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Discrete breathers in transient processes and thermal equilibrium

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Abstract

We study four different aspects of the generation of discrete breathers in one-(1D) and two-dimensional (2D) lattices with soft and hard nonlinearity. Breathers can be generated in thermal equilibrium and in various transient and nonequilibrium situations. We use the numerically obtained information about the spatio-temporal evolution of nonlinear lattices and combine it with analytical and heuristic results and arguments on breather existence, stability and interaction with plane waves to provide with a coherent picture of the complex nature of breather excitation in nonlinear lattices.
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1. Introduction

Discrete breathers (DBs) are time-periodic, spatially localized solutions of equations of motion for classical degrees of freedom interacting on a lattice. Over the last decade much progress has been achieved in the understanding of DB properties [1–4] and their role in various experimental situations ranging from charge-transfer solids, Josephson junctions, photonic structures to micromechanical oscillator arrays [5]. It has been shown that DBs exist due to the discreteness of the lattice and the nonlinearity of the differential equations governing the evolution of the system. There is good understand-

ing in the requirements model parameters should fulfill in order to allow for the existence of DBs. For some system classes existence proofs of breather solutions have been published (see e.g. [2,6–11]). Numerical methods for calculating exact (up to the machine precision) breather solutions were also obtained [2,12–14].

The generic character of DBs as exact solutions raises the question whether DBs can be excited in transient processes and even in thermal equilibrium. Considerable efforts were taken to elucidate this problem. It has been shown that DBs may appear in one-dimensional (1D) lattices due to the modulational instability of a plane wave [15–21]. It has also been shown that when thermalized 1D or two-dimensional (2D) lattices are cooled down, DBs appear and may strongly influence the relaxation properties of the studied systems

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[22–24]. Besides, attempts to observe DBs in thermal equilibrium (a lattice interacting with a thermal bath was simulated) have been successful [17,25]. However most of the results obtained so far leave gaps in the understanding of the role of DBs in transient processes and thermal equilibrium. This in particular is due to the fact that DB properties depend strongly on the chosen system classes and strongly affect the aforementioned processes. Most of the results are spread over these different system classes, leaving us without a clear and detailed systematic understanding of the considered phenomena. Practically nothing is known about the excitation of DBs in equilibrated systems by external local perturbations.

In this paper, we will provide with a systematic analysis of four aspects of DB generation comparing one- and two-dimensional lattices. The considered systems describe the dynamics of coupled oscillators in so-called optical lattices which show up with a gap in the frequency spectrum of small amplitude plane waves. First we will analyze the appearance of DBs in thermal equilibrium. Second we will consider the generation of DBs at various time scales in transient processes of perturbed plane waves. Third we will study the formation of DBs in thermalized lattices which are exposed to external highly local perturbations (think e.g. of a beam of neutrons passing through a crystal). And finally we will study the relaxation of lattices being cooled at their boundaries, which models a heating of a lattice part by e.g. some laser spot and the decay of the excitation after the subsequent switching off the energy source. All the simulation results presented in this paper were obtained using the fourth-order Runge-Kutta method.

The paper is organized as follows. In Section 2 we present numerical simulations of 1D and 2D lattices at non-zero temperatures, and study the existence of DBs in such systems and their properties. In Section 3 we demonstrate how modulational instability of a plane wave can give rise to energy localization in 2D lattices and study the long-time evolution of DBs in one and two dimensions. In Section 4 we investigate the dynamics of thermalized lattices under the action of random in space and time localized short energy impulses, and outline the effects of dimension of the lattice. In Section 5 we discuss the influence of DB excitation on the relaxation of an initially strongly heated lattice part and investigate the dependence of the transient behavior and its outcome upon the initial temperature of the hot region. In Section 6 we summarize the obtained results.

2. DBs in thermal equilibrium

The notion of a DB implies originally an exact time-periodic spatially localized solution. Being generic with respect to the parameters of the model, DBs demand specific initial conditions. It may become quite problematic to provide with these initial conditions in certain physical realizations. This fact stimulates the strong interest for studies of DB solutions in lattices at finite temperatures. The breathers that may be observed in this case can not be exact breather solutions of the model, and thus must have finite lifetimes. The presence of DBs should then be characterized by the existence of long-living localized energy excitations. One should observe then DBs, which appear, grow or decay from time to time at all sites of the lattice.

In the present paper we consider the 1D lattice described by the Hamiltonian

$$H = \sum_n \left(\frac{p_n^2}{2} + V(u_n) + \frac{1}{2}k(u_{n+1} - u_n)^2 \right) \qquad (1)$$

and the 2D lattice which Hamiltonian reads as

$$H = \sum_{n,m} \left(\frac{p_{n,m}^2}{2} + V(u_{n,m}) + \frac{1}{2}k(u_{n+1,m} - u_n)^2 \right.$$
$$\left. + \frac{1}{2}k(u_{n,m+1} - u_n)^2 \right). \qquad (2)$$

The on-site potential is given by

$$V(u) = \tfrac{1}{2}u^2 + \tfrac{1}{3}\alpha u^3 + \tfrac{1}{4}\beta u^4. \qquad (3)$$

Here u stands for the displacement of a particle, p denotes its momentum, $\beta = 0.25$, $k = 0.1$, $\alpha = 0$ for a symmetric potential and $\alpha = -1$ for an asymmetric potential which will be specified in the text. If we linearize the equations of motion (for, say, a 1D lattice) around the classical ground state, we obtain a set of linear coupled differential equations with solutions being small amplitude plane waves:

$$u_n(t) \sim e^{i(\omega_q t - qn)}, \quad \omega_q^2 = 1 + 0.4\sin^2\left(\frac{q}{2}\right). \qquad (4)$$

The dispersion relation $\omega_q(q)$ defines an optical phonon band (the lower squared frequency $\omega_l^2 = 1$, the upper squared frequency $\omega_u^2 = 1.4$) characterized by a nonzero frequency gap below the spectrum. Note that the dispersion relation (4) is periodic in the wave number q and possesses a finite upper bound.

To study the energy distribution in space we define the energy density at each site of the lattice:

$$\varepsilon_{\vec{l}} = \frac{p_{\vec{l}}^2}{2} + \frac{1}{4}k\sum_M (u_M - u_{\vec{l}})^2 + V(u_{\vec{l}}) \tag{5}$$

where $\vec{l} = n$ for a 1D lattice, $\vec{l} = (n, m)$ for a 2D lattice and M denotes neighbors of the site $\vec{l}$.

The microcanonical numerical simulation of the lattice at finite temperatures can be realized (in the most simple way) by setting random initial conditions at all sites:

$$\begin{cases} u_n(0) = c\xi_{2n-1}, \\ p_n(0) = c\xi_{2n} \end{cases} \tag{6}$$

where ξ_k, $k = \overline{1, 2N}$ are random values uniformly distributed in the interval $[-0.5, 0.5]$, c is the parameter that allows to vary the energy (and hence the temperature) of the lattice. Below $\bar{\varepsilon}$ denotes the average energy per site.

