-3\left(\frac{\partial\varphi_1}{\partial\xi_1}\right)^2, \tag{19}$$

we come again to Eqs. (5) and (12) for kink soliton φ_1 and breather φ_2 (with carrier wave number $k=\pi$). The choice Eq. (19) physically means that the interaction effects reduce only to the phase shifts of solitons while the solitons' profiles remain unchanged in the leading approximation.

Finally, in the fourth approximation over ε for the first harmonic the following equality is derived:

$$\frac{\partial\Psi_2}{\partial\xi_1}=\frac{3}{2}\left(\frac{\partial\varphi_1}{\partial\xi_1}\right)^2. \tag{20}$$

According to the last relation the breather acquires group velocity during the interaction process, but as the kink passes it stops. The shift of the breather's position could be calculated from the following simple relations:

$$l_2=\int_{-\infty}^{\infty}v_2dt=\int_{-\infty}^{\infty}\frac{\partial\Psi_2}{\partial t}dt=\int_{-\infty}^{\infty}\frac{\partial\Psi_2}{\partial\xi_1}d\xi_1=\frac{\sqrt{6}}{2}|A|, \tag{21}$$

thus the shift is always positive, i.e., the breather will be shifted opposite to the kink's propagation direction (let us remember that group velocity of the kink has been chosen to be negative) irrespective of the sign of A, therefore the shift is the same for both kink and antikink cases.

Denoting by t_1 and t_2 the times needed for the kink to travel from one side of the chain to the other in the presence or absence of the breather, one can calculate the difference $\Delta t=t_2-t_1$ using relations similar to Eq. (21). Thus one gets

$$\Delta t=2\sqrt{6}|B|. \tag{22}$$

The physical meaning of expressions (21) and (22) could be simply understood by mentioning that in the case of weakly nonlinear solitons' interaction the group velocities of the solitons change only during the interaction process. In particular, the breather acquires the nonzero velocity while interacting with the kink soliton. Simultaneously, during the same small time period the velocity of the kink soliton becomes larger than in the case of its free propagation. These circumstances cause the shift of the low amplitude breather

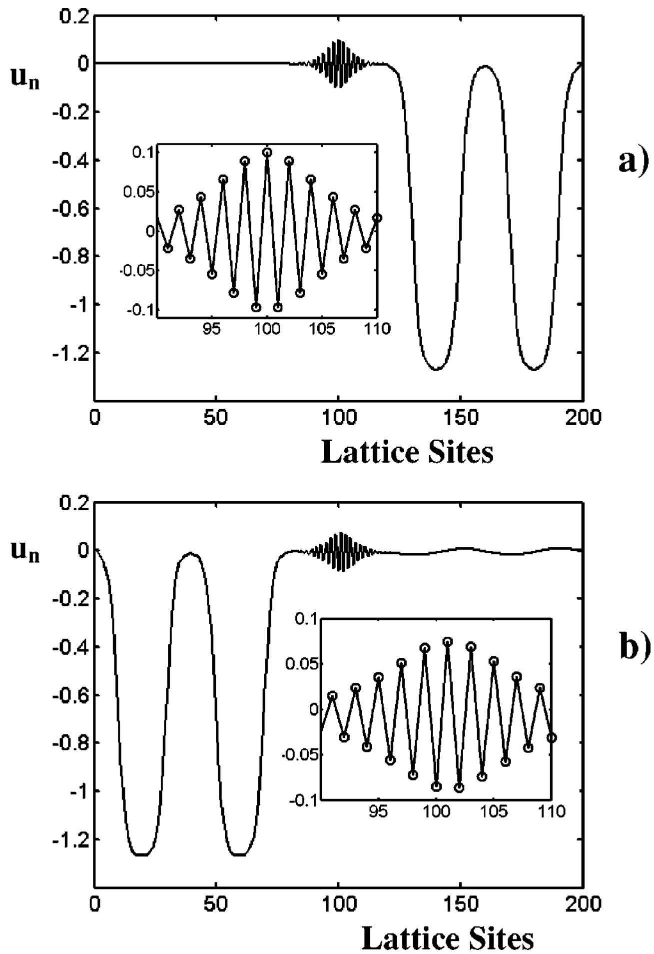

FIG. 1. Shapes and locations of kink-antikink pairs and low amplitude breather: (a) before and (b) after collision. Kink-antikink pairs move from right to the left. Insets show the enlarged view of the breather. u_n is the displacement of the nth site.

position and on the other hand the earlier arrival of the kink soliton at the left side of the chain (see Fig. 1).

