Acoustic Breathers in Two-Dimensional Lattices

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(Received 9 July 1997)

We calculate breather solutions for a two-dimensional lattice with one acoustic phonon branch. We start from the case of a system with homogeneous interaction potentials. We then continue the zero-strain breather solution into the model sector with additional quadratic and cubic potential terms with the help of a generalized Newton method. The breather continues to exist but is dressed with a strain field. In contrast to the ac breather components, which decay exponentially in space, the strain field (which has dipole symmetry) should decay like $1/r^a$, $a = 2$. On our rather small lattice (70×70) we find an exponent $a \approx 1.85$. [S0031-9007(97)04812-6]

PACS numbers: 63.70.+h, 03.20.+i, 03.65.Sq, 63.20.Dj

The understanding of dynamical localization in classical spatially extended and ordered systems experienced recent considerable progress. Specifically time-periodic and spatially localized solutions of the classical equations of motion exist, which are called (discrete) breathers or intrinsic localized modes [1]. The attribute discrete stands for the discreteness of the system, i.e., instead of field equations one typically considers the dynamics of degrees of freedom ordered on a spatial lattice. As already mentioned, the considered systems are spatially ordered, i.e., the lattice Hamiltonian is invariant under discrete translations in space. The discreteness of the system produces a cutoff in the wavelength of extended states, and thus yields a finite upper bound on the spectrum of eigenfrequencies Ω_q (phonon band) of small-amplitude plane waves (we assume that for small amplitudes the Hamiltonian is in leading order usually a quadratic form of the degrees of freedom). If now the equations of motion contain nonlinear terms, the nonlinearity will in general allow us to tune frequencies of periodic orbits outside of the phonon band, and if all multiples of a given frequency are outside the phonon band too, there seems to be no further barrier preventing spatial localization (for a review see [2,3]).

The existence of discrete breathers has been proven so far for (i) weakly coupled anharmonic oscillators [4,5] ordered on a lattice of any dimension and (ii) chains of particles with nearest neighbor interaction whose potential is a homogeneous function $\sim z^{2m}$ with $m = 2, 3, ...$ [6]. While the first case starts from the trivial limiting case of noninteracting oscillators, the second one uses the possibility of space-time separation (due to the homogeneity property) to reduce the consideration to a two-dimensional map. In the first case the phonon band is degenerated in a nonzero frequency value and can grow upon continuation, keeping its optical property (i.e., no conservation of total mechanical momentum). In the second case the phonon band is degenerated in the zero frequency value, so formally it is an acoustic band (total mechanical momentum is conserved) but its width is zero.

As already mentioned, the breather frequency Ω_b should fulfill a nonresonance condition $n\Omega_b \neq \Omega_q$ for all integer $n = 0, \pm 1, \pm 2, ...$. This is necessary in general in order to have spatial localization of the corresponding Fourier mode [7]. In the above mentioned case of weakly coupled oscillators a proper choice of the breather frequency always ensures nonresonance. In the case of homogeneous interaction potentials the symmetry of the potential $\Phi(z) = \Phi(-z)$ is found in also the breather solution, which implies that only odd Fourier components are present in the breather solution. Thus the dc component ($0 \times \Omega_b = 0$), which is in resonance with the mentioned degenerated phonon band, is strictly zero and the resonance is harmless.

It is a widespread expectation that breathers play an important role in the dynamics of anharmonic crystals [8]. Since any crystal has acoustic phonon branches, and the interparticle interaction potentials are not symmetric around their minimum, one has to face the fact that any breather will be accompanied by a strain field (gradient of the dc component of the breather) and that the resonance of the dc component with the acoustic phonon branches has to be incorporated into the consideration.

If any nonzero multiple of Ω_b resonates even with an edge of a phonon band, this leads either to the vanishing of the whole breather or to a delocalization of the breather and to a divergence of its energy [9]. The resonance of the dc component to be considered here is special—it resonates with a Goldstone mode, and one can expect the resonance not to be as destructive to the breather as any resonance at nonzero frequency. From the theory of elastic defects [10] we know the characteristic feature of the strain decay to be algebraic in the distance (from the defect center). The exponent is only depending on the dimension of the system and on the symmetry character of the defect (monopole, dipole, etc.), but independent on the defect strength.

This independence of the exponent on the defect strength implies that if acoustic breathers (breathers with dc components in the presence of acoustic phonon branches) do exist, there will be no parameter limit in which their spatial decay becomes infinitely large. Instead the strain will always decay algebraically; only its amplitude can be varied.

