Energy Localization in Nonlinear Lattices

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We discuss the process by which energy, initially evenly distributed in a nonlinear lattice, can localize itself into large amplitude excitations. We show that the standard modulational instability mechanism, which can initiate the process by the formation of small amplitude breathers, is completed efficiently, in the presence of discreteness, by energy exchange mechanisms between the nonlinear excitations which favor systematically the growth of the larger excitations. The process is, however, self-regulated because the large amplitude excitations are finally trapped by the Peierls-Nabarro potential.

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Many physical phenomena involve some localization of energy in space. The formation of vortices in hydrodynamics, self-focusing in optics or plasmas, the formation of dislocations in solids under stress, and self-trapping of energy in proteins are well known examples. Following the original work by Anderson [1] disorder-induced localization has been widely studied, but, more recently, attention was turned to the possibility to localize energy in a homogeneous system due to nonlinear effects. The process can become dramatic when it leads to collapse in a plasma [2]. In this Letter we are interested in the process by which energy evenly distributed in such a system can concentrate itself spontaneously into spatially localized nonlinear excitations. In some cases this evolution can lead to the formation of topological solitonlike excitations such as dislocations or ferroelectric or ferromagnetic domain walls. However, since there is an energy threshold for the creation of topological solitons, the first step of the evolution is the formation of breathers or envelope modes; we shall therefore focus our attention on such modes.

Nonlinear energy localization in continuous media has been extensively investigated since Benjamin and Feir [3] discovered the modulational instability of Stokes waves in fluids, but very little has been done in lattices although it would be of wide interest for solids or macromolecules. We want to point out here that, in a discrete lattice, nonlinear energy localization is very different from its counterpart in a continuum medium. In particular, we show that, besides the familiar mechanism of modulational instability, which is itself strongly modified by discreteness effects, there is an additional channel for energy concentration, which is specific to lattices, but is not sensitive to the details of the nonlinear lattice model which is considered. Therefore it appears as a very general process leading to localization of energy in a lattice.

The first step toward the creation of localized excitations can be achieved through modulational instability, which exists in a lattice as well as in a continuum medium, although discreteness can drastically change the conditions for instability [4] (e.g., at small wave numbers a nonlinear carrier wave is unstable to *all* possible modulations of its amplitude as soon as the wave amplitude exceeds a certain threshold). However, the maximum energy of the breathers created by modulational instability is bounded because each breather collects the energy of the initial wave over the modulation length λ so that its energy cannot exceed $E_{\max} = \lambda e$ where e is the energy density of the plane wave. Consequently, although modulational instability can lead to a strong increase in energy *density* in some parts of the system, it cannot create breathers with a *total* energy exceeding $E_{\max}$. For a given initial energy density, one can, however, go beyond this limit if one excitation can collect the energy of several breathers created by modulational instability. Such a mechanism is not observed in a continuum medium because there the breathers generated by modulational instability are well approximated by solitons of the nonlinear Schrödinger (NLS) equation which can pass through each other without exchanging energy. On the contrary, when discreteness effects are present, the energy of each excitation is *not* conserved in collisions, and, the important point is that *the exchange tends to favor the growth of the larger excitation.* In order to analyze the growth of the breathers in a lattice, we must therefore examine three of their properties: (i) their stability, (ii) their ability to move in the lattice, and (iii) the nature of their interactions.

In order to discuss these points quantitatively, let us, in a first step, examine a specific model. We consider a chain of harmonically coupled particles situated at positions u_n and submitted to the substrate potential

$$V(u_n) = \omega_d^2 \left(\frac{u_n^2}{2} - \frac{u_n^3}{3} \right) , \tag{1}$$

where ω_d^2 is a parameter which measures the amplitude of the substrate potential, and therefore controls discreteness. We will be interested in motions inside the potential well ($u < 1$). This potential can be viewed as a medium amplitude expansion of any asymmetric potential around a minimum. It can for instance represent the expansion

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of a Morse potential in a nonlinear model for DNA denaturation [5] or the expression around a minimum of the well known ϕ^4 potential [6]. The Hamiltonian of the model is