Numerical simulations of the 1D lattice with the symmetric on-site potential reveal the following results. DBs have finite lifetime and can appear everywhere in the lattice (see Fig. 1(a), compare to the case of harmonic lattice, see Fig. 1(b)). At higher temperatures DBs with longer lifetimes are seen (Fig. 1(c)). For the same case on shorter time scales DBs with shorter
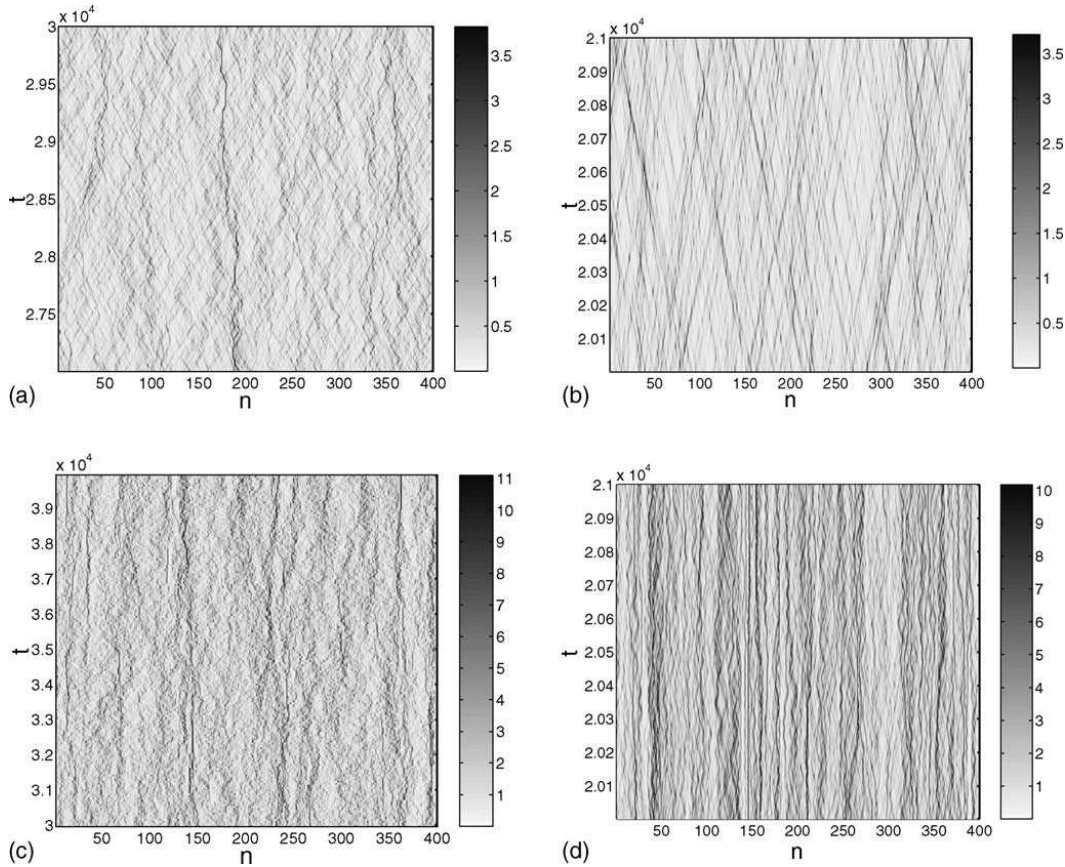

Fig. 1. Energy density evolution in a one-dimensional lattice after giving the system time to equilibrate: (a) $c = 2$, $\bar{\varepsilon} = 0.395$, $\beta = 0.25$; (b) $c = 2$, $\bar{\varepsilon} = 0.374$, $\beta = 0$ (harmonic lattice); (c and d) $c = 4$, $\bar{\varepsilon} = 1.72$, $\beta = 0.25$. Here $\alpha = 0$ and $k = 0.1$. Note that the grey scale coding of the energy density varies for different plots.
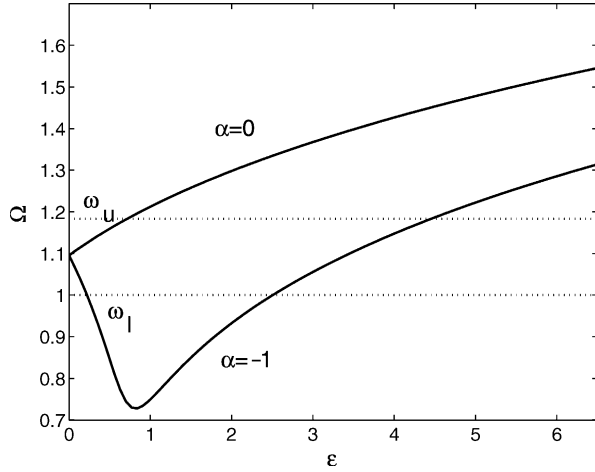
Fig. 2. Frequency vs. energy for the model of the one-site DB. The upper and the lower boundaries of the phonon spectrum are also shown. Here $k = 0.1$ and $\beta = 0.25$.

lifetime are observed (see Fig. 1(d)), which means co-existence of DBs on essentially different time scales.

To get deeper insight into the problem of existence of DBs in one dimension we consider the simplest model of an one-site DB. Let a particle oscillate, while the motion of its neighbors is neglected (this is a rather good approximation when the DB is sufficiently strongly localized [26,27]):

$$\begin{cases} \ddot{u}_n = -V'(u_n) + k(u_{n-1} - 2u_n + u_{n+1}), \\ u_{n-1} = u_{n+1} = \dot{u}_{n-1} = \dot{u}_{n+1} = 0 \end{cases} \qquad (7)$$

and calculate the dependence of the oscillation frequency upon the energy of the particle for the symmetric ($\alpha = 0$) and the asymmetric ($\alpha = -1$) on-site potentials (3) (see Fig. 2).

One usually distinguishes cases $\Omega(E) > \omega_u$ and $\Omega(E) < \omega_l$, calling a DB "hard" in the former case and "soft" in the latter one. The symmetric potential allows only for hard DBs, while the asymmetric one allows for both types of DBs separated by a gap on the energy axis.

This estimation for a one-site DB can be used to predict what types of breathers, if any, will exist at a given value of the average local energy $\bar{\varepsilon}$. Assuming that the whole lattice is populated with DBs with each DB consisting of $(1 + 2d)$ sites, we get a rough estimation of the energy of one DB as $(1 + 2d)\bar{\varepsilon}$, where d is the lattice dimension. Alternatively we can argue that the energy concentration on a given site accumulates
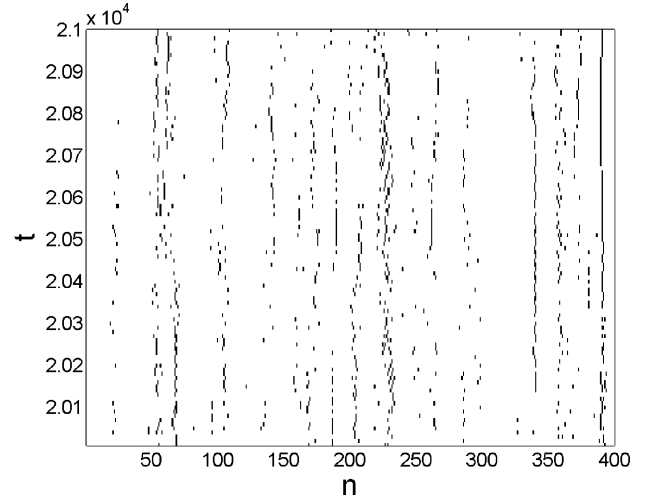

Fig. 3. The energy density evolution in a 1D lattice with a cutoff at small energy densities ($c = 4$, $\bar{\varepsilon} = 1.76$, $\alpha = -1$). The local energy density in plotted points exceeds $3\bar{\varepsilon}$.

the energy of its nearest neighbours, yielding again the same order for the breather energy.

We carried out the following method for detecting one-site DBs in numerical simulations for $d = 1$. When the local energy of a certain site exceeds the threshold of $3\bar{\varepsilon}$ while the energies of the neighboring sites stay below the threshold, we register energy localization. To illustrate the result of this procedure we show a cutoff plot (i.e. only those points at which $\varepsilon_n > 3\bar{\varepsilon}$ are plotted) in Fig. 3. If the lifetime of this localization is long enough, we consider it to be a DB. In the series of experiments with various values of $\bar{\varepsilon}$ we recorded the longest observed lifetimes of breathers. The total observation time in each simulation was 10^6 time units. The dependencies of the longest breather lifetimes on the mean energy density obtained for different types of on-site potential ($\alpha = 0$ and $\alpha = -1$) are presented in Fig. 4. By comparing these data with the simulation of the harmonic chain ($\alpha = \beta = 0$) we found that we can reliably detect those DBs whose lifetime exceeds 100 time units (the characteristic phonon time scale is of the order of 10).

