Cooling nonlinear lattices toward energy localization

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We describe the energy relaxation process produced by surface damping on lattices of classical anharmonic oscillators. Spontaneous emergence of localized vibrations dramatically slows down dissipation and gives rise to quasistationary states where energy is trapped in the form of a gas of weakly interacting discrete breathers. In one dimension, strong enough on-site coupling may yield stretched-exponential relaxation which is reminiscent of glassy dynamics. We illustrate the mechanism generating localized structures and discuss the crucial role of the boundary conditions. For two-dimensional lattices, the existence of a gap in the breather spectrum causes the localization process to become activated. A statistical analysis of the resulting quasistationary state through the distribution of breathers' energies yield information on their effective interactions. © *2003 American Institute of Physics.* [DOI: 10.1063/1.1535770]

Discrete breathers have been widely analyzed as mathematical objects, but the relevance of their role in physical systems is still debated. In fact, any mechanism yielding the spontaneous formation of breathers is expected to provide interesting indications in this direction. In this respect, the phenomenon of relaxation to breather states by cooling lattices from their boundaries is one of the most interesting examples. Here we provide a comprehensive description of this phenomenon in low dimensional lattices. In particular, we review former results and add new information, mainly concerning the two-dimensional case. This study is based on a combination of numerics and theoretical arguments, while we analyze both dynamical and statistical features of the problem to clarify the whole scenario.

I. INTRODUCTION

Nonlinearity has revealed one of the key ingredients for describing many relevant features of different states of matter. In the realm of lattice dynamics, scattering processes among phonons, propagation of solitary waves, and slow energy relaxation are typical examples. Recently, considerable efforts have been devoted to the study of periodic, localized, nonlinear lattice excitations, named ''breathers.'' [1] They are quite peculiar (but generic) objects emerging from the interplay of nonlinearity and space discreteness.[2] Their mathematical properties, like existence, stability, mobility, etc., have been progressively unveiled, while they have been identified in many different scenarios.

Their role in nonequilibrium dynamics seems to be particularly fascinating. An example is the relaxation to energy equipartition of short-wavelength fluctuations.[3] Another interesting scenario where breathers are found to emerge spontaneously is observed upon cooling the lattice at its boundaries,[4–6] i.e., by considering a nonequilibrium process in which energy exchange with the environment is much faster at the surface than in the bulk. The numerical simulations neatly show that the energy dissipation rate may be significantly affected by the spontaneous excitation of breathers. As the latter exhibit a very weak interaction among themselves and with the boundaries, the energy release undergoes a sudden slowing down and is hardly detected on the time scales of a typical simulation. Thus, the lattice remains frozen in a pseudostationary, metastable configuration which is far from thermal equilibrium, which we shall refer to as *residual state*. Despite the absence of disorder, there is a close similarity to the glassy behavior observed in disordered systems, as was already pointed out.[4,5]

But what are the mechanisms leading to spontaneous localization? As we have shown in a previous paper,[6] the latter is intimately related to how dissipation acts on vibrational modes of different wavelengths. If long-wavelength phonons can be efficiently damped out, the modulation instability of short lattice waves[7] becomes highly favored and breathers can easily emerge from an interacting soliton gas.[3,8] In this respect, this type of nonequilibrium condition is much more effective in exciting localized modes than an equilibrium one (see, e.g., Ref. 9 for a related discussion).

Spontaneous localization upon cooling has been observed for both on-site[4,5] and pure nearest-neighbor (nn) interactions.[6,10] The two classes of models are known to behave differently, e.g., as to the mobility of breathers, which is much higher in the absence of local coupling. This is also confirmed by relaxation experiments, where differences in the energy decay laws have been observed. In particular, the

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approach to the residual state follows a simple exponential law in the Fermi–Pasta–Ulam (FPU) system,[6] but turns to stretched exponential in the presence of local coupling.[5]

Our aim in this paper is to provide an up-to-date overview of the phenomenon of breather localization by cooling. Generalities about the energy release process, including models and indicators, will be presented in Sec. II, along with the discussion of the cooling process in an harmonic lattice and the results obtained for one-dimensional (1D) nonlinear systems. In particular we shall survey the different cooling pathways appearing in pure nn and on-site potentials. A specific section will be devoted to clarifying the interpretation of some recent results.[10,11] In Sec. III, we present the results for the nn two-dimensional (2D) FPU model. We want to point out that the 2D is not a straightforward extension of the 1D case. Indeed, the existence of an energy activation threshold for breather solutions[12] leads to conjecture that a thermalized state may be cooled to the residual state only above some initial energy/temperature. Moreover, the residual state is a static multibreather state, whereby in the 1D case it usually contains a single breather. Finally, we perform an analysis of the distribution of breather energies, based on a simple statistical model.

II. RELAXATION AND LOCALIZATION IN 1D

In this section we will describe the lattice models and the generalities of a typical relaxation experiment as well as the relevant indicators used throughout the paper. Let us consider a chain of N atoms of unit mass and denote by u_p the displacement of the pth particle from its equilibrium position pa (a is the lattice spacing). The atoms are labeled by the index $p=0,1,\ldots,N-1$ and their dynamics is given by the equations of motion

$$\ddot{u}_p = V'(u_{p+1}-u_p) - V'(u_p-u_{p-1}) - U'(u_p) - \gamma \dot{u}_p[\delta_{p,0}+\delta_{p,N-1}],$$

where $V(x)$ and $U(x)$ are the interparticle and on-site potentials, respectively. We assume that $V'(0)=U'(0)=0$, denoting with a prime the derivative with respect to x. For convenience, we shall adopt nondimensional units such that a and $V''(0)$ are set to unity. Moreover, as we want to deal with systems in a finite volume, we will impose either free-end ($u_{-1}=u_0$, $u_{N-1}=u_N$) or fixed-end ($u_{-1}=u_N=0$) boundary conditions (BCs).

The last term in Eq. (1) represents the interaction of the atoms with a ''zero-temperature'' heat bath in the form of a linear damping with rate γ. Following Refs. 4 and 5, we restricted ourselves to the case in which dissipation selectively acts only on the atoms located at the chain edges. As mentioned earlier, this choice is crucial and should model a physical situation in which energy exchange with the environment is much faster at the surface than in the bulk.