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

The existence and stability of breathers in nonlinear Klein-Gordon models has been the subject of many investigations [6] and is not yet completely understood. However, we have shown that, provided that discreteness is strong enough, extremely stable large amplitude breathers can exist in such a model [5]. They can be obtained with the Green's function method introduced by Sievers and Takeno [7] for intrinsic localized modes in lattices with anharmonic coupling. The role of discreteness to stabilize the breathers can be understood if one starts from the "anti-integrable" limit where the on-site nonlinear oscillators are decoupled and then turns on a coupling which remains weak with respect to the on-site potential [8]. Thus discrete breathers are sufficiently stable to have a long lifetime which gives them sufficient time to interact, provided that they can move in the lattice. This point is not as trivial as it might seem if one has in mind the picture of solitonlike excitations in a continuum medium because discreteness breaks the translational invariance. This effect is well known for topological solitonlike excitations and has been extensively investigated in the context of dislocation theory [9]. In a lattice a kink cannot move freely. The minimum energy barrier which must be overcome to translate the kink by one lattice period is known as the Peierls-Nabarro (PN) barrier, E_{PN}. It can be calculated by evaluating the energy of a static kink as a function of its position in the lattice. For the various models which have been investigated, two extremal values are generally obtained when the kink is exactly situated on a lattice site (centered solution) or when it is in the middle between two sites (noncentered solution). For a discrete breather very little is known, although the PN barrier has been shown to exist [6]. One of the difficulties is that the breather is a two-parameter solution. While for a kink, the PN barrier depends only on discreteness, i.e., on the model parameters, for a breather it depends also upon its amplitude (or frequency). This amplitude dependence is crucial for our analysis because we are interested in the growth of breathers. As they increase in amplitude, the PN barrier that they feel changes. An accurate value of the PN barrier for a breather can be obtained by calculating the centered and noncentered breather solutions with the lattice Green's functions method [5]. The calculation requires some care because the noncentered solution corresponds to the maximum of the PN barrier. Therefore it is unstable and the breather tends to converge toward the centered solution which has a lower energy. The noncentered solution can, however, be obtained by requesting that the two particles which are around the breather center have the same motion. A typical aspect of the two solutions is shown in Fig. 1.

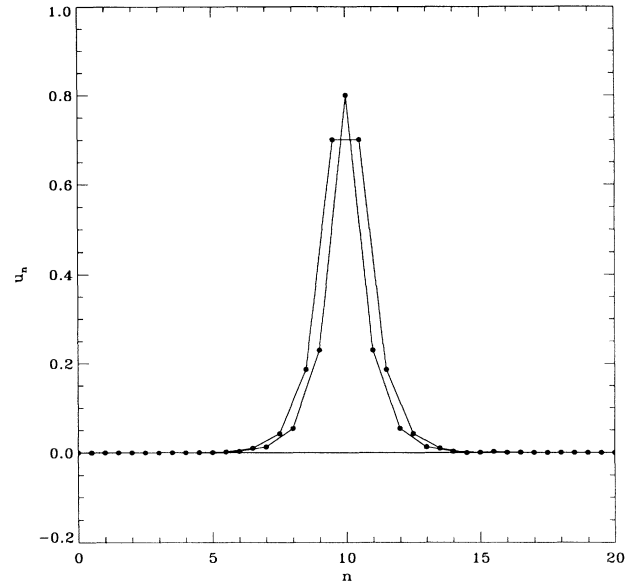

FIG. 1. Profiles of the centered and noncentered breather solutions at the time corresponding to the maximum amplitude, for a breather frequency $\omega_b = 0.873\omega_d$, with $\omega_d^2 = 10$.

