Soliton-breather reaction pathways

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We use a collective coordinate approach to investigate corpuscular properties of breathers in nonlinear lattice systems. We calculate the breather internal energy and inertial mass and use them to analyze the reaction pathways of breathers with kinks that are preformed in the lattice. We find that there is an effective kink-breather intraction potential that, under some circumstances, is attractive and has a double well shape. Furthermore, we find that in some cases the internal energy of a moving breather can be relased during the reaction with the kink and subsequently transformed to kink translational energy. These breather properties seem to be model independent. [S1063-651X(99)05411-2]

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Extended nonlinear lattice systems have been under intense scrutiny recently regarding their dynamical, transport and statistical properties [1–15]. Numerous analytical and numerical studies have demonstrated that intrinsic localized modes, or discrete breathers, forming spontaneously in nonlinear lattices, play a very important role in these properties. Discrete breathers are spatially localized, time periodic solutions of translationally invariant nonlinear lattices that are formed due to the coexistence of nonlinearity with discreteness. Breather solutions exist also in several continuous models but they are not always stable. On the other hand, in discrete models, breathers are typically stable. One very appealing feature of breathers is related to their kinematic properties; they were shown to be mobile and thus contribute to energy transfer processes in the nonlinear lattice. Many lattice systems, on the other hand, with on-site potentials that have more than one degenerate minimum, can also support topological solitons or kinks that also play an important role in the dynamical properties of the system. Kinks are more robust than breathers and require more formation energy. They also have particlelike properties that have been studied extensively over the last several decades. The aim, then, of the present article is to address both breather and kink species formed in an extended nonlinear system, focusing primarily on the particlelike properties of both. We will use the collective coordinate approach to analyze the dynamics of independent kinks and breathers and further use it to address the properties of their mutual interaction. The latter can be considered in analogy with a chemical reaction since, in many cases, the internal breather energy seems to be released to the kink. Our findings demonstrate the complexity of the breather-kink interaction and the occurrence of several reaction pathways that lead to different products. The analytical and numerical results presented here form an attempt to understand this complicated problem.

We consider the classical Hamiltonian in a standard dimensionless form:

$$H=\sum_n \left[\tfrac{1}{2}\dot{u}_n^2+\tfrac{1}{2}\kappa(u_{n+1}-u_n)^2+V(u_n)\right], \qquad (1)$$

where $u_n=u_n(t)$ is the displacement of the nth atom of the chain from its equilibrium position, an overdot stands for differentiation with respect to dimensionless time t, κ is the strength of the nearest-neighbor oscillator coupling, and V is an on-site potential normalized by $V''(0)=1$.

In this work we will be reporting results primarily for sine and double-well nonlinearity on-site potentials. In order to address the particlelike properties of discrete but relatively wide sine-Gordon breathers, we use the well known exact continuous breather solution [18]. To find the center-of-mass dynamics of the breather solution, we introduce the dynamical variables $X_B(t),\dot{X}_B(t)$, representing, respectively, the position and velocity of the breather center of mass. We use the approach of Ref. [16] and work in the continuous limit ($n=x$). Contrary to previous work [19–23], we introduce only *one* collective coordinate, namely, the position of the breather center. Therefore, on the basis of the standing breather solution, we write the following approximate *moving* breather ansatz:

$$u_B(x,t)=4\arctan\left\{\tan\mu\,\sin(\cos\mu t)\times\operatorname{sech}\left[\sin\left(\frac{\mu}{c_0}\right)(x-X_B)\right]\right\}, \qquad (2)$$

where $0<\mu<\pi/2$, and $c_0\equiv\sqrt{\kappa}$ is the dimensionless characteristic velocity. It appears the critical width for the existence of this (standing) breather solution is $\lambda_c=c_0$.