The general layout of a simulation can be summarized as follows. First, an equilibrium microstate is generated by, say, Nosè–Hoover (canonical) method[4] or by letting the Hamiltonian (microcanonical) system ($\gamma=0$) evolve for a sufficiently long transient.[6] In the following we will follow the second strategy. The initial condition for the transient is assigned by setting all displacements u_p to zero and by drawing velocities at random from a Gaussian distribution. The velocities are then rescaled by a suitable factor to fix the desired value of the energy density (energy per particle) e_0. The resulting set of u_p and $\dot{u}_p$ is then used as initial condition to integrate Eq. (1) with $\gamma>0$ (again see Ref. 6 for details).

The result of the relaxation process is the residual state, i.e., a state with a finite fraction of the initial energy stored in the form of breathers. Remarkably, such residual state is characterized by a decay time scale which is several orders of magnitude longer than that of the localization process.

A. The harmonic lattice

A number of features which characterize the relaxation dynamics of nonlinear lattices can be better understood by first studying the harmonic lattice, namely

$$V(x)=\tfrac{1}{2}x^2.$$

We anticipate that the presence of an harmonic on-site potential does not alter the main conclusions. We thus take $U=0$ throughout this section.

For small damping, an approximate analytical solution can be found by time-dependent perturbation theory. Let $\omega_\alpha^2=4\sin^2(q_\alpha/2)$ and η^α ($\alpha=0,1,\ldots,N-1$) denote the eigenvalues and normalized eigenvectors of the unperturbed Hamiltonian problem, where the allowed wave numbers are $q_\alpha=\alpha\pi/N$ and $q_\alpha=(\alpha+1)\pi/(N+1)$ for free-end and fixed-end BCs, respectively. To the lowest order in γ one obtains[6]

$$u_p(t)=\sum_{\alpha=0}^{N-1} c_\alpha e^{-(1/\tau_\alpha+i\omega_\alpha)t}\eta_p^\alpha. \tag{1}$$

where η_p^α is the pth component of the eigenvector η^α and c_α are constant amplitudes fixed by the initial conditions. Notice that, since the number of the damped particles is fixed, the perturbative approximation is expected to improve upon increasing the system size N. The wave-number-dependent damping rates are found to be

$$\frac{1}{\tau_\alpha}=\begin{cases}\dfrac{1}{\tau_0}\cos^2\left(\dfrac{q_\alpha}{2}\right) & \text{for free-end BC}\\[2ex] \dfrac{1}{\tau_0}\sin^2(q_\alpha) & \text{for fixed-end BC}\end{cases} \tag{2}$$

with $\tau_0=N/2\gamma$. The free-end and fixed-end BC systems thus show considerably different behaviors. In the former case, the least damped modes are the short-wavelength ones ($\alpha\approx N$), the largest lifetime being $\tau_{N-1}\approx 2N^3/\pi^2\gamma$, while the most damped modes are the ones in the vicinity of $\alpha=0$, with τ_0 being the shortest decay time. On the contrary, for fixed ends the most damped modes are those around the band center ($\alpha\approx N/2$) while short- and long-wavelength ones dissipate very weakly, being $\tau_{N-1}\approx N(N+1)^2/2\pi^2\gamma$. As we shall illustrate in the following, such difference is crucial for the localization in the nonlinear system.

Using the solution (1), we evaluated the chain energy in the case of equipartition, i.e., by replacing $c_\alpha^2\omega_\alpha^2$ with its

average value $2e_0$. Finally, recalling Eq. (2) and approximating for large N the sum over α with an integral ($\tau_\alpha \to \tau(q)$), we obtained[6]

$$\frac{E(t)}{E(0)} = \frac{1}{\pi}\int_0^\pi e^{-2t/\tau(q)}dq = e^{-t/\tau_0} I_0\left(\frac{t}{\tau_0}\right) = \begin{cases} e^{-t/\tau_0} & \text{for } t \ll \tau_0 \\ \dfrac{1}{\sqrt{2\pi(t/\tau_0)}} & \text{for } t \gg \tau_0 \end{cases} \tag{3}$$

where I_0 is the modified zero-order Bessel function, whose asymptotic expansions have been used to obtain the last equality. We conclude that relaxation is exponential only at short times while a crossover to a power-law decay occurs at $t \approx \tau_0$. Moreover, despite the differences in the relaxation times (2), the decay law for E turns out to be the same in the free and fixed-end systems.

The above-mentioned formulas must be taken with caution when dealing with a large but finite system. In such a case, there is of course a lower cutoff at wave numbers of order π/N. Therefore, after a time of the order of the lifetime of the longest-lived mode, $\tau_{N-1} \sim N^3/\gamma$, formula (3) no longer holds and a further crossover to the exponential decay law $\exp(-2t/\tau_{N-1})$ occurs. This has been also verified numerically.[6]

B. Nonlinear lattices: The role of discreteness

Since the first results of relaxation experiments in nonlinear lattices were reported,[4,5] there has been some debate as to the nature of the decay law of the system energy and its relation with the spontaneously emerging localized modes. In particular, it has been claimed that the phenomenon of energy pinning in the form of discrete breathers would result in a glassy-like relaxation, i.e., stretched exponential decay law. Here we shall describe how the main role in determining the relaxation properties of a nonlinear lattice is indeed played by the type of potential energy. In particular, we will highlight the importance of the relative strength of the interparticle and on-site potentials, i.e., the degree of discreteness of the system. In order to do so, we study the general class of nonlinear lattices obeying the equations of motion (1). In particular, we shall report here the results of numerical simulations performed with

$$V(x) = \tfrac{1}{2}x^2 + \tfrac{1}{4}x^4, \quad U(x) = \tfrac{1}{4}\kappa x^4. \tag{4}$$

In this case, the relative strength of local and interparticle nonlinearities is accounted for by the parameter κ.