For a very discrete breather, an approximate expression can also be obtained by assuming that only a few lattice points enter in the solution. For instance, for a breather centered on site $n = 0$, we look for a solution localized on only three sites by assuming

$$u_0 = A + B\cos(\omega_b t) , \quad u_{\pm 1} = C + D\cos(\omega_b t), \qquad (3)$$
$$\text{and } u_l = 0 \text{ for } |l| > 1 ,$$

where ω_b is the breather frequency and A, B, C, D parameters to be determined. Inserting this *ansatz* into the equations of motion, assuming that the excitation decays sufficiently rapidly, i.e., $A \gg C$ and that adjacent particules move in phase, one gets a relation between the breather amplitude and its frequency

$$\frac{\omega_b^2}{\omega_d^2} = \frac{2}{\omega_d^2} + 1 - A - \sqrt{\frac{2}{\omega_d^4} + A^2} . \qquad (4)$$

Although it is only approximate, this equation gives the general trend, and shows in particular that, as the amplitude increases, the breather frequency decreases as one might expect. From this result the energy of the centered breather can be derived. The noncentered case can be treated similarly by considering 4 sites and assuming $u_0 = u_{-1}$, $u_1 = u_{-2}$. The energies of the centered and noncentered breathers versus the breather frequency for a model with $\omega_d^2 = 10$ are plotted in Fig. 2 which shows

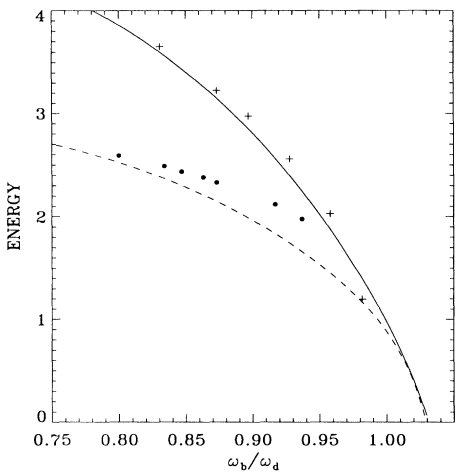

FIG. 2. Variation versus frequency of the energies of the noncentered (full line and crosses) and centered (dashed line and dots) breathers for $\omega_d^2 = 10$. The lines are obtained with the *ansätze* using only 3 or 4 sites, and the points are derived from the exact Green function calculation.

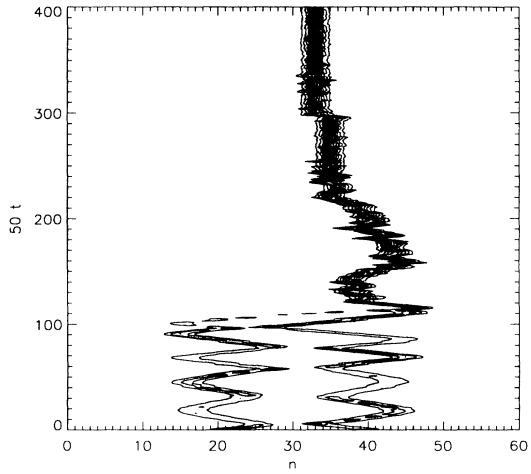

FIG. 3. Numerical simulation of the time evolution of two discrete breathers sent toward each other between two reflecting defects situated at sites 30 and 70. The initial amplitudes of the breathers are in the ratio $A_{\text{right}}/A_{\text{left}} = 1.36$. The figure shows the energy density in the discrete chain using a contour plot. Darker regions correspond to regions where the energy density is higher.

that, while at high frequency, i.e., low amplitude, the two solutions have approximately the same energy, when the frequency decreases, i.e., the amplitude increases, the difference in energy between the two cases increases drastically. Therefore we can expect that small amplitude breathers can move rather freely in the lattice, while the large one will feel the discreteness strongly. This is verified by numerical simulations of the lattice equations.