At this stage it is appropriate to fix the class of Hamiltonians to be considered further. We will treat the simplest case of hypercubic lattices with one degree of freedom per lattice site and nearest neighbor interaction, which can be considered as generalized Fermi-Pasta-Ulam (FPU) systems:

$$H = \sum_l \left[\frac{1}{2} P_l^2 + \sum_{l' \in \mathrm{DNN}} \Phi(X_l - X_{l'}) \right]. \qquad (1)$$

Here P_l and X_l are canonically conjugated scalar momenta and displacements of a particle at lattice site l. Note that depending on the lattice dimension d the lattice site label l is a d-component vector with integer components. The inner sum in (1) goes over all *directed nearest neighbors*, e.g., for $d = 1$ and $l = n$ we sum over $l' = n + 1$, for $d = 2$ and $l = (n,m)$ we sum over $l' = \{(n + 1, m); (n, m + 1)\}$, etc. The interaction potential $\Phi(z)$ is given by

$$\Phi(z) = \frac{1}{2} \phi_2 z^2 + \frac{1}{3} \phi_3 z^3 + \frac{1}{4} z^4, \qquad (2)$$

which turns out to be generic enough for the purposes discussed below.

Breathers for such a system can be represented in the form

$$X_l(t) = \sum_{k=-\infty}^{+\infty} A_{kl} \mathrm{e}^{\mathrm{i}k\Omega_b t}. \qquad (3)$$

We will restrict ourselves to solutions invariant under time reversal, so that all $A_{kl} = A_{-k,l}$ are real. The spatial localization property of (3) implies $A_{k,|l|\to\infty} \to 0$ for $k \neq 0$ and $A_{0,|l|\to\infty} \to$ const. The dc component of the breather is given by A_{0l}.

So far we know about results only for one-dimensional lattices. A lot of numerical and approximative work exists, which shows that the acoustic breather seems to exist as a solution to finite energy [11–13]. Its peculiarity is that the dc component of the breather versus lattice site number has a kink shape $A_{0,l\to\pm\infty} \to \pm$const for free boundaries. For periodic boundary conditions one would find a linear decay of A_{0l} far from the breather, but the gradient of the dc components (the strain) is inverse proportional to the size of the chain, so that in the limit of an infinite chain the result is again a constant for the dc component (zero strain). An analytical proof has been given recently by Livi, Spicci, and MacKay [14]. The proof considers a diatomic chain with asymmetric interaction potential [note that the corresponding Hamiltonian differs from (1) in that one has to introduce an additional parameter $1/M \neq 1$ in front of each kinetic energy term for, say, all even lattice site indices]. The breather is continued from the limit of zero mass ratio (heavy masses are infinitely heavy). The problem of resonance with the Goldstone mode is solved by coordinate transformation and by imposing a strain field of compact support. This means that the dc displacements at this limit are given by a steplike kink. The breather is then continued into a sector of the Hamiltonian with nonzero mass ratio.

The reader might think that we are contradicting ourselves with the previous paragraph and the above statements about the algebraic decay being independent of the breather parameters. Let us explain why that is not so. Suppose that a breather exists, which creates some strain field. The dc displacements A_{0l} will have some dependence on the lattice site vector l. The strain E_l is given by the lattice gradient of A_{0l}. The far field energy stored is given by the integral over the squared strain. Assuming that the strain does decay algebraically, we can use continuum theory far from the breather. The corresponding equation is equivalent to the electrostatic equations in d dimensions. Consider $d = 1$. A monopole far field will yield $E = c \neq 0$ and the corresponding energy diverges. Also in this case the potential $A_{0l} = \mathrm{sgn}(l)a + cl$. This clearly is not what was observed for acoustic breathers in one dimension. A dipole far field instead will yield $E = 0$, $A_{0l} = \mathrm{sgn}(l)a$, and the energy is finite. This is the situation observed. So the known acoustic breather solutions are accompanied by a dipole strain field. Already the demand that the acoustic breather is a solution to finite energy limits the strain fields to dipole or higher order multipole symmetries. In this special case the potential A_{0l} is constant far away from the breather, so the corresponding exponent of the algebraic decay is simply zero. That is the reason why the analytical proof of existence can go through, because a kinklike field for A_{0l} can have the limiting form of a step function, which is precisely the case for the limit of zero mass ratio (see above).

For $d = 2$ (square lattice) the situation is the following. A monopole will generate a strain $E \sim 1/l$ and a potential $A_{0l} \sim \ln(l)$. The energy of such a field diverges. If we search for acoustic breathers with finite energy, we would have to exclude a monopole field. A dipole generates a strain $E \sim 1/l^2$ (we skip direction dependencies here) and a potential $A_{0l} \sim 1/l$. The energy for this field is finite. In any case the predicted exponents of the algebraic decay are nonzero, and no simple limit exists, which makes the strain to be of compact support. So already at this stage it is clear that existence proofs of acoustic breathers in two-dimensional systems are much more complicated than for $d = 1$.

Notice that for $d = 3$ (cubic lattice) a monopole generates $E \sim 1/l^2$ and the energy of this field is finite.