The curve for $\alpha = 0$ in Fig. 4 shows a monotonic increase of the longest DB lifetime with increase of $\bar{\varepsilon}$ (observed deviations are due to the fluctuational nature of detected DBs), while the curve for $\alpha = -1$ exhibits a maximum at quite a low value of $\bar{\varepsilon}$ and a monotonic increase at essentially higher $\bar{\varepsilon}$.
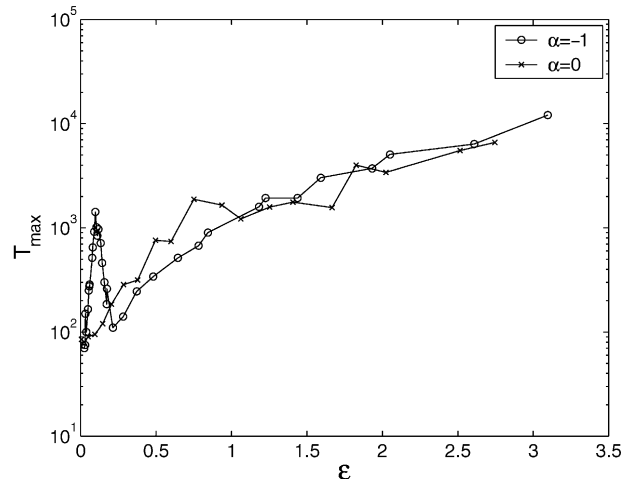
Fig. 4. Maximal detected lifetime of a DB vs. the average energy density for the symmetric and asymmetric on-site potentials in a 1D system. The observation time was 10^6 time units.
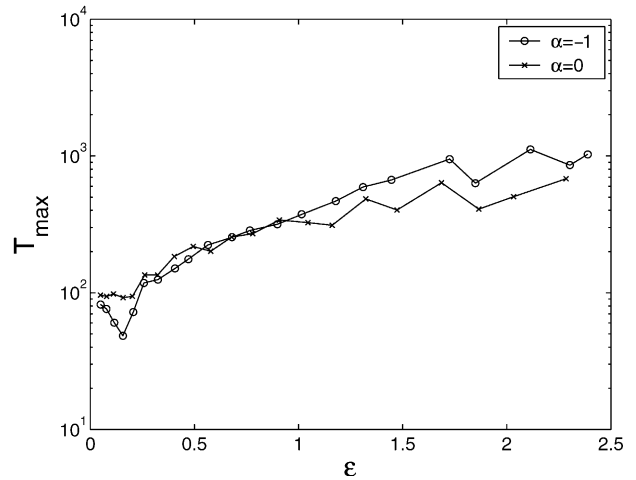

Fig. 6. Maximal detected lifetimes of DBs vs. average local energy density for the symmetric and asymmetric on-site potentials in 2D lattices are presented. The observation time was 2×10^5 time units.

The comparison of the obtained curves with the discussed frequency-energy dependencies for the model of the one-site DB (Fig. 2) allows to identify the maximum on the curve for $\alpha = -1$ with soft breathers and the monotonous increase at longer lifetimes on both curves with hard breathers.

Next we discuss numerical simulations of 2D lattices. The results are quite similar. To give an example we present DBs on various time scales (see Fig. 5). To visualize the DBs we plotted only those sites, in which the local energy exceeded $5\bar{\varepsilon}$.

We also studied the longest living breathers and their lifetime dependence upon the average energy density $\bar{\varepsilon}$ for the 2D case. A one-site breather model should im-

ply then an excited site coupled to four pinned neighbors. The corresponding energy threshold for detecting DBs in numerical experiment equals $5\bar{\varepsilon}$. Results of simulations of 2D lattices are shown in Fig. 6. In contrast to the 1D case (for $\alpha = -1$) no soft breathers were detected. This can be explained by using the frequency-energy dependence for the model one-site breather shown in Fig. 7. In case $\alpha = -1$ the soft DBs must be confined to a narrow energy window. This factor makes the soft DBs much more sensitive to thermal fluctuations than the hard ones. In general, choosing another set of the parameters of the model one may observe soft breathers in thermal equilibrium.
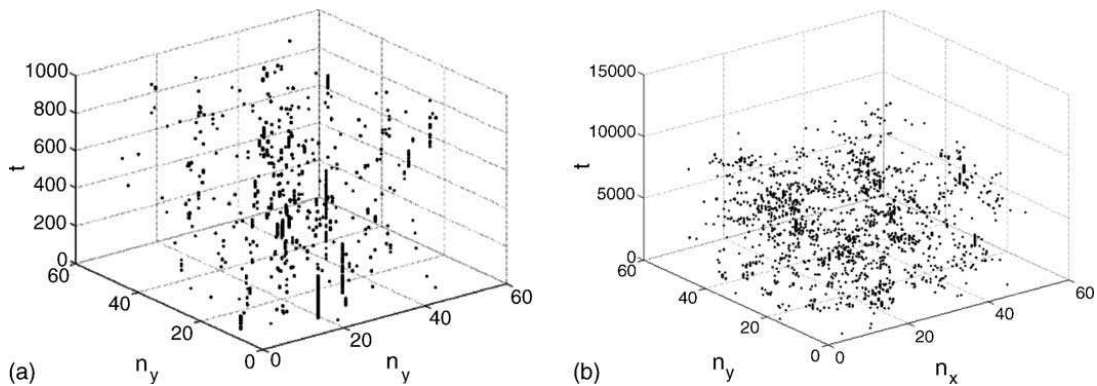

Fig. 5. Energy density evolution in a 2D lattice with a cutoff at small energy densities for various time windows. For both cases $c = 5$ was chosen ($\bar{\varepsilon} = 2.89$). Here $\alpha = 0$. The local energy density in plotted points exceeds $5\bar{\varepsilon}$.
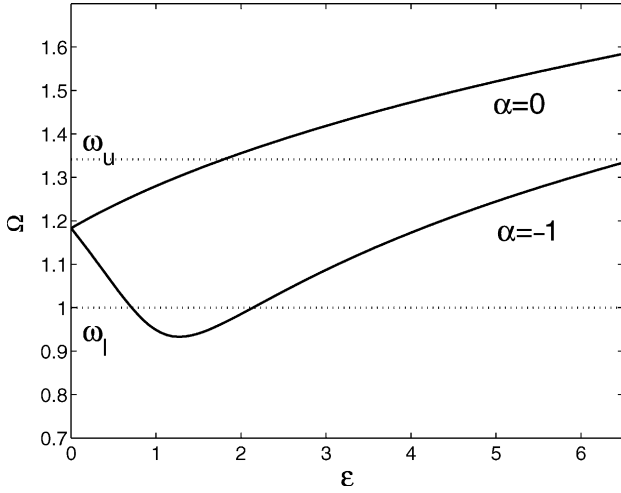
Fig. 7. Frequency vs. energy for the model of a one-site DB in the 2D lattice. The upper and the lower boundaries of the phonon spectrum are also shown.

Another important property of the considered 2D lattice is that DBs have a nonzero lower energy threshold ε_{min} [28]. We performed high accuracy computations of DB solutions using a Newton scheme and obtained the following values for the energy thresholds: for $\alpha = 0$ $\varepsilon_{min} \approx 2.76$; for $\alpha = -1$ soft DBs have a threshold value of $\varepsilon_{min} \approx 0.84$ and hard DBs have a threshold value of $\varepsilon_{min} \approx 8.06$.

In Fig. 6 we find that for $\bar{\varepsilon} < 0.25$ the largest lifetimes of DBs are less than 100, and below this energy lifetimes do not increase with energy. As explained above these data can not be safely interpreted as DB lifetimes when compared to simulations of harmonic lattices. This is in sharp contrast to the 1D results in Fig. 4. There the maximum DB lifetime starts also with a value of 100, but increases with energy even for small energy values. Thus, we conjecture that the observed energy gap in Fig. 6 is due to the presence of a lower energy threshold for DBs in the considered 2D lattice. Note also that energy thresholds for DBs have been observed in 1D systems with higher order nonlinearities in thermal equilibrium [29].

3. Modulational instability

DBs in thermal equilibrium will be generated only if the averaged energy density (or temperature) is large enough for nonlinear terms in the equations of motion to be relevant. In the opposite case of rather small energy densities no breathers are expected to persist. However if the initial conditions are chosen to be nongeneric, the evolution to thermal equilibrium may proceed through transient processes. The duration of these processes can be substantially modified if DBs are generated on the way to equilibrium. A well known transient process in which DBs play a significant role is the decay of a plane wave due to modulational instability [15–19].

This type of instability for discrete 1D lattices of the type (1) was investigated analytically and numerically by Peyrard et al. [16,17]. There numerical simulations were carried out for $\alpha = 0$ and $\beta < 0$ in the on-site potential (3) and on time scales of about 1.5×10^4 periods of the lowest frequency phonon. The results of those simulations indicated, that modulational instability can act as an effective pathway to the formation of breathers when initial conditions are set in the form of a weakly noised plane wave. During the first part of its evolution, the initial wave gets decomposed into wave packets due to modulational instability. During the subsequent second evolution part, which is essentially nonlinear and can not be described by linear stability analysis, multiple collisions of some wave packets tend to increase their energy at the expense of other ones, and finally they get pinned down to the lattice giving rise to breathers.

