Breather Mobility in Discrete ϕ^4 Nonlinear Lattices

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We introduce a systematic approach to investigate movability properties of localized excitations in discrete nonlinear lattice systems and apply it to ϕ^4 lattices. Starting from the anticontinuous limit, we construct localized breather solutions that are shown to be linearly stable and to possess a pinning mode in the double well case. We demonstrate that an appropriate perturbation of the pinning mode yields a systematic method for constructing moving breathers with a minimum shape alteration. We find that the breather mobility improves with lower mode frequency. We analyze properties of the breather motion and determine its effective mass. [S0031-9007(96)01790-5]

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The presence of localized modes in translationally invariant extended nonlinear systems has been under investigation for some time. Spatially localized time periodic modes, or breathers, have been found for a number of continuous [1], as well as discrete, systems [2–4]. A systematic way to find breather solutions in discrete systems and analyze their properties can be done from the anticontinuous limit, i.e., starting from the limit where the coupling between the nonlinear oscillators is zero [5]. It is known rigorously that, under some very general conditions, localized solutions in that limit can be analytically continued to finite couplings [6]. Consequently, finite coupling localized modes can be found and their stability properties investigated [7,8]. Although the existence of moving breathers as mathematically exact solutions is still an open question, very long lifetime moving breathers can be found in some conditions [3,9,10]. The aim of this Letter is to provide a systematic method for constructing mobile localized oscillatory modes and to investigate some of their dynamical properties.

We consider a set of nonlinear oscillators coupled via harmonic springs with a Hamiltonian in one dimension:

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

where we consider two distinct potentials: (i) the double well with $V(u_n) = \frac{1}{4}(1 - u_n^2)^2$ and (ii) the "hard" ϕ^4 potential $V(u_n) = \frac{1}{2}u_n^2(1 + \frac{1}{2}u_n^2)$. In Eq. (1), $u_n(t) \equiv u_n$ is the displacement of the nth unit mass oscillator from its equilibrium position at time t, $\dot{u}_n$ is the corresponding velocity, and k determines the nearest neighbor coupling. To find a breather mode characterized by a frequency ω_b, we use the procedure described in Ref. [8] which we briefly describe here: At the anticontinuous limit $k = 0$, we excite a trivial single-site breather of frequency ω_b at site i by finding the necessary initial energy E_I that satisfies the equation $T_b = \int_0^{T_b} \frac{du_i}{\sqrt{E_I - V(u_i)}}$ with $T_b = 2\pi/\omega_b$. This trivial breather is extended analytically to finite couplings k through the incremental increase of the coupling value k in steps of δk. In this incremental coupling procedure, the initial breather state at coupling $k + \delta k$ is the final breather state at coupling k. At each step δk, the breather solution is a fixed point of a map $\mathcal{T}_{T_b}$ that is obtained from the lattice equations of motion, viz,