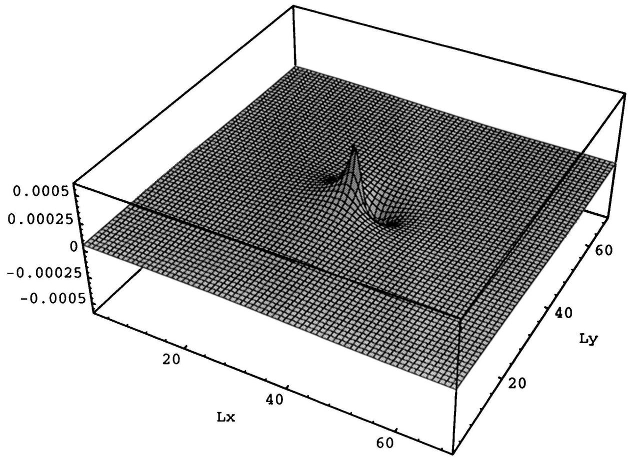

FIG. 1. dc displacement of a breather as a function of the lattice vector l. Parameters are given in the text.

To answer the question "to be or not to be" we will present numerical calculations of acoustic breathers of (1) for $d = 2$. The results show up to numerical accuracy that acoustic breathers exist on finite lattices with free boundaries. The symmetry and spatial decay properties are in accord with the expectations given above. The maximum lattice size is 70×70, but we observed no profound size effects on the existence and symmetry of the acoustic breather when considering smaller systems. The only size effect (to be expected) is observed even for the largest systems with respect to the algebraic decay properties.

We start with $\phi_2 = \phi_3 = 0$. In this case $\Phi(z) = \Phi(-z)$, so $A_{kl} = 0$ for $k = 2m$ and m integer. In particular no dc components are present. Furthermore, due to the degeneracy of the phonon band into a single number the breathers will be localized in space stronger than exponentially. Because of the homogeneity of the interaction potential we can separate time and space $X_l(t) = U_l G(t)$. The master function $G(t)$ satisfies the differential equation $\ddot{G} = -G^3$, and the spatial amplitudes U_l are given by the extrema of a function $S(\{U_l\})$, i.e., $\partial S / \partial U_l = 0$:

$$S = \sum_l \left[\frac{1}{2} U_l^2 - \frac{1}{4} \sum_{l' \in \mathrm{DNN}} (U_l - U_{l'})^4 \right]. \quad (4)$$

The function S has a local minimum at $\{U_l = 0\}$. For large values of the variables U_l it will diverge to $-\infty$ with the fourth power of the distance from $\{U_l = 0\}$ with the exception of some nongeneric directions in the space of $\{U_l\}$, in which S will continue to increase with the second power of the distance from $\{U_l = 0\}$. Thus all nontrivial extrema of S are saddle points, which are located on some rim surrounding the point $\{U_l = 0\}$.

The search strategy is thus to define a certain initial direction in $\{U_l\}$, to find the rim, and then to minimize S staying on the rim. The procedure is very fast, because localized solutions decay in space faster than exponentially. The full solution is obtained by multiplying the found eigenvector for $\{U_l\}$ with the time periodic master function $G(t)$, which can have any period.

After we find a certain solution for $\phi_2 = \phi_3 = 0$ and choose a certain period $T_b = 2\pi/\Omega_b$ for $G(t)$, in the second step we switch on $\phi_2 = \phi_3 = 0.01$. With the help of a generalized Newton method (see, e.g., [15]) we are searching for a periodic orbit with the same period T_b close to the starting solution in phase space. We start with all velocities set to zero, i.e., with the time point when $\dot{G}(t) = 0$. If we find a new periodic orbit, after time T_b all velocities are zero again, so in the Newton algorithm we use only the displacement variables X_l. A periodic orbit is said to be found if

$$\sqrt{\sum_l [X_l(t = 0) - X_l(t = T_b)]^2} < 10^{-8}. \quad (5)$$

The maximum size of the square lattice $N \times N$ with $N = 70$ comes from the circumstance that the rank of

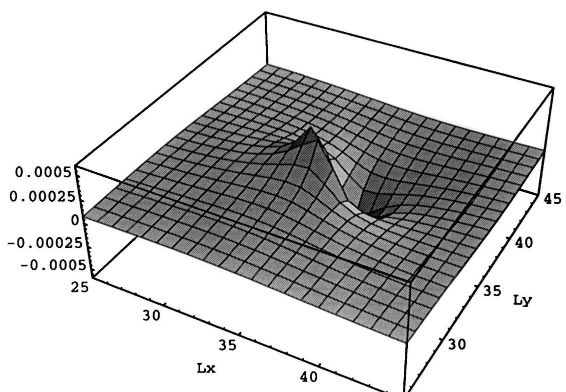

FIG. 2. Zoom of Fig. 1 in the breather center.

