Energy Tresholds for Discrete Breathers in One-, Two-, and Three-Dimensional Lattices

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Discrete breathers are time-periodic, spatially localized solutions of equations of motion for classical degrees of freedom interacting on a lattice. They come in one-parameter families. We report on studies of energy properties of breather families in one-, two-, and three-dimensional lattices. We show that breather energies have a positive lower bound if the lattice dimension of a given nonlinear lattice is greater than or equal to a certain critical value. These findings could be important for the experimental detection of discrete breathers. [S0031-9007(97)02415-0]

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Recently progress has been achieved in the understanding of localized excitations in nonlinear lattices. Discrete breathers (DBs) are time-periodic, spatially localized solutions of equations of motion for classical degrees of freedom interacting on a lattice [1–3]. Nowadays it is known that the reason for the generic existence of DBs is the *discreteness* of the system paired with the *nonlinearity* of the differential equations defining the evolution of the system [4,5]. Thus one can avoid resonances of multiples of the discrete breather's frequency Ω_b with the phonon spectrum Ω_q of the system [6]. If the coupling is weak the phonon spectrum consists of narrow bands. The nonlinearity and the narrowness of the phonon bands allows for periodic orbits whose frequency and all its harmonics lie outside the phonon spectrum. For some classes of system, existence proofs of breather solutions have been published [7–9]. A list of references is given in [10].

For generic Hamiltonian systems, periodic orbits occur in one-parameter families, and discrete breathers are no exception. In many cases, the energy can be used as parameter along the family, but as is well known, the energy can have turning points along a family of periodic orbits. Mathematically, such a turning point in energy is called a *saddle-center periodic orbit*.

The main message of this paper is that in 3D lattices a turning point (in fact, minimum) in energy is almost inevitable for discrete breather families.

One important property of DBs is their generic existence for weak enough coupling, independent of the lattice dimension [5,7]. This means that DBs are not just a 1D curiosity but could be interesting from the point of view of applications. The experimental detection of DBs requires some additional knowledge about their properties. In this contribution we give heuristic arguments that the energy of a DB family has a positive lower bound for lattice dimension d greater than or equal to some d_c, whereas for $d < d_c$ the energy goes to zero as the amplitude goes to zero, and we confirm these predictions numerically. The critical dimension d_c depends on details of the system but is typically 2 and never greater than 2. Furthermore, for $d > d_c$, the minimum in energy occurs at positive amplitude and finite localization length. Consequently, experiments could be designed to look for activation energy thresholds for localized excitations.

Let us consider a d-dimensional hypercubic lattice with N sites. Each site is labeled by a d-dimensional vector $l \in Z^d$. Assign to each lattice site a state $X_l \in R^f$, where f is the number of components and is to be finite. The evolution of the system is assumed to be given by a Hamiltonian of the form

$$H = \sum_l H_{\rm loc}(X_l) + H_{\rm int}(X_l, \{X_{l+s}\}), \qquad (1)$$

where $H_{\rm int}$ depends on the state at site l and the states X_{l+s} in a neighborhood. We assume that H has an equilibrium point at $X_l = 0$, with $H(\{X_l = 0\}) = 0$.

DB solutions come in one-parameter families. The parameter can be the amplitude (measured at the site with maximum amplitude), the energy E, or the breather frequency Ω_b. It is anticipated (and was found both numerically and through some reasonable approximations [1]) that the amplitude can be lowered to arbitrarily small values, at least for some of the families for an infinite lattice. In this zero amplitude limit, the DB frequency Ω_b approaches an edge of the phonon spectrum Ω_q. This happens because the nonresonance condition $\Omega_q/\Omega_b \neq 0, 1, 2, 3, \ldots$ has to hold for all solutions of a generic DB family [6]. In the limit of zero amplitude, the solutions have to approach solutions of the linearized equations of motion, thus the frequency Ω_b has to approach some Ω_q, but at the same time not coincide with any phonon frequency. This is possible only if the breather's frequency tends to an edge Ω_E of the phonon spectrum in the limit of zero breather amplitude. If we consider the family of nonlinear plane waves which yields the corresponding band edge plane wave in the limit of zero amplitude A, then its frequency Ω will depend on A like

$$|\Omega - \Omega_E| \sim A^z \qquad (2)$$

for small A, where the "detuning exponent" z depends on the type of nonlinearity of the Hamiltonian (1), and can be calculated using standard perturbation theory [11].