$$\ddot{u}_n - k(u_{n+1} - 2u_n + u_{n-1}) + V'(u_n) = 0. \qquad (2)$$

If we define a solution vector $\mathbf{X}(t)$ such that $X_n = (\begin{smallmatrix} u_n \\ \dot{u}_n \end{smallmatrix})$, we can view the set of Eq. (2) as the map $\mathbf{Y} = \mathcal{T}\mathbf{X}$ that propagates the initial condition $\mathbf{X}(0)$ to the solution at time t, viz, $\mathbf{X}(t) = \mathcal{T}\mathbf{X}(0)$. In this notation, the breather of period T_b is a fixed point of the map $\mathcal{T}$ *after one breather period*, viz, $\mathbf{X}(T_b) = \mathcal{T}_{T_b}[\mathbf{X}(0)] = \mathbf{X}(0)$. In order to find a fixed point of $\mathcal{T}$ evaluated at the breather period T_b, i.e., $\mathcal{T}_{T_b}$, we perform an iteration procedure. If $\mathbf{X}$ is an initial state close to the desired fixed point of the map, then a small variation $\mathbf{\Delta}$ results in $\mathcal{T}(\mathbf{X} + \mathbf{\Delta}) \approx T(\mathbf{X}) + \partial\mathcal{T}(\mathbf{X}) \cdot \mathbf{\Delta}$. A minimization with respect to $\mathbf{\Delta}$ will yield the optimal approximant to the fixed point at finite k. The variational matrix $\mathcal{M} \equiv \partial\mathcal{T}$ is a square $2N \times 2N$ matrix that forms the tangent map to the original mapping $\mathcal{T}$ while N is the number of sites considered. Since the solution we are seeking is periodic with period T_b, the matrix $\mathcal{M}$ is a Floquet matrix. It is associated with the stability of the periodic breather solutions $\{u_n, \dot{u}_n\}$ of Eq. (2) when we make the change $u_n \rightarrow u_n + \epsilon_n$ away from the same periodic breather solution u_n, with $|\epsilon_n|$ small. The equations for the perturbations $\epsilon_n(t)$ are

$$\ddot{\epsilon}_n - k(\epsilon_{n+1} - 2\epsilon_n + \epsilon_{n+1}) + V''(u_n)\epsilon_n = 0, \qquad (3)$$

where $V''(u_n)$ is a periodic function with period T_b. As a result, through the use of the eigenfunctions and eigenvalues of the Floquet matrix $\mathcal{M}$, we can accomplish two things at the same time, viz, finding the best variational breather solution at finite couplings and studying its linear stability. The symplectic matrix $\mathcal{M}$ has the form

$$\mathcal{M} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}, \qquad (4)$$

where A, B, C, D are $N \times N$ matrices.

We consider first the problem of the construction of the optimal variational breather solution at finite coupling

k. For a given approximate breather solution $\mathbf{X}$ and a variation $\boldsymbol{\Delta}$, we need to minimize the distance between the vectors $\mathbf{X} + \boldsymbol{\Delta}$ and $\mathcal{T}(\mathbf{X} + \boldsymbol{\Delta})$, viz, minimize the norm $\|(\mathcal{M} - 1) \cdot \boldsymbol{\Delta} + [\mathcal{T}(\mathbf{X}) - \mathbf{X}]\|^2$. The vector of variations $\boldsymbol{\Delta}$ has dimension $2N$ since it contains N position and N velocity variables. We perform the variation only with respect to the position coordinates, since, because of time reversibility, the breather solution can be taken initially as the static breather solution. Therefore, we take $\boldsymbol{\Delta} = \binom{\delta}{0}$, where δ is the vector of the position variations only. Minimization with respect to $\boldsymbol{\delta}$ leads to

$$\delta = -(A^*A + C^*C)^{-1}(A^*C^*)[\mathcal{T}(\mathbf{X}) - \mathbf{X}], \quad (5)$$

giving the breather solution as $\mathbf{X}' = \mathbf{X} + \binom{\delta}{0}$. In the expression of Eq. (5), $\mathcal{T}(\mathbf{X}) - \mathbf{X}$ is a vector of dimension $2N$, (A^*C^*) is a $N \times 2N$ matrix formed by placing matrices A^* and C^* adjacently in a new nonsquare matrix, $(A^*A + C^*C)^{-1}$ is an $N \times N$ matrix, and the asterisk denotes conjugation. Repeated application of this procedure and the knowledge of the matrix $\mathcal{M}$ (see below) give the optimal static breather solution at finite couplings k, such as the one shown in Fig. 1(a) for a nonlinear lattice of the double well potentials of case (i). The accuracy used for obtaining the breather was of the order of the standard computer accuracy, viz, 10^{-13}.