In Fig. 1 we show the space–time contour plots of the symmetrized site energies, defined as

$$h_p = \tfrac{1}{2}\dot{u}_p^2 + \tfrac{1}{2}[V(u_{p+1}-u_p) + V(u_p - u_{p-1})] + U(u_p).$$

The instantaneous total energy of the system is then given by $E = \Sigma_{p=0}^{N-1} h_p$. We see that a single localized excitation emerges from the relaxation process for both small and large values of κ. The pathway to localization is the same as the one observed in the FPU model.[6] In particular, the basic mechanism leading to localization is modulational instability of short wavelength modes. The latter can only be effective if dissipation of long wavelength phonons is fast enough. As it shows from Eq. (2), this occurs only in the case of free-end BCs, whereas fixed-end BCs strongly inhibit such process. On the other hand, breather mobility is strongly reduced in the highly discrete system [Fig. 1(b)]. Such difference is even more evident in the decay law of the normalized energy $E(t)/E(0)$, which turns from pure exponential to stretched-exponential behavior upon increasing κ. This is better appreciated by plotting the indicator

$$\mathcal{D}(t) = -\ln[E(t)/E(0)] \tag{5}$$

in a log–log scale, so that a stretched-exponential law of the form $E(t) = E(0)\exp[-(t/\tau)^\sigma]$ becomes a straight line with slope σ that intercepts the y axis at $-\sigma \ln \tau$ [Fig. 2(a)]. The scaling regions correspond to the onset of energy localization, as can be seen by plotting the localization parameter

$$\mathcal{L}(t) = N\frac{\Sigma_p h_p^2(t)}{[\Sigma_p h_p(t)]^2} \tag{6}$$

[Fig. 2(b)]. From its very definition, the fewer sites the energy is localized onto, the closer $\mathcal{L}$ is to N. On the other hand, the more evenly the energy is spread among all the particles, the closer $\mathcal{L}$ is to a constant of order 1. It should be noted that $\mathcal{L}$ is a relative quantity, and bears no information on the amount of energy that is localized. As a matter of fact, the fraction of e_0 that gets trapped in the residual state is found to be greater the higher the degree of discreteness of the system.

To summarize, if the on-site force is weak enough, the behavior is basically the same as the FPU chain which, in turn, exhibits in the approach to the residual state the same exponential decay law of its linearized counterpart, i.e., $E(t)/E(0) \propto \exp(-t/\tau_0)$ [see Eq. (3)]. The reasons for such behavior are the same discussed for the FPU model.[6] First of all, an effective harmonic Hamiltonian with energy-dependent renormalized frequencies is known to account for several equilibrium properties of the FPU chain.[13,14] Second, the harmonic approximation becomes increasingly accurate as time elapses, simply because more and more energy is extracted from the system by the reservoir. On the contrary, if the system is highly discrete, the first relaxation stage is indeed described by a stretched exponential law. A quantitative explanation of it is still lacking, but it is clear that in this case an effective description of such genuine nonlinear phenomenon in terms of quasi harmonic modes breaks down. In other words, the resulting interactions among linear modes inhibit the energy flow from the bulk to the boundaries, thus slowing down the dissipation.

The onset of a pseudostationary state corresponds in Fig. 2 to the almost flat final portions of the curves. Actually, being the system globally dissipative, energy is still at that stage exponentially decreasing but with a huge time constant τ_b. The latter is expected to be inversely proportional to the breather amplitude at the lattice edges, which, in turn, should be of order $\exp(-N/\ell)$, with $\ell \ll N$ being the localization length.

The above-mentioned scenario is generic for large enough systems. Nonetheless, failure to spontaneously local-