We carried out numerical experiments in order to check whether this scenario is valid for 1D and 2D systems described by the equations (1) and (2) respectively for $\beta > 0$ in the on-site potential. Further, we extended the observation time in order to continue the scenario suggested in [17], and in order to find out the effect of the initial energy density value upon the process of formation of breathers.

In the numerical simulations we took $\alpha = 0$, $\beta = 0.25$, $\kappa = 0.1$. The initial conditions for the 1D lattice were taken in the form of a harmonic wave with a small noise added to the amplitude:

$$u_i(0) = A(1 + \xi_i)\cos(qi)$$
$$\dot{u}_i(0) = \omega A(1 + \xi_i)\sin(qi) \tag{8}$$

where $\omega^2 = 1 + 4\kappa \sin^2(q/2) + 3\beta A^2$. The random values ξ_i were distributed uniformly in the interval $(0, 0.001)$. The last term in the expression for ω represents the first-order approximation for the nonlinear frequency shift [17].

The initial conditions in 2D simulations were chosen in a similar way:

$$u_{ij}(0) = A(1 + \xi_{ij}) \cos(q_1 i + q_2 j)$$
$$\dot{u}_{ij}(0) = \omega A(1 + \xi_{ij}) \sin(q_1 i + q_2 j) \tag{9}$$

where $\omega^2 = 1 + 4\kappa(\sin^2(q_1/2) + \sin^2(q_2/2)) + 3\beta A^2$. The noise was specified in the same way as in the 1D case.

The wave numbers of the initial waves were chosen as $q_1 = q_2 = q = 3\pi/4$. The reason for this choice is an analytical result given in [16] from which it follows that a plane wave with a wave number q satisfying $\pi/2 < q < \pi$ in one-dimensional systems of the type (1) with $\alpha = 0$ and $\beta > 0$ is unstable due to modulational instability.

The size of the lattice was 400 sites for the 1D case and 80×80 sites for the 2D case.

The results of our simulations of the 1D chain for $A = 0.5$ ($\bar{\varepsilon} = 0.18$) at time scales of about 10^4 time units (or 10^3 periods of the lowest frequency phonon), see Fig. 8(a), are in good agreement with the scenario described by Peyrard et al.

Long-term simulations (up to 5×10^5 time units, see Fig. 8(b)) demonstrated the decay of most of the breathers formed at the initial stage. Note, that the upper limit of the grey scale code in Fig. 8(b) is about two times higher than the one in Fig. 8(a). It implies an increase of energy of surviving breathers. Furthermore, among the series of 40 simulations each being 5×10^5 time units long, 29 ones demonstrated the emergence of new DBs at large time scales. In 11 of 29 cases DBs with lifetimes longer than 5×10^4 time units were observed (Fig. 8(b) presents a few instances of such DBs). Modulational instability can not describe the nature of this phenomenon, because these 'late' breathers do not
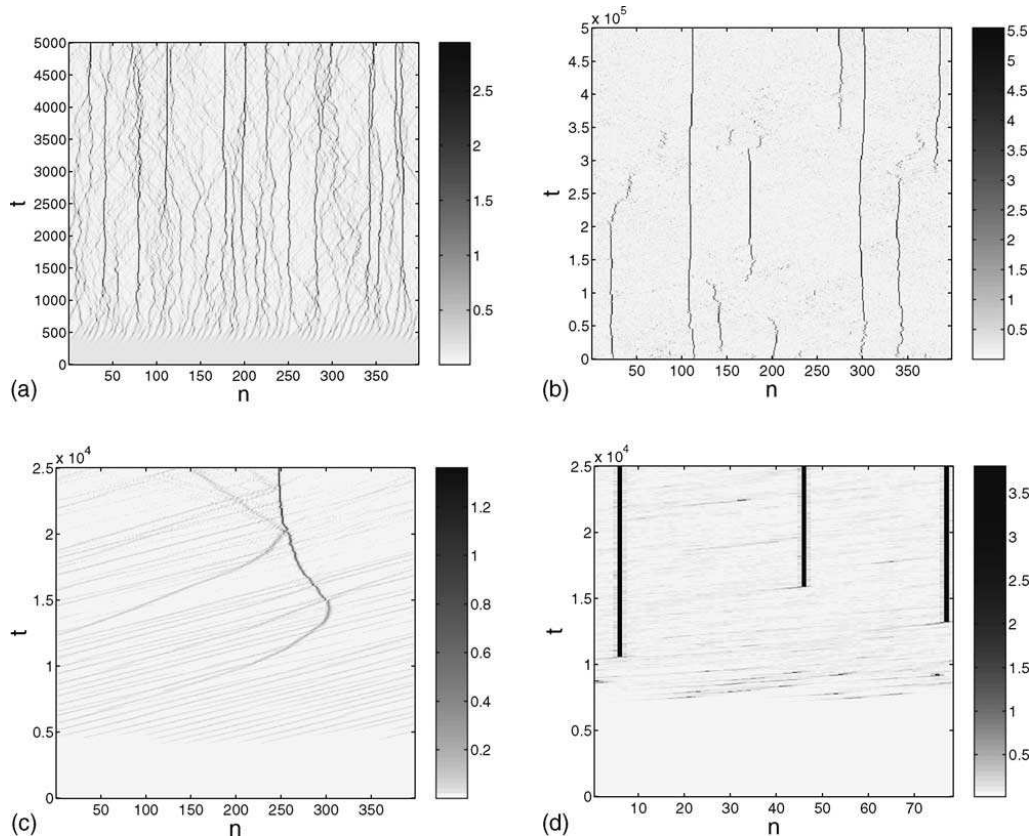

Fig. 8. Energy density evolution in 1D and 2D lattices is plotted in the grey scale. Transient DBs in 1D lattices that result from modulational instability (a) and their long-term evolution (b) are shown ($\bar{\varepsilon} = 0.18$). Character of breather formation in 1D (c) and 2D (d, see comments in the text) at low initial energy density is depicted ($\bar{\varepsilon} = 0.016$). Here $\alpha = 0$.
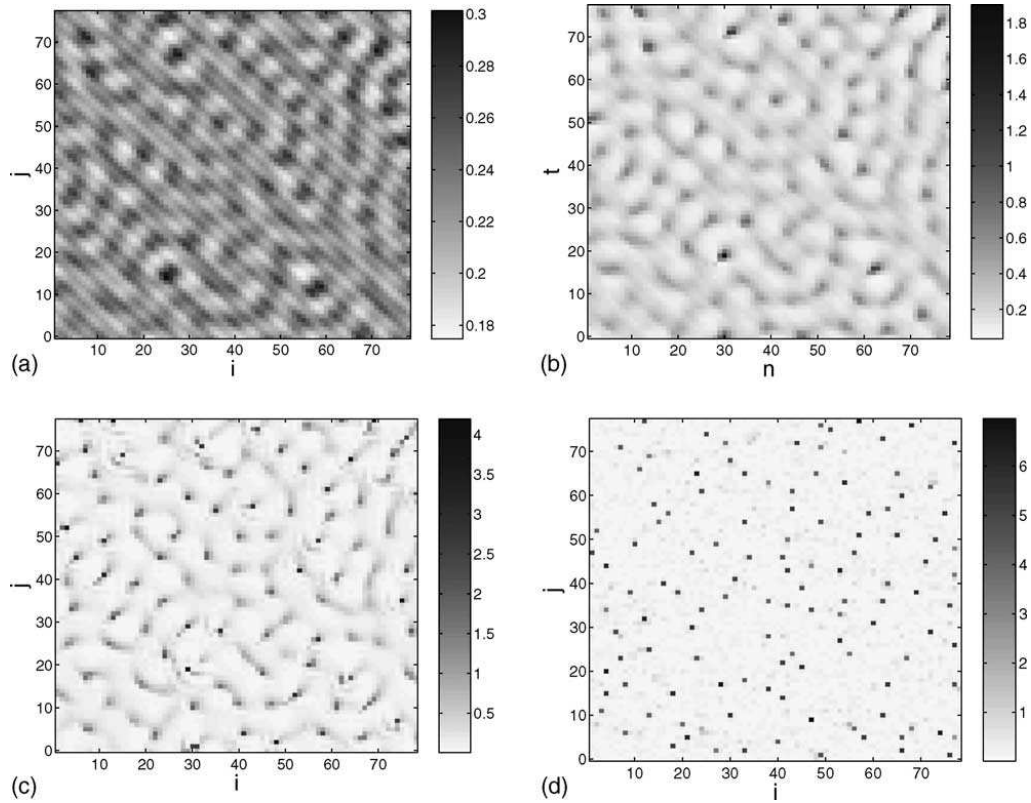
Fig. 9. Energy density evolution in a 2D lattice ($\bar{\varepsilon} = 0.22$). Snapshots taken at $t = 400, 500, 550, 5000$ are shown in (a–d) respectively. Transient DBs that result from modulational instability and their long-term evolution are shown. Here $\alpha = 0$.

originate from a plane wave. Nevertheless, their appearance must be closely connected with the inherent energy concentrating property of the system induced by modulational instability.