The general solution of the breather stability equations of Eq. (3) is

$$\epsilon_n(t) = \sum_m [A_{n,m}\epsilon_m(0) + B_{n,m}\dot{\epsilon}_m(0)], \quad (6)$$

$$\dot{\epsilon}_n(t) = \sum_m [C_{n,m}\epsilon_m(0) + D_{n,m}\dot{\epsilon}_m(0)]. \quad (7)$$

The initial conditions $\epsilon_n(0) = \delta_{n,k}$ and $\dot{\epsilon}_n(0) = 0$ yield, through Eqs. (6) and (7) after time $t = T_b$, $\epsilon_n(T_b) = A_{n,k}$ and $\dot{\epsilon}_n(T_b) = C_{n,k}$ and similarly for matrices B and D. Diagonalization of the thus obtained Floquet matrix $\mathcal{M}$ leads to the breather linear stability spectrum portrayed in Fig. 1(b). The Floquet eigenvalues are distributed in complex conjugate pairs on the unit circle, indicating stability of the corresponding eigenfrequency. The real doubly degenerate eigenvalue at unity indicates that the breather time-reversible velocity vector is also a solution of the stability equation of Eq. (4) while possible isolated eigenvalues correspond to localized internal modes of the breathers.

Whereas in the hard ϕ^4 potential no such mode exists, in the double well case the eigenvalue closest to the real unit eigenvalue marks an isolated odd parity internal breather mode. We found that this latter mode is responsible for *pinning* the breather in a specific crystal site, and thus it is by overcoming this mode that breather motion is possible. For the hard ϕ^4 potential of case (ii) with no pinning mode, breather mobility is not expected.

In order to test for breather mobility we must therefore perturb the breather using the real and imaginary parts