B. Numerical experiments

As it was mentioned above, the direction of the shift of the breather position does not depend on whether the kink or antikink participate in the collision. Therefore in order to increase the interaction effect two kink-antikink pairs are used for collision with the breather. In the numerical experiment the soft kink solution Eq. (6) and low amplitude breather Eq. (14) are separated from each other in the FPU chain with pinned boundary conditions (see Fig. 1). A numerical experiment fully confirms analytical predictions: the nonlinear objects for which analitycal results Eqs. (6) and (14) are valid [i.e., the conditions (7) and (14) are satisfied] behave in full accordance with formulas (21) and (22). In particular, as a series of numerical experiments show, the shift of the low amplitude breather position is proportional to the kink-soliton stiffness and does not depend on its own amplitude. In Fig. 1 the collision process between two kink-antikink pairs with the same stiffness $A=0.2$ and the breather with amplitude $B=0.1$ is expressed. It is clear that the localized objects behave as expected: they retain their shapes and the low amplitude breather changes its position and after interaction becomes static again. According to Fig. 1 the shift is equal to $l_2 \approx 1$ as it expected from formula (21). Note only that as four localized objects with the same stiffness are used (two kink-antikink pairs) the value obtained from expression (21) should be multiplied by a factor of 4. The interaction also causes acceleration of the kink-antikink pair (propagation velocity of the kink-antikink pair is larger during the interaction process in comparison with free propagation) as it follows from formula (22).

Obviously, the weakly nonlinear approach fails, considering the large amplitude breather and/or stiff kink solitons. Therefore it is expected that the results could be different. Indeed, the following phenomena are monitored when colliding the soft kink-antikink pair with the strongly localized odd parity mode. The breather with an amplitude above $B \approx 0.2$ does not change the position if soft kink solitons are used for collision. Moreover, the breather does not change the position if widely separated kink solitons are used for collision. On the other hand, if there is a relatively short distance (by order of inverse stiffness) between kink and antikink the breather starts moving after collision and does not stop. This behavior is expressed in Fig. 2, where the strongly localized odd parity mode $(\ldots 0,-1/2,1,-1/2,0\ldots)$ is placed in the center of the FPU chain and different effects are monitored for different separations between kink-antikink pairs (with stiffness $A=0.25$). Apparently some kind of ''quantum'' phenomenon is caused by the fact that the single soft kink (or antikink) does not carry enough impulse to transform the static breather into the moving one, while the kink-antikink pair is able to do so. This statement is consistent with the observation of chaotic breathers (see e.g., Ref. [1]) and with the lattice quantization procedure recently proposed in Ref. [24]. It should be mentioned that all localized objects retain their shapes after interaction and the acceleration of the kink-antikink pair is still observed during the interaction process.

Considering the breathers with larger amplitudes, naturally, the stiffer kink-antikink pairs will be required to displace the breather. A number of numerical experiments have been made for breathers with larger amplitudes. The general feature is represented in Fig. 3, where the collision of odd parity mode $(\ldots,0,-1,2,-1,0,\ldots)$ and kink-antikink pair with stiffness $A=0.35$ is demonstrated. As in the previous case the breather does not change its position, colliding with the widely separated kink-antikink pair. However, in contrast to the previous case, although the breather starts to move because of the collision with the closely placed kink-antikink pair, after some time it is trapped by the lattice sites and stops.

It should be mentioned that according to the analytical results and numerical experiments the low amplitude breather acquires the group velocity only during the interaction process, while the large amplitude breather once starting to move does not stop (for intermediate amplitudes) or it will become further trapped by the lattice sites (for larger amplitudes, approximately $B>1.4$).