As with the breather solution, we also introduce the kink solution with a set of collective coordinates, respectively, $X_K(t), \dot{X}_K(t)$. The moving kink ansatz is

$$u_K(x,t) = 4 \arctan \exp[\pm(x - X_K)/c_0]. \tag{3}$$

Upon substitution in the continuous system Hamiltonian, summing these solutions ($u = u_B + u_K$) and elimination of all but the center-of-mass dynamical variables of the breather and kink, we obtain the averaged effective breather-kink energy that, for small velocities, reads

$$E = E_B + \frac{1}{2} M_B \dot{X}_B^2 + E_K + \frac{1}{2} M_K \dot{X}_K^2 + U(R), \tag{4}$$

with the effective interaction potential

$$U(R) = -8 \tan^2\mu \int_{-\infty}^{\infty} dx \, \mathrm{sech}^2 \frac{x-R}{c_0} \times \mathrm{sech}^2\left(\frac{\sin\mu}{c_0} x\right)\left[1 + \tan^2\mu \, \mathrm{sech}^2\left(\frac{\sin\mu}{c_0} x\right)\right]^{-3/2}, \tag{5}$$

where $R = X_B - X_K$. In these equations the expected stationary breather and kink energies and masses are given by

$$E_B = 16 c_0 \sin\mu, \quad M_B = (16/c_0)\cos\mu(\tan\mu - \mu), \tag{6}$$

$$E_K = 8 c_0, \quad M_K = 8/c_0. \tag{7}$$

For $\mu \to \pi/2$ we have $M_B = 2M_K$, while in the other extreme $\mu \to 0$ we have $M_B \to 0$.

For the kink and breather collective coordinates we calculated also the field momentum P given by

$$P = -\int_{-\infty}^{\infty} dx \overline{u_t u_x} = M_B \dot{X}_B + M_K \dot{X}_K, \tag{8}$$

where the overbar denotes the time-averaged quantity over one breather period.

These equations approximate the complicated problem of a breather interacting with a sine-Gordon kink as a problem of two classical particles of masses M_B and M_K, respectively, with internal energies E_B and E_K interacting through the complex potential $U(R)$, where R is the relative distance between the particles. In Fig. 1 we plot the breather-kink interaction potential for various breather frequencies. We observe that the potential has a double-well structure for smaller breather frequencies but switches to a single well at higher frequencies. The double-well structure signifies that there is an equilibrium distance from the kink at which the system of breather-kink can be at rest, or that the breather can excecute bounded oscillations around this minimum. This result does not seem to be specific to the sine-Gordon system. For instance, for the case of a ϕ^4 lattice with the on-site potential $V(u) = (1-u^2)^2/8$, a similar approach can be used, although the analytical calculations are considerably more difficult, since the ϕ^4 breather is not symmetric [17]. To find, in the continuum approximation, a small-amplitude breather solution to this model, we can also use the multiple-scale asymptotic expansion (for details, see, e.g., Refs. [24]) in the small parameter $\epsilon = \sqrt{1-\Omega^2}$, where Ω is the breather frequency. Substituting the expansion

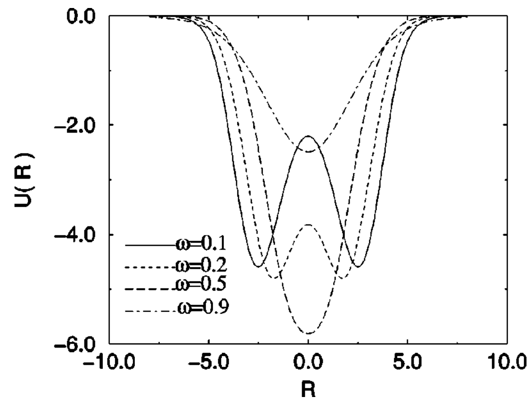

FIG. 1. Kink-breather attractive potential as a function of the dimensionless kink-breather distance R, for breather frequencies $\omega_b = 0.1$, 0.2, 0.5, and 0.9. In the regime $\omega_b \leqslant \omega_0/3$ the potential has the form of a double well.

$$u_n(t) = \pm 1 + \frac{1}{2}\epsilon[A_n e^{i\Omega t} + \epsilon D_n e^{2i\Omega t} + \text{c.c.}] + \epsilon^2 C_n + \cdots \tag{9}$$

[where the upper (lower) sign stands for oscillations in the right (left) well of the double-well on-site potential] into the discrete equation of motion and equating coefficients at the same powers of the parameter ϵ, one finds the equation

$$\kappa\epsilon^{-2}(A_{n+1} - 2A_n + A_{n-1}) - A_n \mp 3A_n C_n \mp \frac{3}{2} A_n D_n - \frac{3}{8} A_n^3 = 0 \tag{10}$$

and the relations $C_n = \mp 3A_n^2/4$ and $D_n = \pm A_n^2/4$. Using the solution in the continuum limit of these equations, one can write the corresponding (standing) breather solution:

$$u_B(x,t) = \pm 1 + \frac{2c_0}{\sqrt{3}\lambda} \mathrm{sech}\frac{x}{\lambda} \cos(\Omega t) \mp \left(\frac{c_0}{\lambda}\right)^2 \mathrm{sech}^2 \frac{x}{\lambda}\left[1 - \frac{1}{3}\cos(2\Omega t)\right], \tag{11}$$

where $\lambda = c_0/\epsilon$ is the correlation length of oscillations and the breather frequency Ω is given by $\Omega^2 = 1 - (c_0/\lambda)^2$. In the continuum limit, $\lambda \gg 1$.