It is tempting to check then whether the breather appears through a bifurcation from a periodic orbit which is a normal mode of the linearized equations of motion for any system with finite N. Band edge plane waves of the linearized equations of motion can be continued to nonzero amplitudes for the general nonlinear system. The stability analysis of these periodic orbits yields the possibility of tangent bifurcations (collision of Floquet multipliers at +1) if some algebraic inequalities of the expansion coefficients of H in (1) are met [12]. It has been also shown that the orbits which bifurcate from the plane wave are not invariant under discrete translations and have the shape of discrete breathers [12]. It has been conjectured that the new bifurcating orbits *are* discrete breathers. Subsequently it was successfully explained why discrete breathers exist or not for certain models by analyzing the above-mentioned algebraic inequalities [12]. Numerical studies confirm these findings [13] for some one-dimensional models.

The above-mentioned analysis of stability of band edge plane waves was carried out for systems with detuning exponent $z = 2$ and large N. The critical amplitude A_c of the plane waves at the bifurcation point depends on the number of lattice sites as $A_c \sim N^{-1/d}$ [12]. We see that the amplitudes of the new orbits bifurcating from the plane wave become small in the limit of large system size. If the energy of the system is given by a positive definite quadratic form in the variables X in the limit of small values of X it follows for the critical energy of the plane wave at the bifurcation point [12]

$$E_c \sim N^{1-2/d}. \tag{3}$$

Result (3) is surprising, since it predicts that for $z = 2$ the energy of a DB for small amplitudes should diverge for an infinite lattice with $d = 3$ and stay finite (nonzero) for $d = 2$, whereas if $d = 1$ the breather energy will tend to zero (as initially expected) in the limit of small amplitudes and large system size. The whole construction depends on the validity of the assumption that the new periodic orbits bifurcating from the plane wave through the above-mentioned tangent bifurcation are indeed DBs.

It is not known how to prove this assumption. But we can estimate the discrete breather energy in the limit of small amplitudes and compare the result with (3). Define the amplitude of a DB to be the largest of the amplitudes of the oscillations over the lattice. Denote it by A_0 where we define the site $l = 0$ to be the one with the largest amplitude. The amplitudes decay in space away from the breather center, and by linearizing about the equilibrium state and making a continuum approximation, the decay is found to be given by $A_l \sim CF_d(|l|\delta)$ for $|l|$ large, where F_d is a dimension-dependent function

$$F_1(x) = e^{-x}, \qquad F_3(x) = \frac{1}{x}\, e^{-x}, \tag{4}$$

$$F_2(x) = \int \frac{e^{-x\sqrt{1+\zeta^2}}}{\sqrt{1+\zeta^2}}\, d\zeta\,, \tag{5}$$

δ is a spatial decay exponent to be discussed shortly, and C is a constant which we shall assume can be taken of order A_0. To estimate the dependence of the spatial decay exponent δ on the frequency of the time-periodic motion Ω_b (which is close to the edge of the linear spectrum) it is enough to consider the dependence of the frequency of the phonon spectrum Ω_q on the wave vector q when close to the edge. Generically, this dependence is quadratic $(\Omega_E - \Omega_q) \sim |q - q_E|^2$ where $\Omega_E \neq 0$ marks the frequency of the edge of the linear spectrum and q_E is the corresponding edge wave vector. Then analytical continuation of $(q - q_E)$ to $i(q - q_E)$ yields a quadratic dependence $|\Omega_b - \Omega_E| \sim \delta^2$. Finally, we must insert the way that the detuning of the breather frequency from the edge of the linear spectrum $|\Omega_b - \Omega_E|$ depends on the small breather amplitude. Assuming that the weakly localized breather frequency detunes with amplitude as the weakly nonlinear band edge plane wave frequency this is $|\Omega_b - \Omega_E| \sim A_0^z$. Then $\delta \sim A_0^{z/2}$.