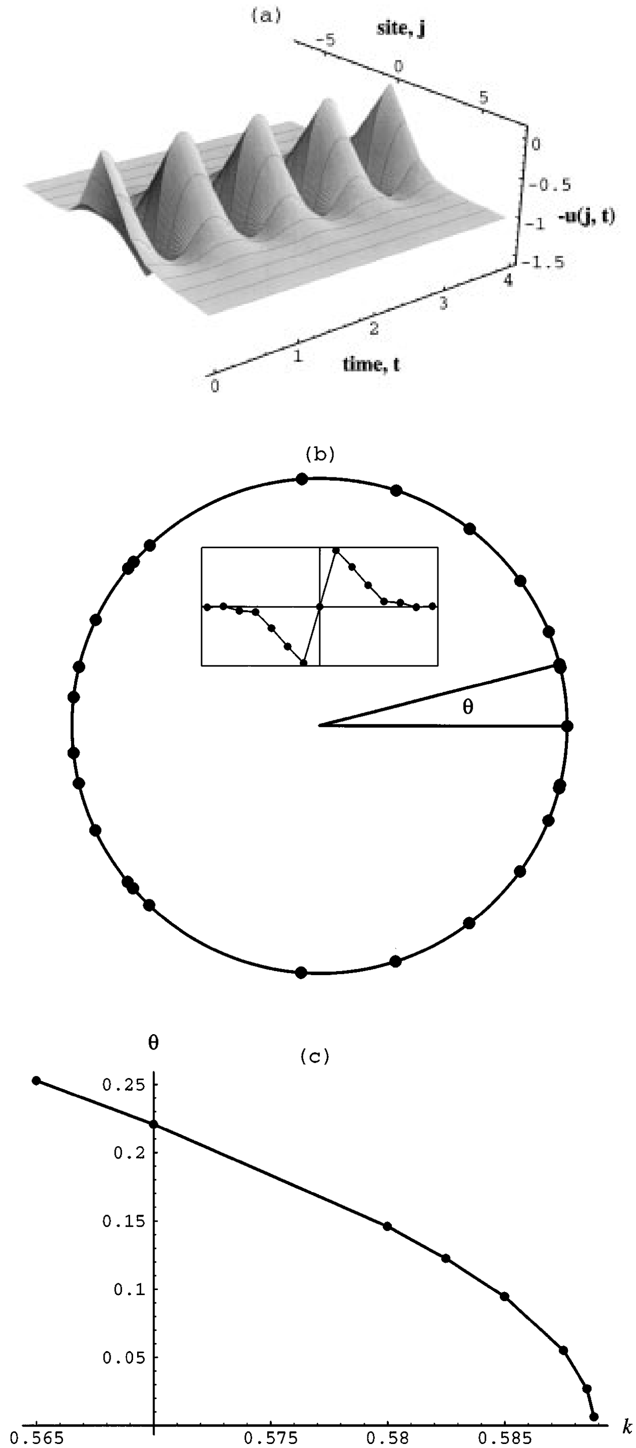

FIG. 1. Spatial breather configuration and stability. (a) Spatiotemporal display of a breather of period $T_b = 6.0$ for the double well lattice with $k = 0.5650$. (b) Distribution of the Floquet eigenvalues of the stability matrix of the breather. The distributed modes on the unit circle correspond to phonon modes that for the infinite system form two symmetric bands. The isolated eigenvalue closest to the real unity eigenvalue (denoted through the radial line) is an antisymmetric pinning mode. In the inset we show the parity of the mode. (c) Dependence of the pinning mode location in the unit circle on the coupling k. We plot the angle of the mode with respect to the positive real axis as a function of the coupling. Larger proximity to the real axis results in higher mobility.

of the Floquet eigenvector that correspond to the pinning mode found previously. Breather mobility is possible when a pinning mode is overcome by a perturbation. To find an optimal way to perturb the breather and render it mobile, the intuitive analogy with the pendulum is helpful: In order for the latter to reach the rotating solutions above the separatrix, a *kinetic* perturbation must be exerted. Thus perturbing the breather in the direction determined by the N velocity components of the $2N$-dimensional pinning mode eigenvector favors its depinning while well preserving its shape. The perturbation takes the form

$$\begin{pmatrix} u' \\ \dot{u}' \end{pmatrix} = \begin{pmatrix} u \\ 0 \end{pmatrix} + \lambda \begin{pmatrix} 0 \\ \delta p \end{pmatrix}, \quad (8)$$

where λ is the variable perturbation strength, u is the exact static breather vector (with velocity vector $\dot{u} = 0$), while the prime denotes the new values after the application of the perturbation. The perturbation vector δp corresponds to the (normalized) velocity part of the pinning mode eigenvector. We now apply this perturbation on a breather obtained through the previously described method, and follow its time evolution, integrating numerically the general equations of motion of Eq. (2). The resulting breather evolution in the lattice is portrayed in Fig. 2. In Fig. 2(a) we plot the local energy in each lattice site and observe its coherent movement in time. In Fig. 2(b) we plot the first (n_1) and second (n_2) moments of the energy distribution as a function of time. We observe that the breather moves with constant velocity in the lattice, while its shape, determined primarily through the second moment, remains intact.

A critical parameter that induces breather motion is the perturbation parameter λ. We note that the mobility of the breather depends on the proximity of the pinning mode to the real unit eigenvalue of the Floquet matrix. This, in turn, depends on the value of λ. We have found that the critical value for having a mobile breather of period $T_b = 6.0$ at $k = 0.5888$ is $\lambda_c \approx 0.0015$. For $\lambda < \lambda_c$ the breather remains pinned, while for $\lambda \geq \lambda_c$ it moves with a velocity that depends on the value of the perturbation. We have also tested perturbation forms that are more general than the one of Eq. (7) and that involve alterations of both the position and velocity part of the pinning eigenvector. We found that, in some cases, when the spatial perturbation is very large the breather still moves while emitting a substantial amount of radiation.