Consider now the (anti)kink motion in the ϕ^4 model with sufficiently small velocities and denote the (anti)kink position by $X_K(t)$. Then for sufficiently small velocities the (anti)kink solution of Eq. (1) in the continuum limit can approximately be represented by

$$u_K(x,t) = \pm \tanh[(x - X_K)/2c_0], \tag{12}$$

where the upper (lower) sign corresponds to the kink (antikink). We are interested in the breather-(anti)kink interaction. Note that the ansatz for this interaction cannot be assumed in the *additive* form because of topological arguments. Using Eqs. (11) and (12), the additive form should be modified to

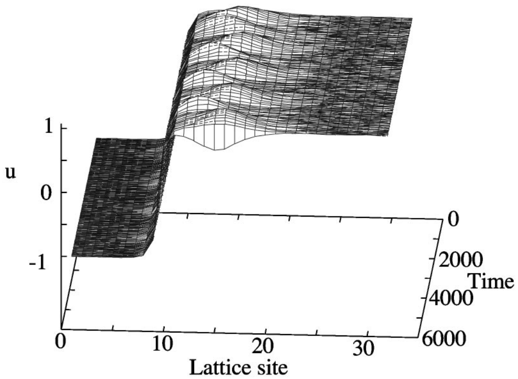

FIG. 2. Trapping of an initially static breather in the vicinity of a ϕ^4 kink. Parameters are $\omega_0^2=2$, $\omega_b=1.37819$ and coupling $k=0.301$.

$$u(x,t)=\frac{2c_0}{\sqrt{3}\lambda}\mathrm{sech}\frac{x-X_B}{\lambda}\cos(\Omega t)\pm\left\{1-\left(\frac{c_0}{\lambda}\right)^2\mathrm{sech}^2\frac{x-X_B}{\lambda}\right.$$
$$\left.\times\left[1-\frac{1}{3}\cos(2\Omega t)\right]\right\}\tanh\frac{x-X_K}{2c_0}, \tag{13}$$

where the upper (lower) sign corresponds to the interaction of a breather with a kink (antikink).

The total energy can be represented to lowest order in λ by the same sum of Eq. (4), but with

$$U(R)=\left(\frac{c_0}{\lambda}\right)^2\int_{-\infty}^{\infty}dx\,\mathrm{sech}^2\frac{x-R}{\lambda}\mathrm{sech}^2\frac{x}{2c_0}$$
$$\times\left(\frac{c_0}{\lambda}\tanh\frac{x-R}{\lambda}\tanh\frac{x}{2c_0}-\frac{1}{4}\mathrm{sech}^2\frac{x}{2c_0}-\frac{1}{2}\right). \tag{14}$$

This effective potential has the form of a single well, centered at $R=0$. Here in the lowest orders of ϵ, the breather and kink energies and masses are given by

$$E_B=4c_0^2/3\lambda,\quad M_B=4c_0^2/9\lambda^3, \tag{15}$$

$$E_K=2c_0/3,\quad M_K=2/3c_0. \tag{16}$$

Except for the well known kink relation $E_K=M_Kc_0^2$, we note a similar breather relation with low amplitudes. Indeed, for small amplitudes the correlation length of the SG breather $\lambda=c_0/\sin\mu\simeq c_0/\mu$. Using the last relation, one finds for both models the following equation: $E_B=3M_B\lambda^2$.