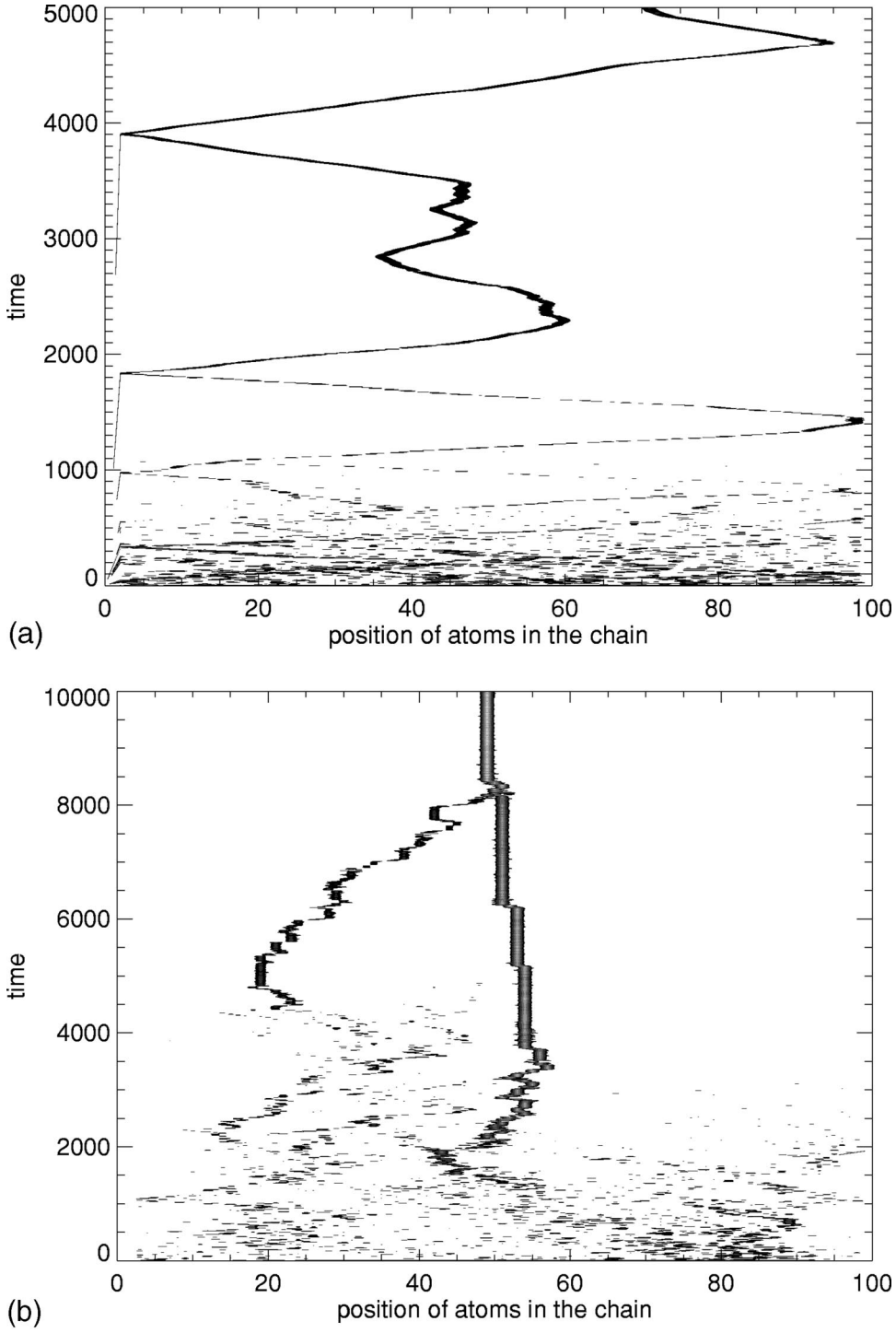

FIG. 1. Relaxation in a FPU chain with quartic on-site potential, $\gamma=0.1$, $N=100$, $e_0=1$. Space–time contour plots of the symmetrized site energies. (a) $\kappa=0.1$. (b) $\kappa=10$.

ize energy occurs the more frequently the smaller is the lattice. This is because the probability of occurrence of large enough energy fluctuations at a given energy density decreases with the number of particles. In other words, given a number of different initial equilibrium conditions, only a fraction n of them will give rise to breathers. To give a quantitative idea, for the FPU model with $e_0=1$, n is only about 50% for a chain of $N=20$ particles but rapidly approaches 100% already for $N\gtrsim 100$. In the absence of spontaneous localization, the nonlinear systems show no difference with respect to the linear ones and $E(t)$ decays according to Eq. (3).

C. The effective-exponent analysis

We have repeatedly mentioned that for the FPU model no stretched exponential relaxation is observed, even in presence of a weak on-site force. In this section we wish to expand on this statement by reporting a more detailed analysis of the energy decay. This can be accomplished by defining an effective exponent $\zeta(t)$ through the logarithmic derivative

$$\zeta(t)=\frac{d[\ln \mathcal{D}(t)]}{d[\ln t]}. \tag{7}$$

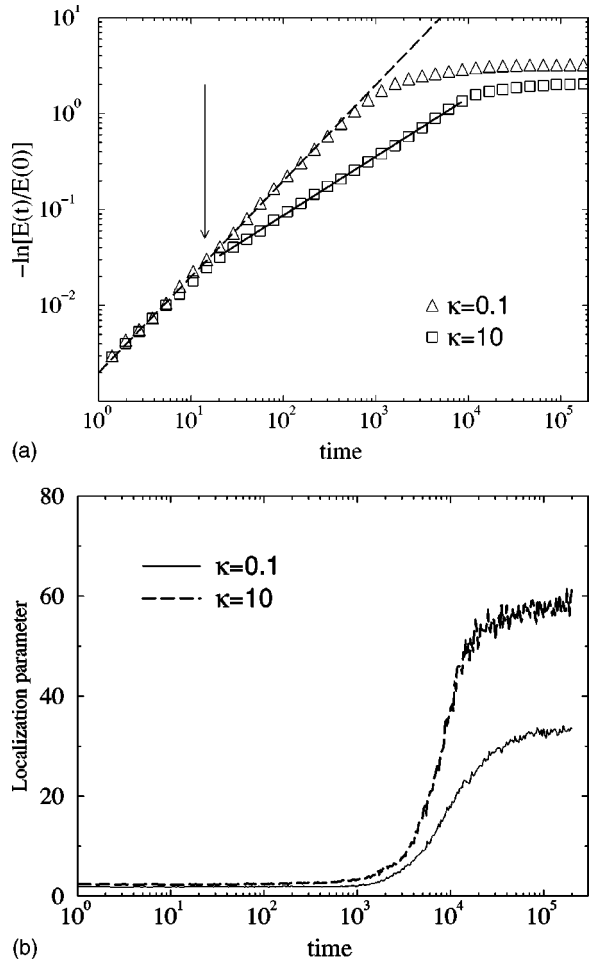

FIG. 2. FPU chain with quartic on-site potential, $N=100$, $\gamma=0.1$, and $e_0=1$. (a) Plot of $\mathcal{D}$ vs time. The dashed line is the exponential $\exp(-t/\tau_0)$, while the solid line is a fit with the stretched exponential law $\exp[-(t/\tau)^{\sigma}]$ ($\sigma\approx 0.61$). The arrow marks the time at which the system with $\kappa=10$ departs from the initial exponential trend. (b) Localization parameter vs time for different values of the on-site coupling κ. The data of both $\mathcal{D}$ and $\mathcal{L}$ are averaged over 32 initial conditions.