Now we are able to calculate the scaling of the energy of the discrete breather as its amplitude goes to zero by replacing the sum over the lattice sites by an integral

$$E_b \sim \frac{1}{2} C^2 \int r^{d-1} F_d^2(\delta r)\, dr \sim A_0^{(4-zd)/2}. \tag{6}$$

This is possible if the breather persists for small amplitudes and is slowly varying in space. We find that if $d > d_c = 4/z$ the breather energy diverges for small amplitudes, whereas for $d < d_c$ the DB energy tends to zero with the amplitude. Inserting $z = 2$ we obtain $d_c = 2$, which is in accord with the exact results on the plane wave stability [12] and thus strengthens the conjecture that discrete breathers bifurcate through tangent bifurcations from band edge plane waves. Note that for $d = d_c$ logarithmic corrections may apply to (6), which can lead to additional variations of the energy for small amplitudes.

An immediate consequence is that if $d \geq d_c$, the energy of a breather is bounded away from zero. This is because for any nonzero amplitude the breather energy cannot be zero, and as the amplitude goes to zero the energy goes to a positive limit $(d = d_c)$ or diverges $(d > d_c)$. Thus we obtain an energy threshold for the creation of DBs for $d \geq d_c$. This new energy scale is set by combinations of the expansion coefficients in (1). If $z = 2$ with $|\Omega - \Omega_E| \sim \beta A^2$ for the nonlinear plane waves, and the energy per oscillator $E \sim gA^2$ and the spatial decay exponent δ is related by $|\Omega_b - \Omega_E| \sim \kappa\delta^2$, then the energy threshold $E_{\min}$ is of the order of $\kappa g/\beta$, and the minimum energy breather in 3D has spatial size of the order of the lattice spacing, independently of

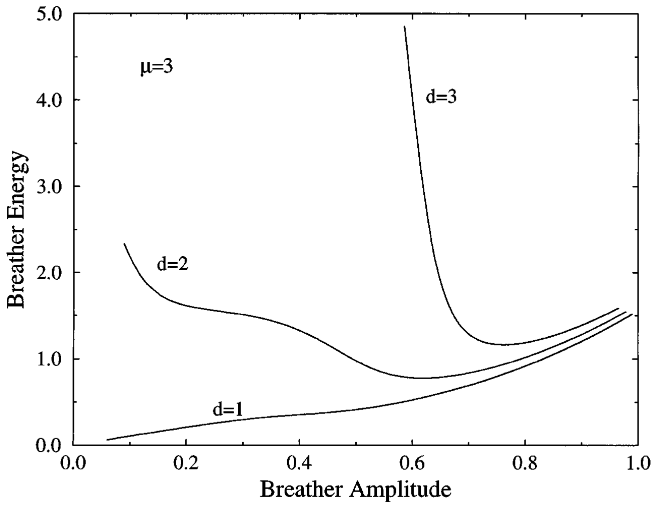

FIG. 1. Breather energy versus amplitude for the DNLS system in one, two, and three lattice dimensions. Parameters $C = 0.1$ and $\mu = 3$ for all cases. System sizes for $d = 1, 2, 3$: $N = 100$, $N = 25^2$, $N = 31^3$, respectively. The estimated points $(A; E)$ of bifurcation of the band edge plane wave for $d = 1, 2, 3$ are (0.014; 0.024), (0.064; 5.53), (0.097; 237), respectively.

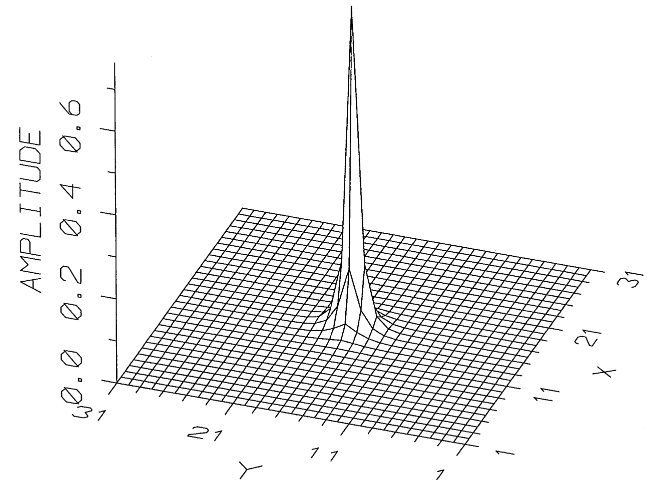

FIG. 2. Amplitude distribution of the minimum energy breather solution of the DNLS system with $d = 3$, $\mu = 3$, $C = 0.1$, and $N = 31^3$. Actually, only a distribution in a cutting $(x; y)$ plane is shown (the plane cuts the center of the breather). The intersections of the grid lines correspond to the actual amplitudes, the rest of the grid lines are guides to the eye.