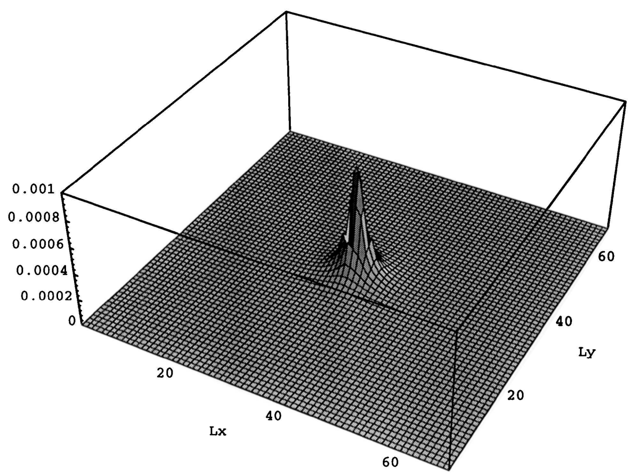

FIG. 3. Absolute value of the strain of the breather solution of Fig. 1 as a function of the lattice vector l.

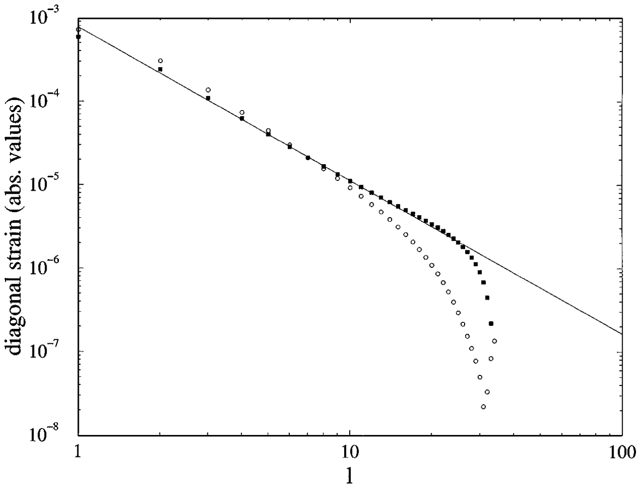

FIG. 4. Variation of the absolute value of the strain (Fig. 3) along the diagonals of the lattice on a double-logarithmic plot. Open circles: (1,1) direction; filled squares: $(-1, 1)$ direction.

the Newton matrix is N^2 and the operative memory size needed for calculation with double precision is $8N^4$ bytes.

The numerical results shown below apply to the above mentioned initial vector in $\{U_l\}$ space for which all U_l are zero except one elementary plaquette of four lattice sites on which $|U_l = 1|$ and the signs are alternating between nearest neighbors. We obtained similar results with an initial vector where all U_l are zero except for one single lattice site where $U_l = 1$.

As already mentioned, the Newton search algorithm successfully produced solutions in all cases considered. The ac components of the found solution decay exponentially in space and essentially vanish at a distance of 5–7 lattice constants from the center of the breather. In Fig. 1 we show the dc displacements of one solution with a period obtained by initial conditions $G(t = 0) = 1$ and $\dot{G}(t = 0)$ for the master function $G(t)$. We do observe dipole symmetry of the dc field. In Fig. 2 a zoom of the center of the dc field is shown.

Let us turn to the strain. In Fig. 3 we show the absolute values of the strain field of the found acoustic breather. To analyze the spatial behavior of the strain, we plot in Fig. 4 the variation of the absolute values of the strain along the two diagonals, as in those directions we have the largest distance and can hope that the boundary effects are suppressed in some bulk region. The results depend on the choice of the diagonal. The diagonal which is directed along the dipole moment gives poor results—the finite size effects are too strong to observe any power law in the double logarithmic plot in Fig. 4. The second diagonal perpendicular to the dipole moment, however, though still with strong influence from the boundaries, allows us to fit some part of the "bulk" data with a power law (solid line in Fig. 4). The resulting exponent is 1.85, and, considering the small system size, quite close to the expected value 2.

In conclusion we can say that acoustic breathers can be obtained for finite two-dimensional lattices up to numerical precision. The symmetry is the one expected from general argumentations. The dc components (and thus the strain) decay much slower than the exponentially decaying ac components of the breather, and a fit along one of the diagonals of the surprisingly small system under study yields a power law with an estimated exponent of 1.85 to be compared with the exponent of 2, which follows from the assumption that the strain field has dipole symmetry.

These results should support the expectations that breathers can exist in real crystals. Moreover at any finite temperature excited breathers will decay after some time. Since they are accompanied by a strain field, those strain fields will be dispersed in the form of low-lying acoustic modes after the decay of a breather. Thus breathers can act as an efficient energy transfer from high-lying excitations into low-lying acoustic phonons.

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