There is clear numerical evidence presented in Fig. 2 showing the breather trapped in the vicinity of the kink and executing small oscillations around the minimum of an effective potential. These minima can be seen in Fig. 1 in the Sine-Gordon model, but only for very small frequencies, where the breather is unstable. Numerical evaluation of the expression of Eq. (14) for the same parameters as in Fig. 2 results in a single attractive well centered around $R=0$. This indicates that for the case of the asymmetric ϕ^4 breather, additional collective coordinates are necesary for explicit prediction of the double-well feature of the kink-breather attractive potential that is seen numerically in Fig. 2. By plotting the average over one period of the breather oscillation,

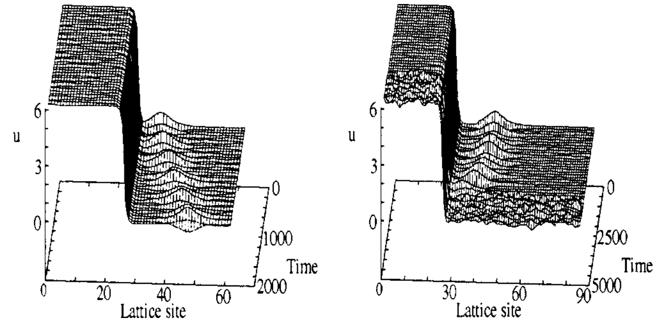

FIG. 3. (a) Breather repulsion when placed close to the center of the kink with zero initial velocity ($\omega_0=1.0$, $\omega_b=0.9844$, $k=0.251$). (b) Breather absorbion by the kink, while breather internal energy is transformed into phonons. ($\omega_0^2=2$, $\omega_b=1.3921$, $k=0.691$).

of the potential energy of the system, we see that when the breather comes close to the kink, it sees a potential barrier and it is forced to return.

The trapping of a breather in the vicinity of a kink is not the only possible breather-kink dynamical configuration. For an initially static breather-kink system, depending on the parameter regime and additional perturbations due to proximity to the discreteness regime, we may have a detrapped situation. In Fig. 3 we present numerical simulations for the sine-Gordon system with an initially static breather-kink configuration. When the breather is placed close to the kink, it is

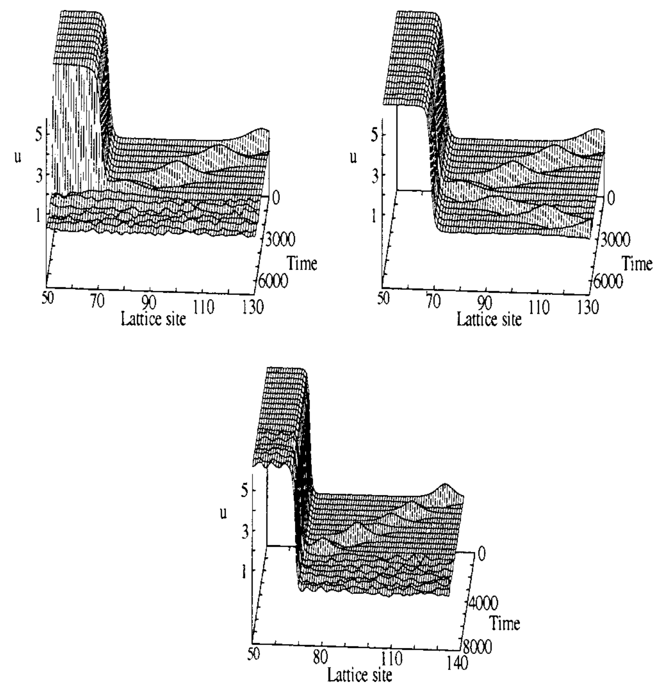

FIG. 4. (a) The breather is absorbed by the kink while its internal energy is transformed into kinetic energy for the latter. We also see that some phonons are excited. The values of the parameters are $\omega_0=1$, $\omega_b=0.9844$, coupling $\kappa=0.649$, perturbation strength $l=0.161043$ [13]. (b) In this case we increase the perturbation strength and see that the breather is reflected from the kink. The parameters are the same as in Fig. 4(a) except that $l=0.161172$. (c) In this figure we see that the breather is absorbed by the kink, and the internal energy of the kink is transformed into outgoing phonons. Parameters are $\omega_0^2=2$, $\omega_b=1.3921$, coupling $k=0.691$, and $l=0.166813$.

repelled [Fig. 3(a)], while when placed further it is attracted to the kink. In the last case, shown in the figure, we note that the breather is actually destroyed with a subsequent generation of linearized modes.