κ, g, and β. One should allow for a factor of $(2 + d)$ for underestimating the true height of the minimum and the contributions of nearest neighbors.

To confirm our findings, we performed numerical calculations. First, we study the discrete nonlinear Schrödinger (DNLS) equation

$$\dot{\Psi}_l = i\left(\Psi_l + |\Psi_l|^{\mu-1}\Psi_l + C\sum_{m\in N_l}\Psi_m\right), \qquad (7)$$

where N_l denotes the set of nearest neighbors of l. The detuning exponent z is easily seen to be $\mu - 1$. Making the substitution $\Psi_l = A_l e^{i\Omega_b t}$ we solve the algebraic equations for the real amplitudes A_l. Numerically this is implemented by considering the case of large breather amplitude A_0 first. Then the breather is essentially given by $A_0 \approx (\Omega_b - 1)^{1/(\mu-1)}$ and $A_{l\neq 0} = 0$. Next we define a functional G which is the sum over the squares of differences between left hand and right hand parts of all algebraic equations for the amplitudes. This functional is minimized by gradient descent, where the initial guess is the large amplitude approximate solution. Finally, the frequency Ω_b is varied in small steps and the breather solution is traced. In Fig. 1 we show the resulting breather energy as a function of the amplitude A_0 for $\mu = 3$ and $d = 1, 2, 3$. The results are in full accord with the predictions. For $d = 3$ the above estimate of the minimum energy yields a value of 0.2 with $\beta = g = 1$ and $\kappa = C = 0.1$. The mentioned factor $(2 + d) = 5$ accounts for the deviation from the true value of 1. Figure 2 shows the amplitude distribution of the discrete breather with minimum energy in the (x, y) plane crossing the breather center for $d = 3$. The minimum energy breather is strongly localized—its spatial width is only a few lattice spacings. In Fig. 3 we show results for $d = 1$ and $\mu = 3, 5, 7$. Again we find full agreement. Note that even one-dimensional lattices exhibit positive lower bounds on breather energies if $\mu \geq 5$. This $d = 1$ result has also been predicted using variational techniques [14].

To demonstrate that the numerical results are not an artifact of the DNLS case, we study the three-dimensional

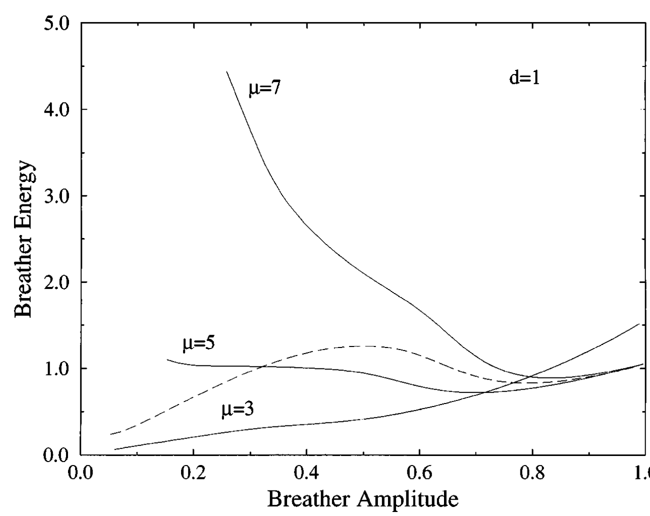

FIG. 3. Breather energy versus maximum amplitude for the DNLS system in one lattice dimension and for three different exponents $\mu = 3, 5, 7$ (solid lines). The system size is $N = 100$ and the parameter $C = 0.1$. The dashed line is for the modified system (cf. text).