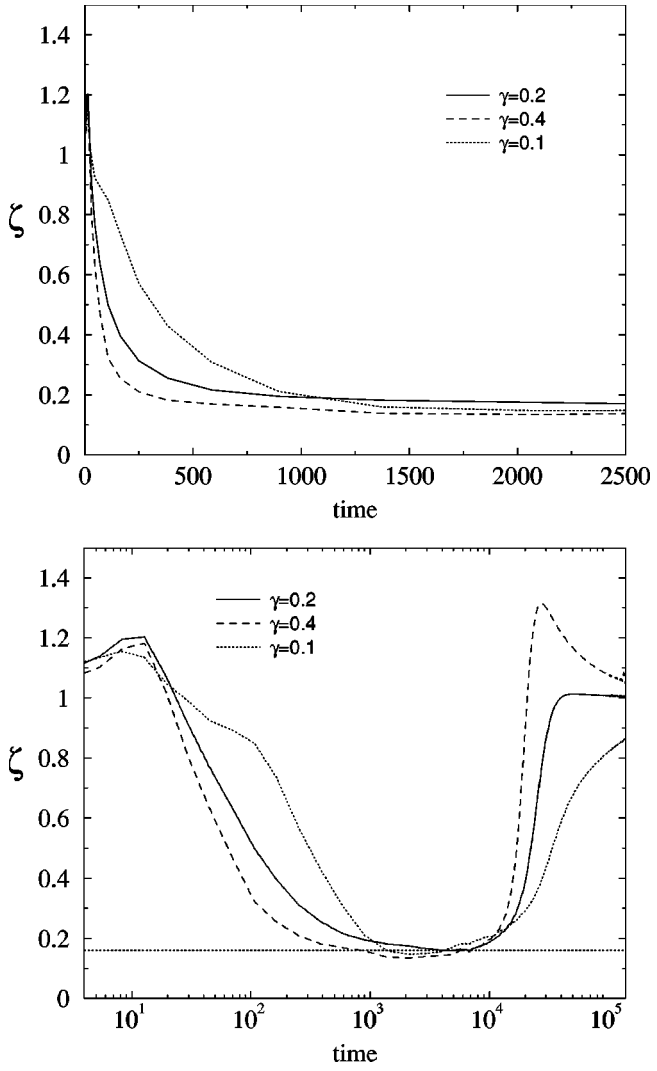

FIG. 3. Plot of $\zeta(t)$ for a short FPU chain ($N=20$) for different γ's and $e_0=2$. (a) Short linear time scale. (b) Long logarithmic time scale. The dotted line is the γ-independent minimum $\zeta_{\min}$ (see the text). Localization does not even occur for this initial condition but one can incorrectly conclude in favor of a stretched-exponential law.

It is clear from definition (7) that if a portion of the energy decay curve goes as $E(t)=E(0)\exp[-(t/\tau)^{\sigma}]$ this would result in a plateau of height σ in the corresponding $\zeta(t)$ curve. For the problem at hand, interpretation of numerical data with this indicator is however a delicate matter. Actually, we want to remark that a naive analysis can lead to misleading or even incorrect conclusions.[10,11]

The most convincing way to illustrate this is to discuss the case of the harmonic chain where localization and stretched-exponential behavior are obviously excluded *a priori*. From Eq. (3), it is easily seen that ζ should start from 1 and monotonically vanish as $1/\ln t$ for $t\gg\tau_0$. On the other hand, we already learned that in a finite chain a further crossover to an exponential law $\exp(-2t/\tau_{N-1})$ occurs so that ζ must again approach 1 for $t\gg\tau_{N-1}$. The net results of those competing trends is that, for a finite N, ζ displays a broad minimum $\zeta_{\min}$, at $t\sim\tau_{N-1}$. The value $\zeta_{\min}$ (which is independent of γ) can be estimated by noting that from Eqs. (7) and (3) one has $\zeta(t)\approx 1/\ln[2\pi t/\tau_0]$ for $t\gg\tau_0$, and hence $\zeta_{\min}\approx 1/2\ln[4N/\pi]$. A simple plot of the curves shows how the minimum $\zeta_{\min}$ can be incorrectly interpreted as a plateau if observed on a too short time scale. Of course, the same scenario is likely to appear in relatively short FPU chains whenever the chosen initial conditions do not yield localization (see Fig. 3).

When localization does occur, the residual state decays exponentially.[6] Therefore one expects ζ to converge to 1 as the residual state is approached. Actually, one observes first very small values of ζ, while such a convergence does occur only on much longer time scales. To see why, let us consider a one-breather residual state. The total energy decays as $E(t)=E_b e^{-t/\tau_b}$, where E_b is the initial energy of the breather and τ_b its characteristic decay time. The time constant τ_b is huge: in fact, it is roughly inversely proportional to the breather amplitude at the edge sites of the chain. From definitions (7) and (5) one has

$$\zeta=\frac{t/\tau_b}{t/\tau_b-\ln[E_b/E(0)]}. \tag{8}$$

Since $-\ln[E_b/E(0)]$ is a number of order 1, we see that, at times such that $t \ll \tau_b \ln[E_b/E(0)]$, ζ is very small. The numerical results in this case are just a deceptive by-product of the wrong normalization. The exponent ζ will start converging to 1 only when $t \gg \tau_b \ln[E_b/E(0)]$, which is a huge time, being also $E_b \ll E(0)$. In this case the ζ analysis may be misleading in identifying the nature of the decay law. The way around such problem would be to calculate the effective exponent by normalizing the total energy to E_b. However, this solution is in turn complicated by the intrinsic uncertainty in locating the time origin for the decay of the breather state.

III. 2D LATTICES

Since a careful study of the 2D Klein–Gordon model has already been presented,[5] we focus here on the 2D FPU model. In this respect, the most natural extension of model (1) should involve a two-component displacement vector. For the sake of simplicity, we rather consider here a scalar model with only one degree of freedom $u_{i,j}$ per lattice site. Actually, a preliminary series of simulations of the 2D vector version showed no appreciable differences with what is reported here, and will be discussed elsewhere.

With the same choice of nondimensional units introduced in Sec. II, the model on an $N \times N$ lattice $(i,j = 0,\ldots,N-1)$ with damping on all edges is defined by the equations of motion

$$\ddot{u}_{i,j} = V'(u_{i+1,j} - u_{i,j}) - V'(u_{i,j} - u_{i-1,j}) + V'(u_{i,j+1} - u_{i,j}) - V'(u_{i,j} - u_{i,j-1}) - \sum_{p,q=0}^{N-1} \Gamma_{i,j}^{p,q} \dot{u}_{p,q},$$

where $\Gamma_{i,j}^{p,q} = \gamma[g_{i,p}\delta_{j,q} + \delta_{i,p} g_{j,q} - g_{i,p} g_{j,q}]$, with $g_{i,p} = \delta_{i,p}[\delta_{p,0} + \delta_{p,N-1}]$. Since localization has been shown to be strongly inhibited by fixed-end boundary conditions, we consider here free-end BCs.

Calculations identical to the one described in Sec. II A can be easily extended to the case of a simple 2D harmonic lattice. It turns out that the contributions from the two spatial coordinates are identical for an $N \times N$ lattice, and therefore factorize, yielding

$$\frac{E(t)}{E(0)} = \left[e^{-t/\tau_0} I_0\left(\frac{t}{\tau_0}\right) \right]^2 \approx \begin{cases} e^{-2t/\tau_0} & \text{for } t \ll \tau_0, \\ \dfrac{1}{2\pi(t/\tau_0)} & \text{for } t \gg \tau_0, \end{cases} \quad (9)$$

with $\tau_0 = N/2\gamma$. In particular, the law (9) applies in the absence of localization, as well as during the first stage before the onset of localization. In Fig. 4 we plot the energy decay curves of a FPU lattice with $N=32$ relaxing from different values of the energy density e_0. The first stage of the decay indeed follows the theoretical prediction Eq. (9). Moreover, it is clear that localization does not occur below a finite value of e_0 (located between $e_0 = 0.2$ and $e_0 = 0.3$ in this case). In particular, in the absence of localization the energy decay is again described by the two-crossover scenario. Notice that, also in this case, failure to spontaneously localize energy results in a minimum of the effective exponent ζ, due to the competition of the power law decay $1/t$ and the exponential law $\exp(-2t/\tau_{N-1})$.