A useful concept for describing the breather dynamics is that of the dynamical breather mass that corresponds to the inertia of the breather to external forces. A direct way to measure the mass is by comparing the breather kinetic energy, considering the breather as a particle of mass m_b, with the perturbation kinetic energy. For the perturbation of Eq. (7) we have $m_b = (\lambda/v)^2$, where v is the breather velocity. We find that $m_b \approx 4.0$ for $\lambda \geq \lambda_c$ [Fig. 2(c)]. We can thus form

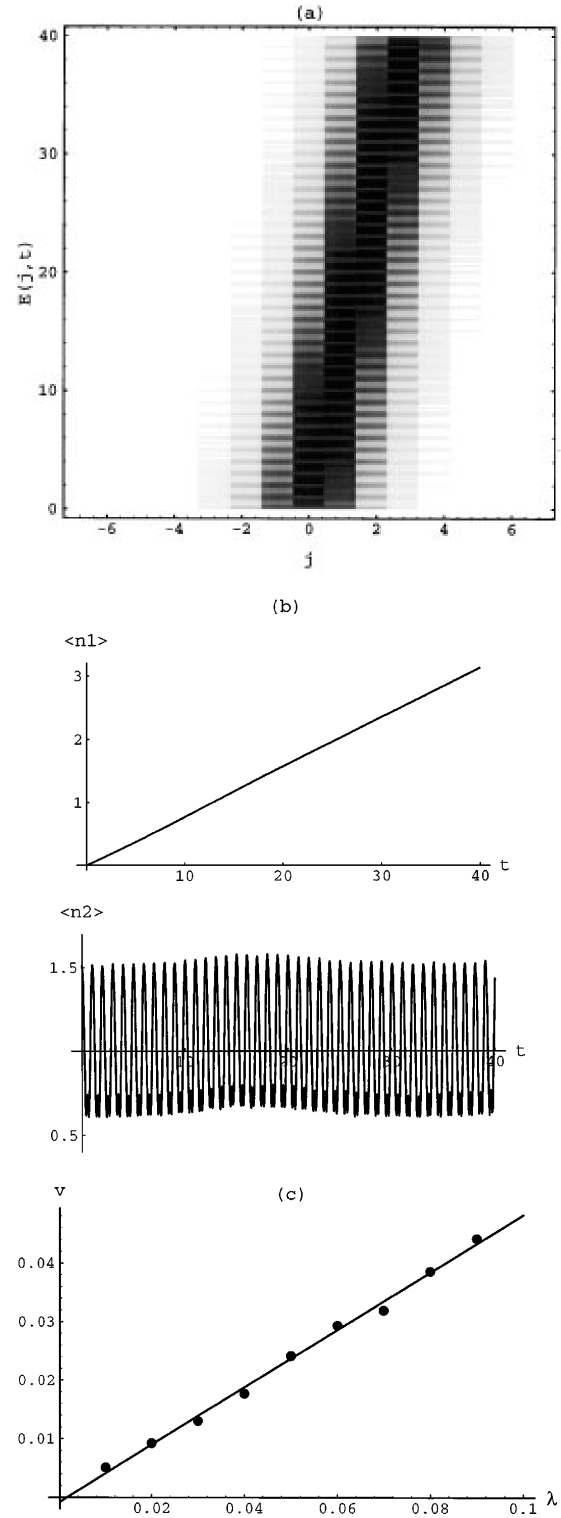

FIG. 2. Breather mobility in the double well chain. (a) Time evolution of the perturbed breather as a function of time in a periodic lattice with $N = 16$, $k = 0.5888$, and $T_b = 6.0$. The ordinate corresponds to local lattice energy at each site and the abscissa in propagation time in units of the breather period. Dark regions denote energy maxima. (b) First (n_1) and second (n_2) moments of the breather energy distribution as a function of time. (c) Linear dependence of the breather velocity on the perturbation λ for $\lambda \geq \lambda_c$. The inverse slope determines the constant inertial mass of the breather.