Let us finally consider the case of moving breathers impinging on the kink. To generate moving breathers we use the method of Ref. [13]. We recall that the moving breather, in addition to an inertial mass, also carries internal energy E_B. This energy can, in principle, be deposited in any lattice location whenever the breather ''reacts'' with another species, such as, for instance, a kink. This situation is seen in Fig. 4(a), where a kinetic breather reacts with the kink, releasing all internal and kinetic energy to the kink, which then begins moving. In this case, breather energy is transformed into kink kinetic energy. In Fig. 4(b), on the other hand, we observe a breather-kink elastic collision, where the breather is simply reflected from the kink with very little distortion. Finally, in Fig. 4(c) we observe a third kink-breather reaction pathway through which the breather energy is released to the vicinity of the kink with subsequent generation of linearized modes. In this case, the breather is destroyed without passing its internal energy to the kink in the form of kinetic energy.

From the previous analysis we observe that the breather-kink interaction is a complex one, leading to a variety of outcomes. From the energy transfer point of view, a breather is an efficient agent that acts as a particle with its internal structure characterized by a given amount of internal energy. It is also characterized by certain reactivity features that enable it to transfer and deposit this energy in lattice regions with kinks. The kink-breather reaction is complex, characterized by a trapping potential that depends on the breather frequency and the breather initial momentum and possibly the relative phase. For breathers with low frequencies, we find that a length scale is created within which a breather-kink bound state can be formed. Moving breathers, on the other hand, can react with kinks transforming all their energy into kink kinetic energy, or having an elastic collision with the kink. Finally, complete breather annihilation is also possible with subsequent generation of linearized extended modes.

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[1] S. Flach and C. R. Willis, Phys. Rep. **295**, 182 (1998).
[2] D. Hennig and G. P. Tsironis, Phys. Rep. **307**, 333 (1999).
[3] D. K. Campbell and M. Peyrard, Physica D **18**, 47 (1986).
[4] A. J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988).
[5] T. Dauxois and M. Peyrard, Phys. Rev. Lett. **70**, 3935 (1993).
[6] S. Aubry, Physica D **71**, 196 (1994).
[7] R. S. MacKay and S. Aubry, Nonlinearity **7**, 1623 (1994).
[8] D. Hennig, K. O. Rasmussen, G. P. Tsironis, and H. Gabriel, Phys. Rev. E **52**, 4628 (1995).
[9] D. Cai, A. R. Bishop, and N. Gronbech-Jensen, Phys. Rev. E **52**, 5784 (1995); **53**, 4131 (1996); **56**, 7246 (1997).
[10] S. Takeno and M. Peyrard, Physica D **92**, 140 (1996).
[11] S. Aubry, Physica D **103**, 201 (1996).
[12] J. L. Marin and S. Aubry, Nonlinearity **9**, 1501 (1994).
[13] Ding Chen, S. Aubry, and G. P. Tsironis, Phys. Rev. Lett. **77**, 4776 (1996).
[14] G. P. Tsironis and S. Aubry, Phys. Rev. Lett. **77**, 5225 (1996).
[15] D. W. Brown, L. Bernstein, and K. Lindenberg, Phys. Rev. E **54**, 3352 (1996).
[16] G. Kalosakas, A. V. Zolotaryuk, G. P. Tsironis, and E. N. Economou, Phys. Rev. E **56**, 1088 (1997).
[17] A. R. Bishop, P. Maniadis, G. P. Tsironis, and A. V. Zolotaryuk (unpublished).
[18] See, e.g., L. D. Faddeev and L. A. Takhtajan, *Hamiltonian Methods in the Theory of Solitons* (Springer-Verlag, Berlin, 1987).
[19] B. A. Malomed, Physica D **15**, 385 (1985); **27**, 113 (1987).
[20] Yu. S. Kivshar and B. A. Malomed, Rev. Mod. Phys. **61**, 763 (1989).
[21] Z. Fei (unpublished).
[22] E. Mann, J. Phys. A **30**, 1227 (1997).
[23] St. Pnevmatikos, Yu. S. Kivshar, M. J. Velgakis, and A. V. Zolotaryuk, Phys. Lett. A **173**, 43 (1993).
[24] A. M. Kosevich and A. S. Kovalev, Z. Éksp. Theor. Fiz. **67**, 1793 (1974) [Sov. Phys. JETP **40**, 891 (1975); T. Kawahara, J. Phys. Soc. Jpn. **35**, 1537 (1973); N. Flytzanis, St. Pnevmatikos, and M. Remoissenet, J. Phys. C **18**, 4603 (1985).