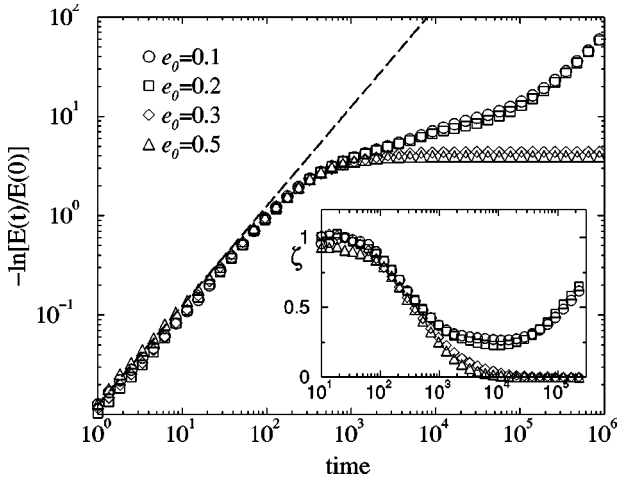

FIG. 4. 2D FPU lattice, $N=32$, $\gamma=0.1$. Plot of $\mathcal{D}(t)$ for different values of the initial energy e_0 (symbols). The dashed line is a plot of Eq. (9) for $t \ll \tau_0$. The inset shows the corresponding effective exponents $\zeta(t)$ calculated from Eq. (7). Notice the minimum associated with the absence of localization.

A. Fluctuation-activated localization

The relaxation process described in terms of the energy decay curves is identical to the two-crossover picture which applies to the 1D FPU case. Nonetheless, the scenario markedly differs from the 1D case in two respects. First of all, the mobility of the localized excitations which spontaneously emerge is drastically reduced. In fact, after a first stage in which strong interaction is observed, they arrange on a ''random lattice,'' which, on the time scale of our typical simulations, appears indeed to be frozen. One such state is illustrated in Fig. 5(a). This is presumably due to a smaller ''scattering section'' in 2D. Obviously, due to the presence of dissipation, this state decays on a much longer time scale, which (as discussed earlier) scales exponentially with the linear size of the lattice.

The second important difference with the 1D case stems from the appearance of a finite energy threshold Δ for the existence of breathers (akin to envelope solitons in the small-amplitude limit) in 2D.[12] As a consequence, we expect that localized modes are generated in the relaxation dynamics only by fluctuations that are large enough to overcome such threshold. The spontaneous excitation of breathers can thus be seen as an activated process. Accordingly, their number will be exponentially small in the ratio between Δ and some quantity measuring the strength of fluctuations. Therefore, one expects the average density of breathers (i.e., the average number of breathers per lattice site) in the residual state to follow an Arrhenius law of the form

$$\langle n_B \rangle \propto \exp(-\beta\Delta). \quad (10)$$

From Eq. (10), it is tempting to identify β with some inverse temperature. However, one has to keep in mind that we are dealing with a nonequilibrium process and this identification can only make sense if energy release is adiabatically slow. If

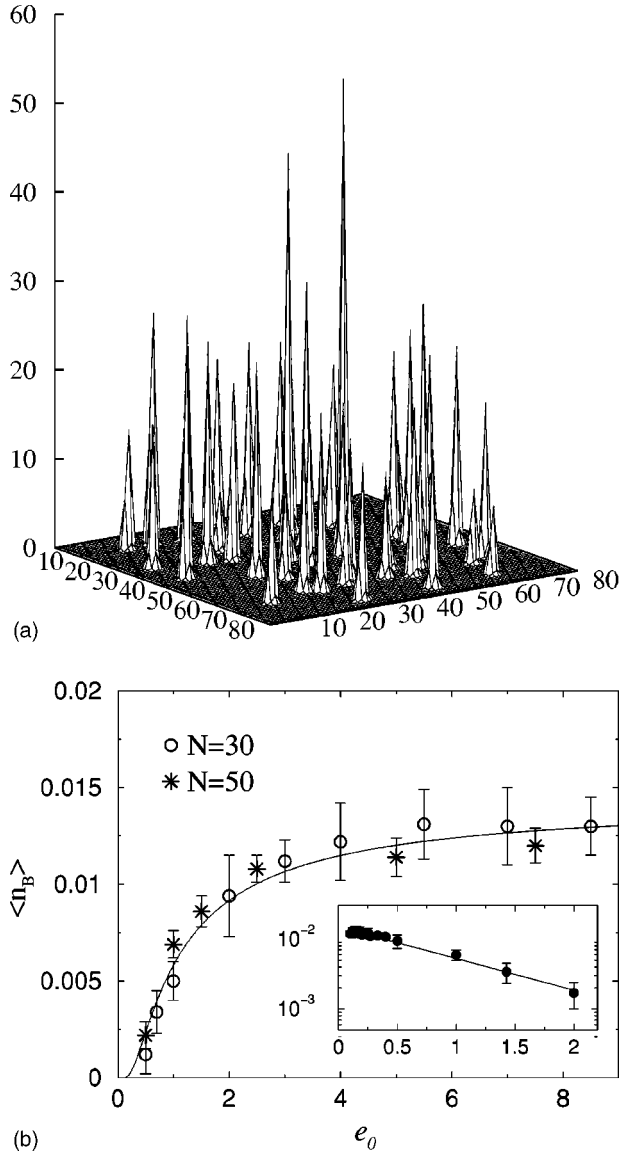

FIG. 5. 2D FPU lattice. (a) $N=80$, $\gamma=0.1$, $e_0=1$, symmetrized site energies in the residual state state. (b) Average breather density $\langle n_B \rangle$ vs initial energy density for $N=30$ and $N=50$ and Arrhenius plot. The inset shows the average density measured in the $N=50$ system vs $1/e_0$ in lin–log scale, and an exponential fit.

this is true, $1/\beta$ should be proportional to (and smaller than) the initial temperature, which, in turn, is roughly proportional to the initial energy density.