To study the interactions between the breathers, we must rely on numerical simulations since, in the discrete model, no exact solution is available. In the energy localization process that we propose, small amplitude breathers are generated by spontaneous modulation of some energy initially evenly distributed in the system, and then collisions favor the growth of some of the excitations at the expense of the others. The process requires generally several collisions. In order to study this effect in a controlled manner, we have confined two breathers between two impurity sites where the on-site potential $V(u)$ is removed. These sites act as perfectly reflecting walls for the breathers which bounce back and forth between the defects. If two solitons were sent toward each other in such a system they would simply pass through each other many times as they oscillate in the "box." For discrete breathers, the picture is very different. Figure 3 shows a typical numerical simulation result. To generate this figure, two breathers of unequal amplitude have been sent toward each other. After 5 collisions, only a large amplitude breather subsists in the system and the smaller excitation can no longer be distinguished from the small amplitude waves which have been radiated during the collisions. Moreover, as one of the breathers grows in amplitude, its PN barrier increases and the breather is finally completely trapped by discreteness. It is important to notice, however, that it is still slowly growing as shown in Fig. 4 because it collects some energy of the small amplitude waves generated in the collision. The detail of the interaction between discrete breathers depends on the precise conditions of the collision, and in particular on the relative phases of the two breathers when they collide. It may even happen that, in a single collision, the bigger breather loses some energy. However, we have

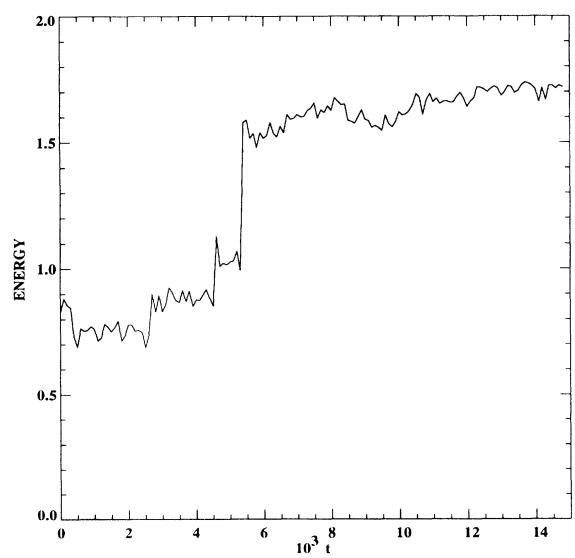

FIG. 4. Time evolution of the energy of the three central particles of the biggest breather in the numerical simulation of Fig. 3.

observed that the average effect of multiple collisions occurring randomly in a lattice, is always to increase the amplitude of the larger excitations. *This phenomenon is very general and very robust to perturbations.* In particular, the same behavior is found in a thermalized system, which is important for physical applications. To check this point, we have prepared thermalized lattices by running constrained temperature numerical simulations with the Nosé scheme [10].

Then we have launched couples of breathers in the chain and noticed again that the bigger breather grows at the expense of the smaller one. In fact, we observe that its growth rate is larger in the presence of thermal fluctuations because it collects some energy from the fluctuations. The results do not depend on the boundary conditions. Multiple collisions can also be generated by periodic boundary conditions and the same results are found. More importantly, the results do not depend on the particular nonlinear lattice model which is considered. Using the more physical Morse potential instead of $V(u)$ given by Eq. (1) leads to the same general conclusions.

Discreteness can be viewed as a perturbation of the integrable NLS equation which can be derived for many nonlinear lattice models in the continuum and medium amplitude limit. Therefore, one might have expected that the usual property of the solitons of passing through each other without energy exchange would be destroyed as the integrability is lost. This is, however, not so obvious because, in the first order of perturbation, conservative perturbations do not cause energy exchange in two-soliton collisions [11]. Moreover, the most remarkable result is that the world of discrete solitons is as merciless for the weak as the real world: in the presence of discreteness, breather interactions show a systematic tendency to favor the growth of the larger excitation at the expense of the others.

However, the process contains also its own regulation mechanism because of the fast increase of the Peierls barrier with the amplitude of the breathers. When they become large enough, the breathers stay trapped by discreteness. As a result, energy initially evenly distributed over the lattice tends to concentrate itself into large amplitude breathers, but the localization stops before all the energy has collapsed into a single very large excitation. The mechanism of discreteness-induced energy localization that we have described here can appear in a large variety of physical systems involving lattices. In particular, it is clearly at work in a model of nonlinear DNA dynamics that we have investigated recently [12]. Numerical simulations of the model at constrained temperature show that, in the steady state, thermal energy tends to localize itself around some sites and consequently the lattice in equilibrium is very far from equipartition of energy.

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