The overall scenario of emergence and evolution of breathers observed in 2D lattices is qualitatively the same as in the 1D case. The decay of the initially homogeneous energy distribution into energy lumps is accompanied by a drift of the energy pattern as a whole in the direction of the initial wave vector. Snapshots of the energy distribution during the simulation with the initial wave amplitude $A = 0.5$ ($\bar{\varepsilon} = 0.22$) at $t = 400$, $t = 500$, $t = 550$ and $t = 5000$ are shown in Fig. 9(a–d). Note again, that the grey scale coding is different for plots at different times. Long-term simulations (up to 10^6 time units) showed the process of breathers collapsing, but formation of new breathers was also observed.

In none of the simulations carried out did we observe the decay of all the DBs initially formed. This

indicates, that formation of breathers can stretch transient processes dramatically, thus preventing us from observing the ultimate relaxation to the true thermal equilibrium in our simulations.

A challenging problem is to determine what will happen to the described transient process if the energy density of the initial wave ε_0 is decreased, in particular, whether any kind of energy threshold exists or not. First, as it was proven in [16] for 1D systems, under a proper choice of the wave number (see above), a harmonic wave solution of any amplitude is subject to modulational instability. Therefore, the question is whether this instability can lead to the formation of breathers at arbitrary small values of ε_0. The answer to this question is most likely to be positive for both 1D and 2D systems as suggested by the character of transient processes observed in our simulations.

Indeed, lowering the energy density by one order of magnitude in the 1D case, modulational instability still leads to the formation of wave packets being a few

sites in size, which are moving afterwards monotonically along the chain, from time to time interacting with each other due to some randomness in initial conditions (Fig. 8(c)). At some times, this interaction leads to an energy increase and motion slowdown of certain wave packets. Then other packets moving at their usual speed start to collide with the slow ones, feeding them with energy as described in [16,17]. This leads to a further slowdown of the slow packets, thus the process becomes avalanche-like. The slow packets can even once or several times change the direction of their motion due to collisions with the faster ones. After the energy density in a slow packet exceeds a certain threshold (being about 1.0–1.5, which is in good agreement with the results obtained for the one-site breather model, see Fig. 2), the packet turns into an immobile breather, keeping on collecting energy of the moving low energy packets. The characteristic time required for slow packets and then breathers to appear is increasing rapidly with the decrease in ε_0; nevertheless there seems to be no reason for the described scenario to fail for some small but finite values of ε_0.

In 2D lattices, modulational instability results in the concentration of energy into small (again, a few sites in size) energy lumps. The simulations show that the time needed for these lumps to emerge is about 1.5 times as long and the energy density in a lump about 10 times as high as in the 1D case, the value of ε_0 being equal. The major peculiarity of the 2D case as compared to the 1D one is that the lumps, unless their energy is above a threshold being about 2.0–2.5 (which again perfectly agrees with the one-site breather model, see Fig. 7), collapse again very fast, while 1D lumps keep on moving, preserving their shape and staying quite localized in space. Nevertheless, simulations reveal, that the energy in the 2D lattice after the collapse of the mentioned lumps tends to organize into a larger number of lumps with smaller energy which collide with each other chaotically. Moreover, this late concentration of energy appears to be able to give rise to breathers. Despite the fact that the avalanche process characteristic to 1D systems is no longer observed in the 2D case, the typical time needed for breathers to appear is found to be 1.5–2 times shorter than in the 1D case at the same ε_0. In Fig. 8(d) the maximal energy density value in a column of the lattice is plotted in the grey scale against the number of the column and time (the horizontal and the vertical axes, respectively). Thus, the figure represents the evolution of a sort of a one-dimensional projection of the energy density pattern in the lattice. The dark tilted strokes in this figure denote moving packets. Some of these strokes, especially those appearing at $t \simeq (0.8/0.9) \times 10^4$, end up with dark spots, which indicate the formation and immediate collapsing of energy lumps, while three of them give rise to breathers, appearing as dark vertical lines.

4. External perturbations–energy kicks

In this section we study the emergence of breathers due to external perturbations. We will consider a part of the infinite lattice being exposed to an incoming energy flux in the form of random kicks (think e.g. about a crystal lattice being exposed to a neutron beam).

A kick implies an instantaneous increase of the kinetic energy of a randomly chosen element at a random time (the interval between two kicks is a random value uniformly distributed in the interval $(0, 2\tau)$). In our simulations each kick increases the absolute value of velocity, thus providing a fixed increment $\Delta\varepsilon$ of the local energy of some chosen element. The value of the velocity of an element after a kick is given by

$$\tilde{\dot{u}}_n = \text{sign}\,(\dot{u}_n)\sqrt{\dot{u}_n^2 + 2\Delta\varepsilon}. \tag{10}$$

Thus, the incoming energy flux is characterized by two parameters $\Delta\varepsilon$ and τ.

Since the kicks increase the energy of the system, we allow for some radiation of this energy into outer undisturbed parts of the system. We introduce dissipation in a number of oscillators at the boundaries of the finite lattice considered in numerical experiments:

$$\ddot{u}_n + \lambda_n\dot{u}_n + V'(u_n) = k(u_{n+1} - 2u_n + u_{n-1}) \tag{11}$$

where the dissipation parameters λ_n are zero in the active region and are linearly increasing from the boundary of the active region towards the edges of the lattice.

The initial conditions correspond to zero temperature:

$$u_n(0) = \dot{u}_n(0) = 0. \tag{12}$$

Depending on the value of $\Delta\varepsilon$, a kick can either immediately generate a breather or not. In the latter case the energy of the kick is radiated into the lattice. We restrict ourselves to kick energies $\Delta\varepsilon < 0.3$ for $\alpha =$
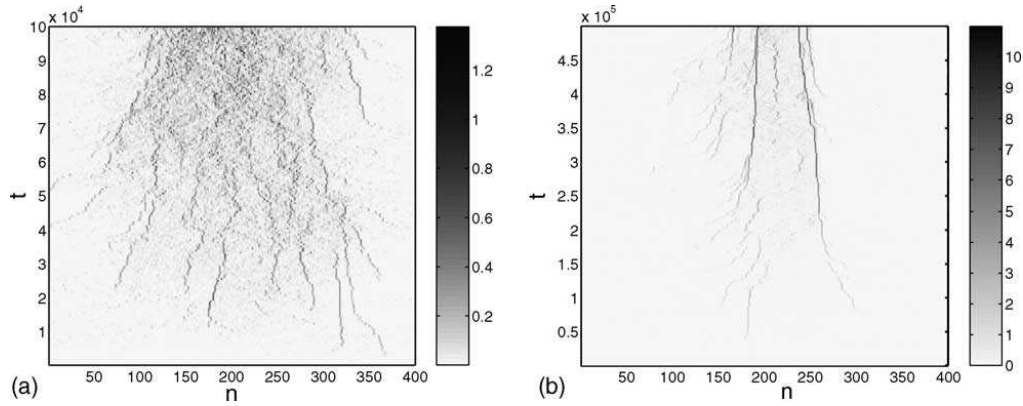
Fig. 10. Energy density evolution in a 1D lattice for (a) $\alpha = -1$, $\tau = 200$, $\Delta\varepsilon = 0.2$ and (b) $\alpha = 0$, $\tau = 200$, $\Delta\varepsilon = 0.4$.