In our numerical simulations we clearly observe that n_B strongly depends on the initial specific energy. In Fig. 5(b) we plot $\langle n_B \rangle$ for two system sizes as a function of e_0, along with a fit performed with the law $\langle n_B \rangle = C \exp(-\Delta'/e_0)$, with $\Delta' \propto \Delta$. As it shows, the agreement is good. We conclude that the spontaneous localization of energy in our system is indeed an activated process. In particular, the fit gives $\Delta' \approx 0.9$. We note that a quantitative analysis of the time t_0 required to reach the residual state (localization time) reveals that $t_0 \propto 1/\langle n_B \rangle \propto \exp(\beta\Delta)$.[15] By fitting the numerical data for the localization time, it is possible to get an independent confirmation of the thermal activation scenario. In particular, we get $\Delta' \approx 0.7$, in good agreement with the above-obtained value.

B. Statistics of breathers' energies

It is important to realize that the ''pseudostationary'' distribution of breathers in the residual state emerges as a result of two competing mechanisms, namely the birth out of fluctuations from the homogeneous state and the decay due to both the coupling with the external reservoir and to the various inelastic interactions (phonon–breather, breather–breather, etc.). Although the former can be safely neglected, it is very difficult to understand the latter in full detail. Indeed, to the best of our knowledge, only a few studies are available[16,17] and a full description in terms of elementary interactions seems hardly feasible. Nonetheless, simple statistical arguments can be of help in understanding the energy distribution to a greater detail. Let us consider the fraction of breathers $\mathcal{P}(\epsilon,t)$ having energy between ϵ and $\epsilon+d\epsilon$ with $\epsilon \geqslant \Delta$ (in the FPU model breathers of arbitrarily large energy exist due to the unboundedness of the interaction potential) and let us define $B(\epsilon)$ and $D(\epsilon)$ to be some phenomenological birth and decay rates, respectively. Furthermore, let us assume that birth of a breather can only occur by a spontaneous fluctuation from the ground state ($\epsilon=0$). Stationarity requires the flux-balance condition

$$B(\epsilon)\mathcal{P}(0) = D(\epsilon)\mathcal{P}(\epsilon). \tag{11}$$

Since the birth is an activated process we expect $B(\epsilon) \propto \exp[-\beta\epsilon]$. (In principle, one could have a further energy-dependent prefactor in front of the exponential. That would affect the form of the distribution. We neglect it for simplicity.) This assumption yields (for a constant $\mathcal{P}(0)$)

$$\mathcal{P}(\epsilon) = \frac{\mathcal{P}(0)}{D(\epsilon)} \exp(-\beta\epsilon). \tag{12}$$

In this simplified description, the prefactor of the exponential term is thus interpreted as a measure of the effective breather lifetime $\tau(\epsilon)$ ($\mathcal{D}(\epsilon) \propto 1/\tau(\epsilon)$) and is *a priori* unknown. In all simulations we observe that small-amplitude breathers decay more easily. This observation agrees with the accepted existence of a preferred energy flow from small-amplitude breathers to large-amplitude ones in breather–breather collisions.[17] Moreover, Eq. (12) requires that $\tau(\Delta)=0$. Thus, we postulate

$$D(\epsilon) \propto (\epsilon-\Delta)^{-z}, \tag{13}$$

where the exponent $z>0$ can be estimated by measuring the distribution of breather energies in the vicinity of the threshold Δ. We can estimate the average density of breathers in the residual state from Eqs. (12) and (13) as

$$\langle n_B \rangle = \int_{\Delta}^{\infty} \mathcal{P}(\epsilon)\, d\epsilon \propto \beta^{-(z+1)} e^{-\beta\Delta}. \tag{14}$$

This result is consistent with our initial hypothesis [Eq. (10)].

From Eqs. (12) and (13) it follows that the average breather energy $\langle \epsilon \rangle$ can be expressed as a function of β and

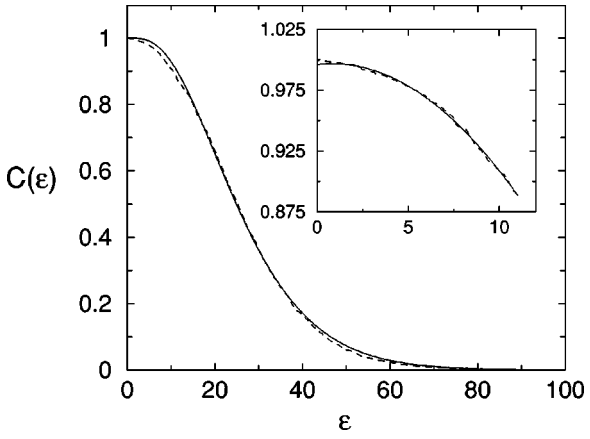

FIG. 6. 2D FPU lattice, $N=70$, $\gamma=0.1$, and $e_0=1$. Experimental cumulative distribution of breather energies (dashed line) and fit with formula (16) (solid line). Both curves have been shifted to the left by $\epsilon_{\min}$. The breather population is here of 1742 breather "events," recorded in 50 different realizations of the initial condition. The inset shows a quadratic fit of the small-energy portion of the distribution.

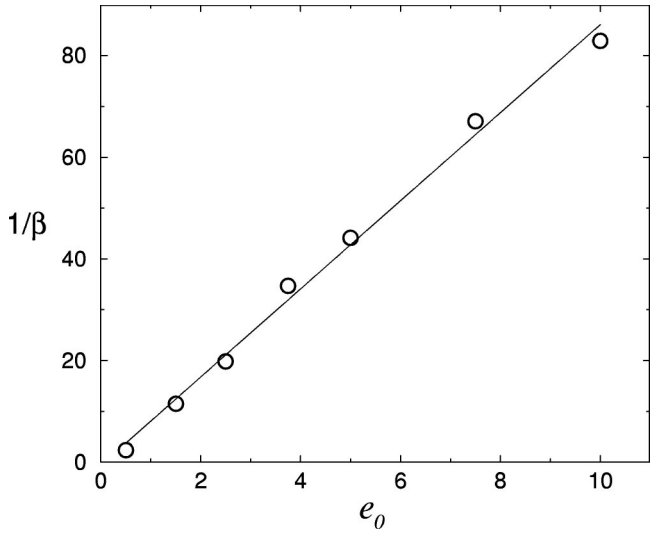

FIG. 7. 2D FPU lattice, $\gamma=0.1$, $N=50$. Plot of Eq. (18) evaluated from the best-fit values of the floating parameters z and $\langle\epsilon\rangle$ vs initial energy density (symbols) and linear fit.