nonlinear Klein-Gordon lattice

$$\ddot{U}_l = -U_l - U_l^{\mu} - C \sum_{m \in N_l} (U_l - U_m). \quad (8)$$

The detuning exponent z is given by $\mu - 1$ for μ odd and $2\mu - 2$ for μ even. Again the discrete breather with large amplitude is essentially an on-site excitation and given by $\ddot{U}_0 = -U_0 - U_0^{\mu}$ and $U_{l\neq 0} = 0$. The equations of motion are integrated numerically for a given set of initial conditions $\{U_l(t=0), \dot{U}_l(t=0)\}$ over the breather period $T_b = 2\pi/\Omega_b$. The functional $G = \sum_l \{[U_l(T_b) - U_l(0)]^2 + [\dot{U}_l(T_b) - \dot{U}_l(0)]^2\}$ is minimized with respect to the initial conditions using gradient descent. This method allows us to perform a reliable numerical calculation of DBs in three-dimensional arbitrary lattices. The result in Fig. 4 for $\mu = 3$ and $d = 3$ is again in full accord with the predictions.

We can predict that a modified DNLS system with an additional term $v_{\mu'} |\Psi_l|^{\mu'-1} \Psi_l$ can exhibit complex curves $E_b(A_0)$. For example, for $d = 1$, $\mu = 7$, $\mu' = 3$, and $v_{\mu'} = 0.1$, the $E_b(A_0)$ dependence will be nearly identical to the case $v_{\mu'} = 0$ already considered, if the amplitude A_0 is not too small. Then $E_b(A_0)$ will show a minimum at a nonzero value of A_0. For small A_0, however, the energy of the breather will ultimately decay to zero, so the curve has a maximum for smaller amplitudes! The dashed line in Fig. 3 shows the numerical calculation, which coincides with our prediction.

Our findings should help to detect discrete breathers in experimental realizations like the dynamics of atoms in crystals. For a three-dimensional crystal we predict a positive energy threshold for the excitation of discrete breathers.

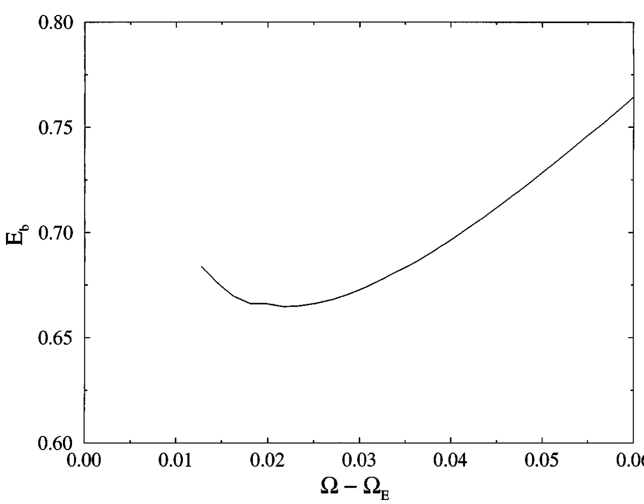

FIG. 4. Breather energy E_b versus frequency detuning $(\Omega - \Omega_E)$ for a 3D Klein-Gordon lattice. Parameters $\mu = 3$ and $C = 0.1$. System size $N = 10^3$.

Another consequence of our work is that breather solutions belonging to parts of the family where the energy is decreasing with increasing amplitude are dynamically unstable, whereas those in the other parts have a good chance of being dynamically stable. This can be seen from a Poincaré map of the phase space flow around the breather orbits. The minimum energy breathers correspond to saddle-center bifurcations, since no breather solutions will exist if the energy is lowered beyond the minimum breather energy.

A similar phenomenon occurs in polaron theory. In a three-dimensional lattice, two polarons of unit electric charges exist above a certain parameter threshold (large and small polaron) [15].

Summarizing, we have shown that discrete breather families have positive lower energy bounds if the dimension of the lattice is larger than or equal to some critical value which in turn is defined by the power of the first nonlinear expansion term in the equations of motion. These results are expected to be of importance for the experimental detection of discrete breathers, because the minimum energy of a breather family should show up as an activation energy.

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