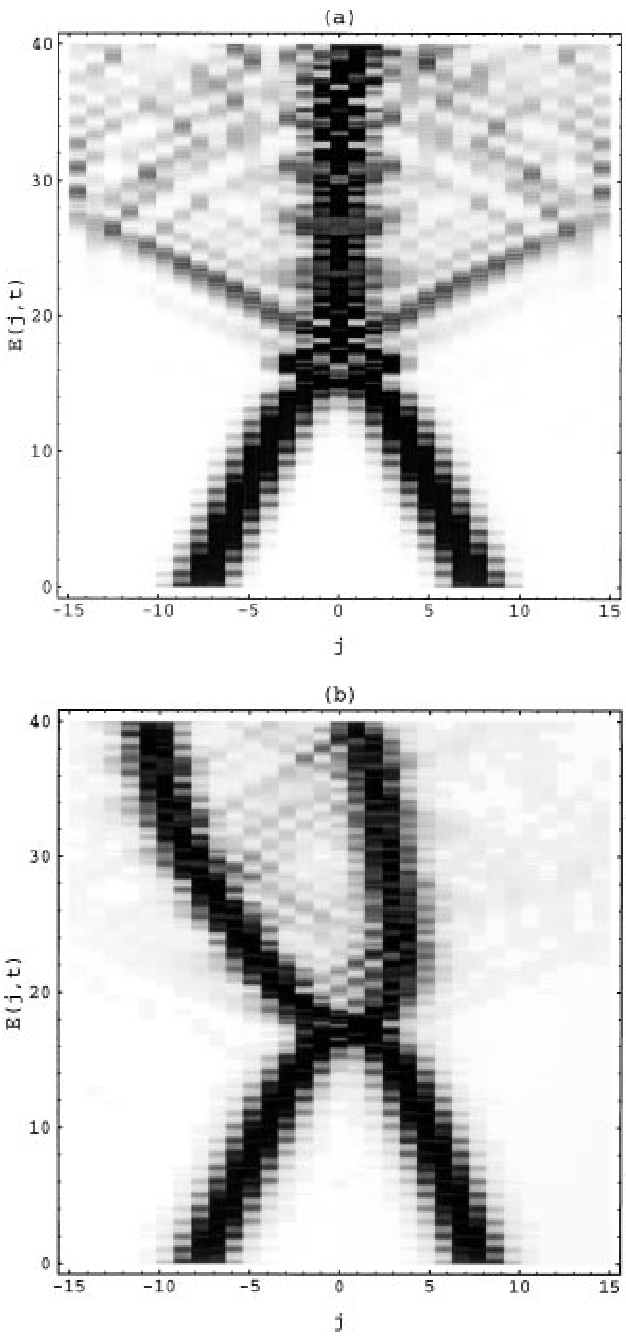

FIG. 3. Discrete breather collisions as a function of time. (a) Two identical breathers with $T_b = 6.0$ and $k = 0.5650$ are perturbed with the same (opposite in sign) perturbation with $\delta = 0.15$. After the collision they form a new localized breather mode. (b) The same breathers are given different initial perturbations with $\delta = 0.15$ (left) and 0.12 (right). Traveling breathers emerge after the collision with slightly altered velocities.

the picture of the breather being a pinned localized vibration that in the presence of an appropriate perturbation becomes mobile and moves as a classical particle of mass m_b. In this picture, it is useful to consider also interactions between mobile breathers. In Fig. 3 we show an energy density diagram with the collision of two identical breathers perturbed initially through the same [Fig. 3(a)] or different [Fig. 3(b)] velocity perturbations. At the collision site a new complex is temporarily formed that, depending on the perturbation, remains localized or emerges as two moving breathers.

The systematic method for mobile breather construction through perturbation in a pinning mode eigendirection that was demonstrated for the ϕ^4 cases applies in general and also for small amplitude breathers [11]. Furthermore, only external forces that have nonzero overlap with a pinning mode eigenvector can induce breather mobility. In particular, spatially uniform fields do not lead to breather mobility.

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