Δ. Hence, we can write the normalized distribution Eq. (12) as a function of the three parameters z, $\langle\epsilon\rangle$, and Δ in the following fashion:

$$\mathcal{P}(\epsilon)=\frac{(z+1)^{z+1}}{\Gamma(z+1)(\langle\epsilon\rangle-\Delta)}\left[\frac{\epsilon-\Delta}{\langle\epsilon\rangle-\Delta}\right]^{z}\times\exp\left(-(z+1)\left[\frac{\epsilon-\Delta}{\langle\epsilon\rangle-\Delta}\right]\right), \tag{15}$$

where $\Gamma(z)$ is the gamma function and $\langle\epsilon\rangle=\Delta+(z+1)/\beta$. From the point of view of the numerics, it is more accurate to deal with the cumulative (integrated) distributions. These are easily obtained from the histograms without actually performing the integration, by noting that they are nothing but rank-size plots with the axes inverted. The cumulative distribution of the function (15) is

$$\mathcal{C}(\epsilon)=\int_{\epsilon}^{\infty}\mathcal{P}(\epsilon')d\epsilon'=\frac{1}{\Gamma(z+1)}\gamma\left(z+1,(z+1)\left[\frac{\epsilon-\Delta}{\langle\epsilon\rangle-\Delta}\right]\right), \tag{16}$$

where $\gamma(z,\epsilon)$ is the incomplete gamma function, defined as

$$\gamma(z,\epsilon)=\int_{\epsilon}^{\infty}y^{z-1}e^{-y}dy. \tag{17}$$

In principle one could evaluate Δ explicitly by calculating the energy of exact breather solutions of vanishing amplitude.[12] However, we expect that $\Delta\ll\langle\epsilon\rangle$. Therefore, if the population of breathers used to calculate the experimental distribution $\mathcal{C}(\epsilon)$ is large enough, we can assume that the smallest breather energy recorded $\epsilon_{\min}$ is close to the threshold Δ. Hence, we can perform a two-parameter fit with the theoretical prediction Eq. (16) with $\Delta=\epsilon_{\min}$. The quality of such fits is illustrated in Fig. 6 for a lattice with $N=70$. As it shows, the agreement of our simple model with the numerics is excellent. In particular, the analysis of the small-energy portion of the distributions yields $z=2$ (see the inset in Fig. 6). We stress that the result of our fits were well reproduced irrespective of the particular realization of $\epsilon_{\min}$. The fit of the experimental distributions over the whole range of available energies yields a slightly greater value, $z\approx 2.6$. This is because the large-energy tail of the distributions accounts for the rarest events, which are under-represented within reasonably large breather populations. (The main constraint comes from the time required to numerically integrate the equations of motion of large lattices for a large number of realizations of a given initial condition.) In order to convince oneself that this is the case, it is enough to introduce an energy-dependent weight function in the fit, which gauges the relative weights of the small-energy and large-energy portions of the curves. In this case, the best estimates of z monotonically decrease toward the value $z=2$ upon lowering the relative weight assigned to the large-energy region.

The analysis of energy distributions also provides an independent confirmation that localization is in the present case an activated process. To check this, we fitted the distributions obtained by letting systems of given size relax from different values of e_0. Then, we evaluated β from the best-fit values of the fitting parameters z and $\langle\epsilon\rangle$ according to

$$\frac{1}{\beta}=\frac{\langle\epsilon\rangle-\epsilon_{\min}}{z+1}. \tag{18}$$

As shown in Fig. 7, β turns out to be inversely proportional to e_0 as expected.

IV. CONCLUSIONS

The mechanisms yielding the spontaneous formation of localized periodic excitations, i.e., breathers, in spatially discrete nonlinear dynamical systems are of primary importance for the understanding of their physical interest. In this paper we have focused on the phenomenon of relaxation to breather states by cooling from the boundaries 1D and 2D lattices. We have provided a detailed description of the many facets of this phenomenon by combining numerical studies

with theoretical arguments. In particular, we have shown that in models with sufficiently weak ''substrate'' forces the energy loss process can be explained on the basis of a simple perturbative analysis, which applies independently of the boundary conditions and of the nature of the nonlinearity. In this sense, we can claim that this is a general feature of this class of models, where an initial exponential decay is followed by a power-law behavior. In the second stage of the decay process, boundary conditions play a crucial role in allowing for the formation of a long-living breather state, when they are taken free. On the contrary, fixed ends yield complete cooling of the lattice eventually ruled by the exponential decay rate of the longest-lived Fourier mode. We have also pointed out that the presence of a sufficiently strong ''substrate'' force can turn the initial exponential decay to a stretched-exponential law, while maintaining all the other features of the previously described scenario. A theoretical explanation of the origin of this stretched exponential behavior and its dependence on the strength and on the nature of the local potential is a problem that deserves further and more refined investigations. We have also commented about the technical difficulties that can be encountered for identifying the correct time behavior in these models, where the crossover between different regimes can be easily mistaken for an indication in favor of other scaling laws.

Another crucial aspect that we have widely analyzed concerns the main differences between 1D and 2D systems. At variance with the former case, in 2D we have found numerical evidence of the existence of a finite energy threshold for breather formation. We have also proposed a statistical model that provides an effective agreement with numerical results concerning the breather residual state. This state eventually sets in as an almost static stationary configuration, where breathers of different amplitudes coexist. The statistical model is based on the hypothesis that this state emerges as a result of the competition between breather activation and mutual interaction. Moreover, it allows one to determine an effective breather lifetime and its dependence on energy. In this framework the initial energy density plays the role of the control parameter regulating the strength of fluctuations.

In our opinion these results provide a satisfactory understanding of the phenomenon of spontaneous breather formation by cooling. As a final remark, it seems worth investigating experimentally the capability of real systems to store energy in the form of long-lived localized excitations.

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