-1 and $\Delta\varepsilon < 1.7$ for $\alpha = 0$, which implies the second case, as computations show.

Numerical simulations of one- and two-dimensional lattices show that even though the kick energy is not enough to generate a DB from scratch, DBs are generated in the system (see Figs. 10 and 11). Let us explain the reason for that. The first kicks heat the cold lattice, and, failing to create DBs, generate wave packets travelling towards the dissipative boundaries. Reaching the boundary takes the wave packet some time which is
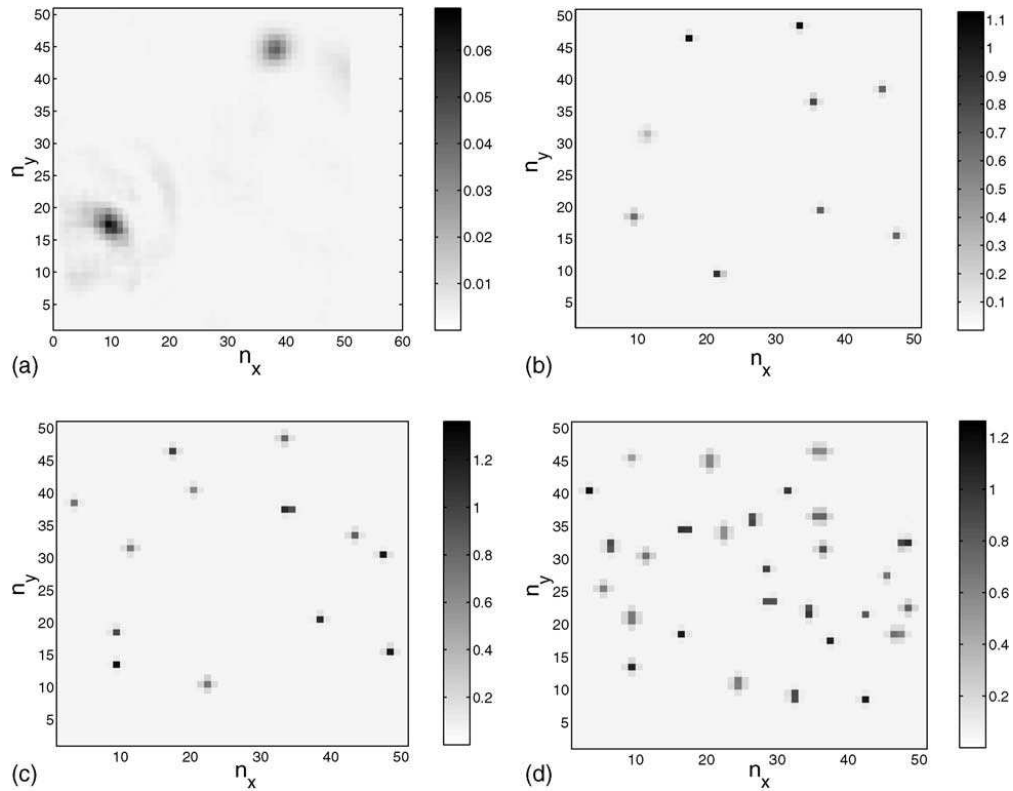

Fig. 11. Energy density evolution in a 2D kicked lattice ($\tau = 200$, $\Delta\varepsilon = 0.9$). Snapshots taken at $t = 2400, 9800, 19800, 59800$ are shown in (a–d) respectively. Here $\alpha = -1$.

long enough for subsequent kicks to take place. Thus, we observe a gradual heating of the lattice, numerous wave packets colliding with each other and thus (see previous section) leading to the formation of DBs.

Although the emergence of DBs looks similar in one- and two-dimensional lattices, their future behavior is completely different.

In a chain generated DBs act as strong scattering centers for travelling wave packets [30–32]. Two or more breathers can block the travelling packets and store the energy between them (Fig. 10). In the case of the asymmetric potential the following scenario is observed. As the local energy gradually increases (see Figs. 10(a) and 12) breathers become subject to increasingly stronger perturbations and eventually get destroyed. This is due to the above discussed energy gap between soft and hard breathers. As a result the chain gets thermalized. However due to following kicks the thermalized hot region again generates soft DBs and so on. Another remarkable effect is that these breathers attract each other. Indeed, breathers in a one-dimensional system effectively backscatter plane waves (see [30–32]). This leads to a trapping of the radiation between them and also to some enhanced retarded interaction between the breathers mediated by the radiation, probably being the cause for the observed attraction. A quite different type of interaction between DBs and wave packets is observed for $\alpha = 0$ (Fig. 10(b)). Here we observe opaque stable DBs, guarding the hot region, which reflect and partially consume energy and stay almost immobile.

We think that the destruction of the soft DBs ($\alpha = -1$) is caused by the existence of the relatively low upper bound of the energy they can possess (see Fig. 2). If the amount of the energy, contributed by wave packets, exceeds this limit, the DB's frequency gets in resonance with the phonon band. Together with the growing thermal fluctuations inside the hot region this process will inevitably destroy the breather. On the other hand, hard DBs may accumulate an arbitrary large amount of energy. The growth in energy of the hard breathers that we observe in Fig. 10(b) helps them preserve their stability in the presence of increasing perturbations and fluctuations.

In a 2D lattice breathers cannot block travelling wave packets as efficiently as in 1D systems. Thus, the radiation can easily reach the dissipative boundaries and disappear. The local energy stays low and
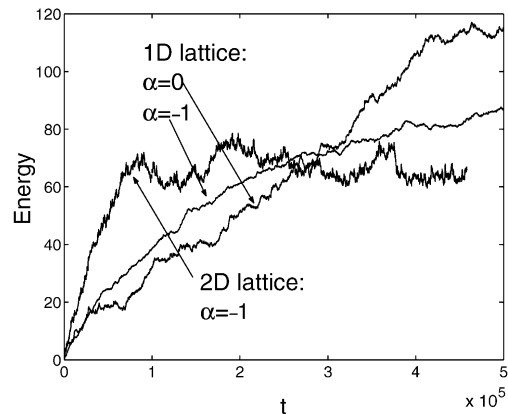

Fig. 12. Evolution of the total energy of the kicked lattice over a long time interval: 1D ($\tau = 200$, $\Delta\varepsilon = 0.2$ for $\alpha = -1$, $\Delta\varepsilon = 0.4$ for $\alpha = 0$) and 2D lattices ($\alpha = -1$, $\tau = 200$, $\Delta\varepsilon = 1.0$).

existing breathers are subject to small perturbations. Long-time simulations show that the lattice becomes saturated with breathers (Fig. 11). The energy is almost completely stored in breathers and also shows saturation (see Fig. 12). From time to time two neighboring breathers can merge or collide and disappear. The appearing free space will be occupied by a new breather soon, as the number of breathers does not seem to decrease substantially with time.

5. Hot spot decay

Yet another way of generating breathers is to heat a certain part of the lattice, and after a subsequent switching off the heating source (e.g. a focused laser beam) to cool the hot spot down by radiation of energy into the neighbouring cold parts of the lattice. The idea is that if breathers are generated in the hot spot, they will simply stay there, and only plane waves will disappear [22–24].

We carried out numerical simulations of the 1D and 2D lattices using both forms of the on-site potential ($\alpha = 0$ and $\alpha = -1$) and observed this effect in our model too. The infinite cold part of the lattice was imitated by a dissipative layer on the boundaries of the hot lattice (see Section 4). We show experiments for a 1D lattice of 400 sites and a 2D lattice of 50×50 sites plus friction boundaries, with model parameters as above.