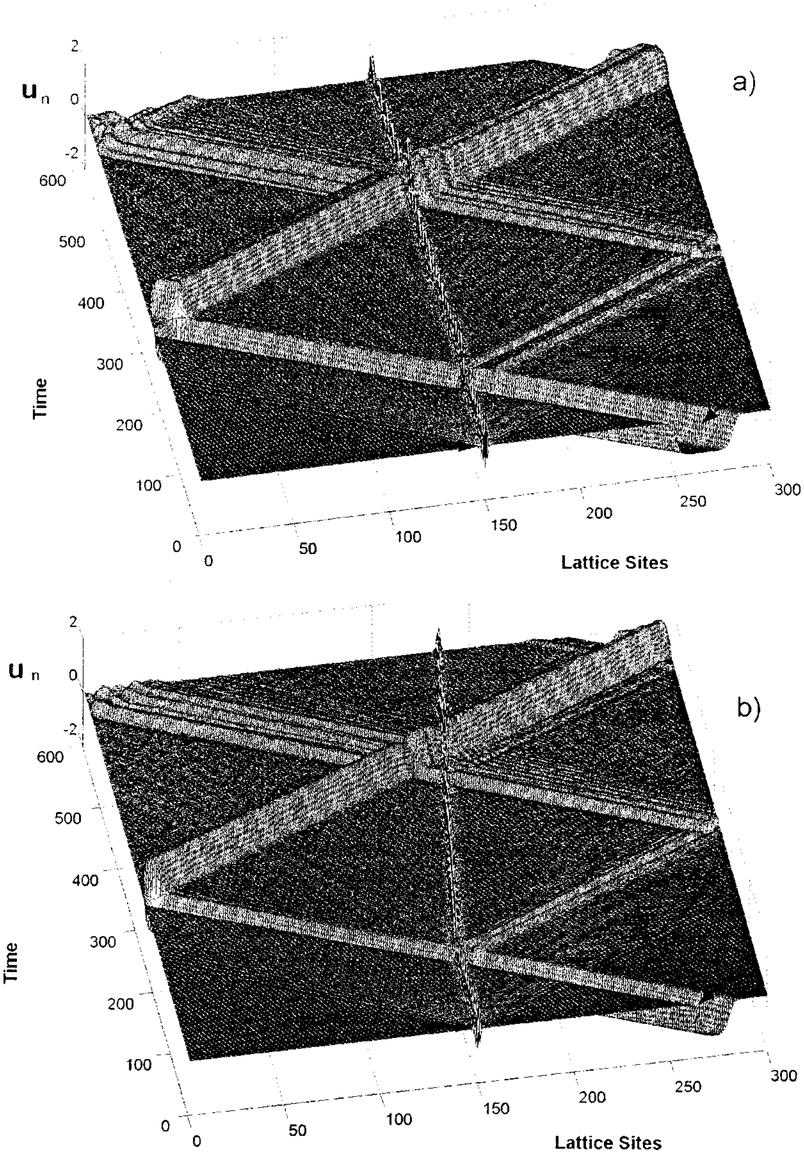

FIG. 2. (a) Collision of widely separated kink-antikink pair (stiffness $A=0.25$) with strongly localized odd parity mode (amplitude $B=1$). (b) Collision of the same breather with the closely placed kink-antikink pair. Arrows show the initial position of the kink-antikink pair.

In the present paper only the results concerning the colli sion process with odd parity mode are presented because, as numerical simulations show [21], the even parity mode spontaneously starts to move and decays after a finite time period, while the odd parity mode remains well localized in the absence of collisions with other nonlinear objects. At the same time only soft kink solitons are the subject of this study because stiff kinks sufficiently perturb the background and it is hard to see what causes displacement or pinning of the breather.

Let us mention also that reflected kink-antikink pairs almost return the low amplitude breather to its initial position, while they are unable to change the picture in the case of a large amplitude odd parity mode. As it is seen from Fig. 2, the odd parity mode with amplitude $B=1$ does not react on collision with the reflected kink-antikink pair and remains moving with the same velocity. On the other hand, the reflected kink-antikink pair cannot displace the larger amplitude breather ($B=2$) (see Fig. 3).

IV. CONCLUSIONS

Summarizing, as it is shown above, the kink solitons could be used to displace or move the static localization without the destruction of the latter. The direct analogy to the quasi-one-dimensional easy-plane magnetic structures should be quoted again. The existence of continuous U(1) symmetry in magnetization vector space for this systems allows the presence of the broken symmetry Goldstone mode, which because of the existing nonlinearity forms the kink soliton. These large wavelength nonlinear excitations have been studied for easy-plane antiferromagnets in the presence of applied magnetic field along the anisotropic axis [15] and in spiral structures [13]. On the other hand it is known [12] that the band edge excitations in easy-plane type antiferromagnets form stable intrinsic localized spin wave modes (ILSMs) having an odd parity structure in a large amplitude limit. Thus, a theoretical study and corresponding realistic experiments could be planned in order to investigate and observe the effects caused by the interaction between mag-

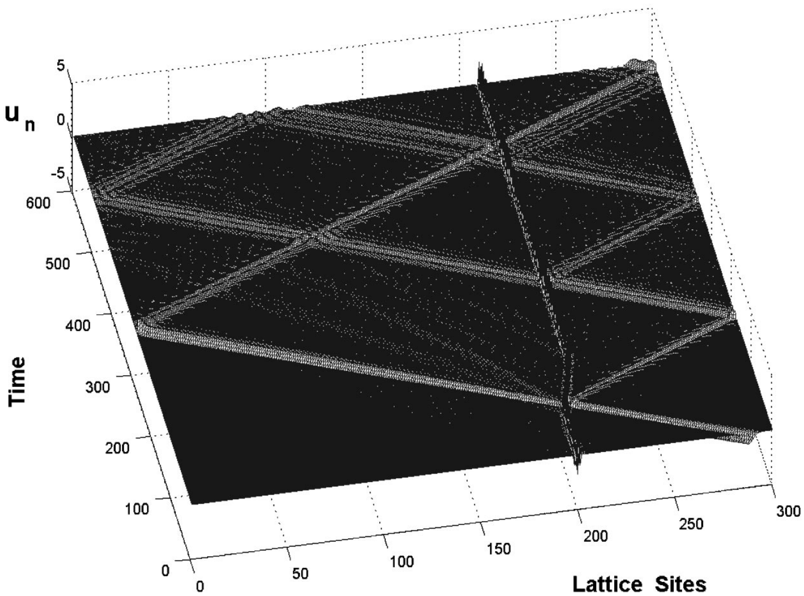

FIG. 3. Collision of closely placed kink-antikink pair (stiffness $A=0.35$) with larger amplitude ($B=2$) odd parity mode. Note that although the breather starts to move after collision (as in Fig. 2), it is further trapped by the lattice.

netization kink solitons and ILSM in quasi-one-dimensional easy-plane structures. As the analogy is almost straightforward it could be predicted that kink solitons in the easy-plane magnetic structures should cause the same effect as in FPU chains. In particular, they can displace or move the strongly localized objects without their destruction.

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