In Fig. 13(a) we plot the energy density distribution versus time for the case $\alpha = 0$ and initial average en-
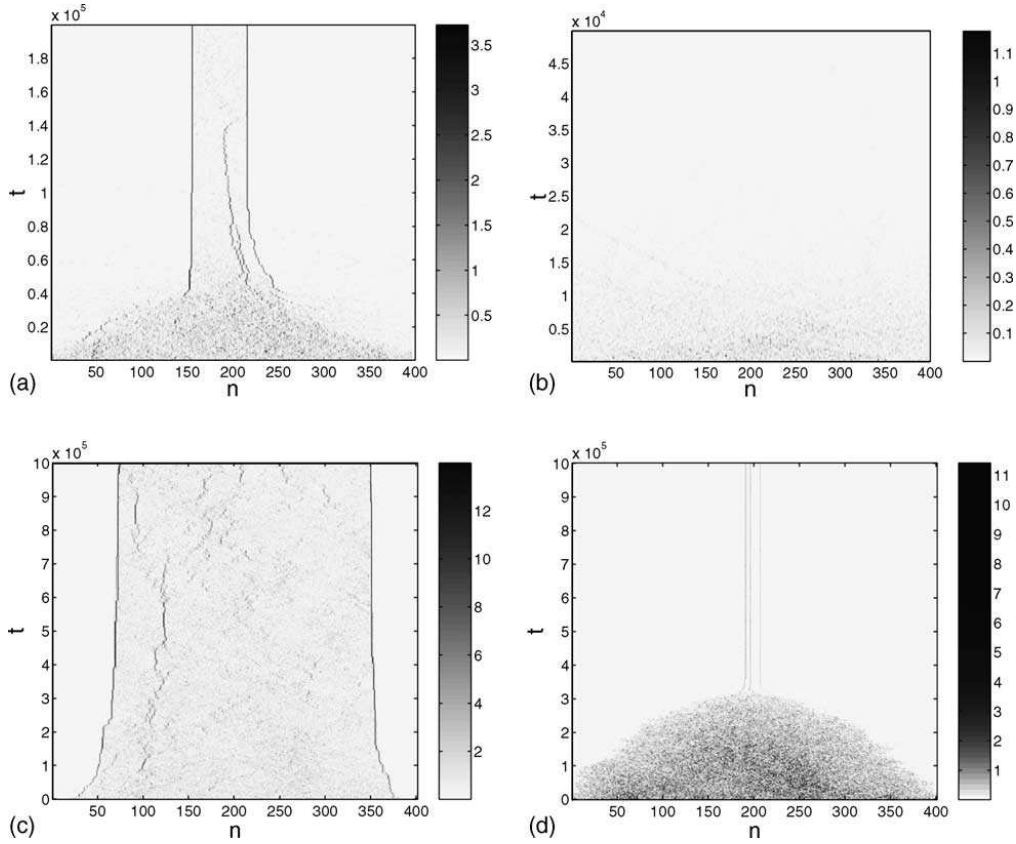
Fig. 13. Energy density evolution in the hot spot of a one-dimensional lattice during cooling. For relatively big energy densities DBs appear after a transient process (a) $\bar{\varepsilon}_0 = 0.389$, $\alpha = 0$; for smaller energy densities they are not observed after cooling down (b) $\bar{\varepsilon}_0 = 0.09$, $\alpha = 0$; for high energy densities, the evolution of systems with $\alpha = 0$, $\bar{\varepsilon}_0 = 0.96$ (c) and $\alpha = -1$, $\bar{\varepsilon}_0 = 0.97$ (d) differs essentially.

ergy per site $\bar{\varepsilon}_0 = 0.389$. We observe the emergence of breathers, which survive on large time scales. Note, that some amount of delocalized energy becomes trapped between the DBs. Although there are no energy thresholds for exact DB solutions in this 1D system, we find that lowering the value of $\bar{\varepsilon}_0$ to 0.09 (Fig. 13(b)) no DBs are detected. The reason is that even if DBs are excited, there energy will be small, they will be weakly localized, close to continuum soliton solutions and can easily move. Moreover in this limit their scattering potential of plane waves is weak also. So simply all the excited energy – plane waves and weakly localized DBs – can quickly leave the hot spot region. Increasing the initial energy density to $\bar{\varepsilon} = 0.96$ we find that for $\alpha = 0$ the size of the hot spot part preserved for long times by large amplitude DBs increases (Fig. 13(c)). At the same time the case $\alpha = -1$ shows the surprising result that

almost all the energy leaves the system, with just a few DBs in the center of the hot spot region (Fig. 13(d)).

In Fig. 14 the energy density distribution in the 2D lattice (here $\alpha = -1$) is shown at four times $t = 0, 4900, 11900, 19900$ and $c = 3$. We observe a fast leakage of plane waves out of the hot spot region, with a number of long-living DBs remaining inside.

To provide better understanding of the dependence of breather excitation upon the initial energy density in the hot spot, we performed simulations of the 1D and 2D lattices at various $\bar{\varepsilon}_0$. After a transient process that takes $t = 10^6$ in the 1D lattice and $t = 2 \times 10^4$ in the 2D lattice we measured the stored energy per site $\bar{\varepsilon}$. The results shown in Fig. 15(a) and (b) show the existence of an average energy density threshold for the appearance of DBs in hot spots especially for the 2D case.
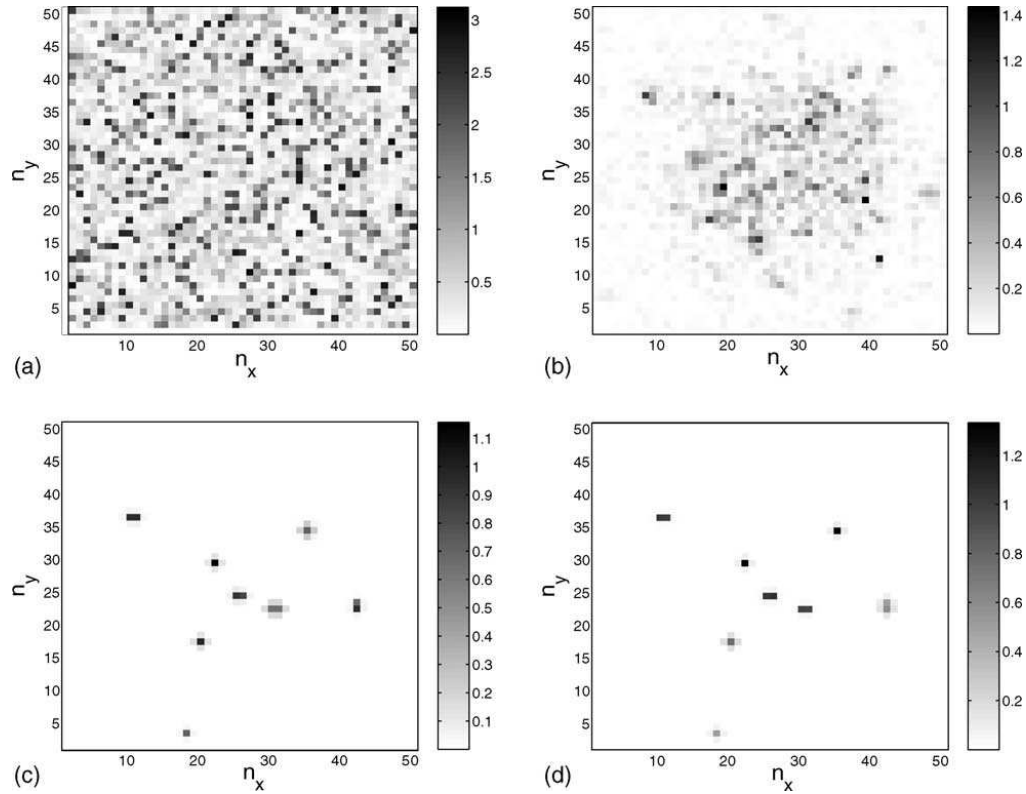
Fig. 14. Energy density evolution in the hot spot of a 2D lattice during cooling. Snapshots taken at $t = 0, 4900, 11900, 19900$ are shown in (a–d) respectively. Here $c = 3$ ($\bar{\varepsilon}_0 = 0.97$), $\alpha = -1$.

Let us discuss the results for the 1D lattice. A comparison with the results of simulations of lattices in thermal equilibrium (Fig. 4) implies that the appearance of DBs in the hot spot with subsequent cooling is closely related to the existence of pronounced DBs in thermal equilibrium. Especially, if the initial energy density was too low to generate DBs, no DBs are expected to appear during the subsequent cooling. DBs appear in the case $\alpha = -1$ as soon as the energy density is large enough for the soft DBs to form. For $\alpha = 0$ one
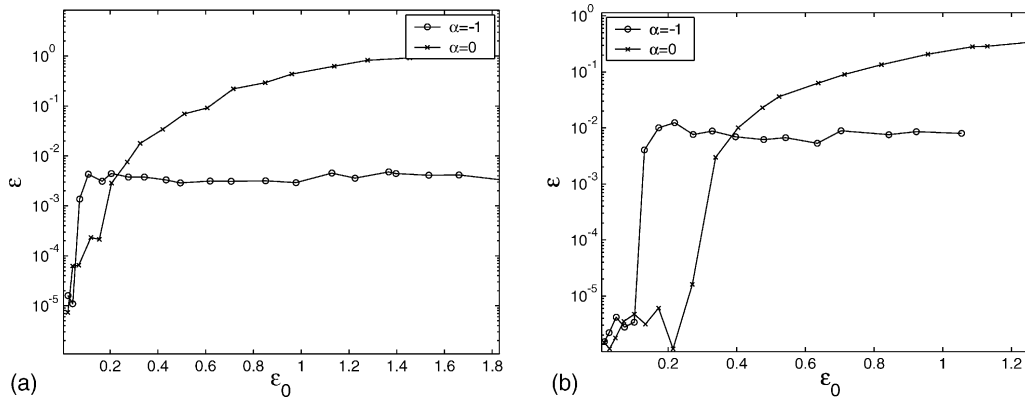

Fig. 15. Average energy per site after a transient process versus initial average energy for (a) 1D (at $t = 10^6$) and (b) 2D (at $t = 2 \times 10^4$) lattices.
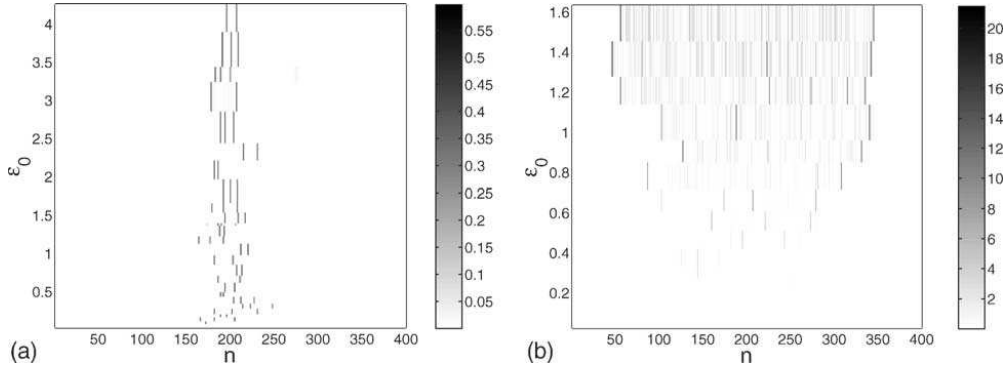
Fig. 16. Spatial distribution of the energy density after a transient process (at $t = 10^6$) is shown. Initial energy density $\bar{\varepsilon}_0$ is changed along the vertical axis. Here (a) $\alpha = -1$, (b) $\alpha = 0$.

needs larger values of $\bar{\varepsilon}_0$ to observe hard breathers, in analogy to the case of thermal equilibrium.

The dynamics of the lattice becomes far more puzzling as $\bar{\varepsilon}_0$ is increased further (see Fig. 13(c) and (d) for $\bar{\varepsilon}_0 = 0.96$ with $\alpha = 0$ and $\bar{\varepsilon}_0 = 0.97$ with $\alpha = -1$, respectively). To obtain further insight we plot in Fig. 16 the spatial energy distribution as a function of the initial energy density $\bar{\varepsilon}_0$ after a cooling time of 10^6. For the asymmetric on-site potential (Fig. 16(a)) several soft breathers are pinned down in close neighborhood of each other, in the center of the hot spot region, which is also reflected by a constant value of the total energy left in the system. If $\bar{\varepsilon}_0$ is low enough, then soft DBs may be observed at the edges of the hot spot region (moving towards each other during the cooling). These DBs are weakly localized and do not act as efficient backscatterers of waves which leak into the cold region. For the case of the symmetric on-site potential hard breathers successfully appear, grow in energy (as $\bar{\varepsilon}_0$ is increased) and efficiently backscatter wave packages, storing some amount of energy between them (see Fig. 16(b)).

A possible reason for the fact, that soft DBs do not appear on the edges of the hot region at high energies and (when they do at lower $\bar{\varepsilon}_0$) do not prevent it from getting cooled, is that soft DBs appear only on intermediate energy scales (see Figs. 2 and 4). Even if they appear on the edges of the hot spot, the plane waves inside this region will heat them up and lead to their disappearance. Only if the soft DBs are generated in the center of the hot spot, they can survive, simply because there is no further significant interaction with radiation.

This also explains why the final energy left in the region after cooling is quite constant (Fig. 15(a)). In the case of hard DBs nothing prevents them from raising their energy on the expense of radiation and still remaining (even more) robust and localized.

Finally, let us discuss in more detail the result for the 2D case in Fig. 15(b). For $\alpha = 0$ we find the presence of an energy threshold for DBs. Essentially no DBs are observed for $\bar{\varepsilon}_0 < 0.3$. This corresponds to DB energies larger than $5 \times 0.3 = 1.5$, and is of the order of the minimum hard DB energy 2.76. The monotonous increase of ε for $\bar{\varepsilon}_0 > 0.4$ is due to the increasing number and energies of DBs excited. Thus, we confirm thermal equilibrium studies from Section 2 and again observe DB energy thresholds affecting the statistics of the system, this time concering relaxations. For $\alpha = -1$ no DBs are observed for $\bar{\varepsilon}_0 < 0.1$, which is three times less the threshold value for $\alpha = 0$. Note that soft DBs have here an energy threshold of 0.84, roughly three times smaller the hard DB threshold for $\alpha = 0$. This is a strong indication that for $\alpha = -1$ we observe the soft DB energy thresholds. The plateau behaviour of ε for $\bar{\varepsilon}_0 > 0.2$ can be explained by the fact that soft DBs are excited only from a narrow energy interval. Further increase of the input energy density simply leads to an excess of plane waves which are radiated away. The hard DB energy threshold of 8.06 implies that possible changes due to the additional excitation of hard DBs are expected for input energy densities $\bar{\varepsilon}_0 > 1$. The detailed investigation of these intricate issues is beyond the scope of the present work.

6. Conclusions

The results presented in this paper demonstrate the complex and intricate way of DB excitation in nonlinear lattices. They include the novel modulational instability scenario in 2D lattices, the observation of DB energy thresholds in 2D lattices both in thermal equilibrium and in hot spots during cooling, and the generation of DBs in lattices with external energy kicks. Our studies show that while results for exact DB solutions and their small perturbations help in interpreting some of the data, some cases are less clear. Especially the fact that thermal equilibrium studies suggest that for small enough temperatures DBs do not exist, but reappear during a subsequent cooling of a corresponding hot spot region, remain puzzling. While there exist several publications with related results, only the coherent choice of potentials allows to reveal the complexity of the processes under consideration.

Our results show how different DBs behave in 1D and 2D lattices. Since DBs act as strong scattering centers in 1D systems, they trap radiation. But precisely this radiation starts to interact with the DBs, perturbing them in various ways (cf. [33,34]). This interaction often leads to a DB destruction. Contrary DBs in 2D systems interact only weakly with radiation. This implies that DBs in 2D systems are much more robust in the presence of various fluctuations. We can safely conjecture here that this will be even more true for 3D systems.

We have indirectly observed the presence of energy thresholds for DBs in 2D systems. For special models such thresholds can be also obtained in 1D systems. Recent efforts to observe these thresholds in 1D systems in thermal equilibrium were less conclusive (cf. [29]). We think that a possible reason for that is the above mentioned effect that 1D breathers trap radiation and thus are easier destroyed.

One of the outcomes of the present work is that time-resolved pump-probe spectroscopy is a possible method to observe DBs e.g. within the scenario of hot spot cooling in thin film insulators, if DBs survive for 4–6 orders of the phonon time scales as obtained in our numerical studies. Possible links exist also with the long discussed issue of hole burning, where radiation causes long time changes in the spectral properties of absorption of crystals.

To conclude we think that despite of a growing number of results on DB properties in lattices in and out of equilibrium, we are just at the beginning of understanding the complex ways dynamical localization may take to influence statistical properties of nonlinear lattices. The best is yet to be done.

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