DISCRETE BREATHERS AND ENERGY LOCALIZATION IN NONLINEAR LATTICES

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Abstract

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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I. INTRODUCTION

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, 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 attracted on the possibility to localize energy in an homogeneous system due to nonlinear effects. the process can become dramatic when it leads to collapse in a plasma \[2\]. In this paper 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 num-
bers 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 $\lambda$ so that its energy cannot exceed $E_{\text{max}} = \lambda e$ 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 $E_{\text{max}}$. 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, 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

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

where $\omega_d^2$ 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 of a Morse potential in a nonlinear model for DNA denaturation or the expression around a minimum of the well known $\phi^4$ potential. The hamiltonian of the model is
\[ H = \sum_n \left[ \frac{1}{2} \ddot{u}_n^2 + \frac{1}{2} (u_n - u_{n-1})^2 + V(u_n) \right]. \quad (2) \]

The existence and stability of breathers in nonlinear Klein-Gordon models has been the subject of many investigations \[1\] 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 \[2\]. They can be obtained with the Green’s function method introduced by Sievers and Takeno \[4\] 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 \[3\]. 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.

II. PEIERLS-NABARRO BARRIER FOR A BREATHER

The trapping effect of the discreteness is well known for topological solitonlike excitations and has been extensively investigated in the context of dislocation theory \[3\]. 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 (non-centered solution).

For a discrete breather very little is known, although the PN barrier has been shown to exist \[4\]. One of the difficulties is that the breather is a two-parameter solution. While for a kink, the PN barrier depends only on discreteness, \textit{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. The definition of the Peierls barrier itself is not as simple for a breather as for a kink. In principle, its value can be obtained by monitoring the breather as it is translated along one lattice constant. While for a kink the path followed by the particles in the multidimensional phase space of the system can be obtained by minimizing the energy while the position of the central particle is constrained in all intermediate states, in the case of the breather, the path in the phase space is not a minimum energy path but a succession of saddle points. The energy of a kink which is exactly centered on a site or in the middle between two sites is defined without ambiguity. For a breather with a given frequency when it is centered on a site, there is no obvious constraint which imposes that it should have the same frequency when it is situated in the middle between two sites. We have used, as a working definition of the PN barrier for a breather the difference between the energies of a centered and a non-centered breather with the same frequency. This definition gives results which agree with the observations of the breather motion made by molecular dynamics simulations, but the notion of PN barrier for a breather will require further analysis.

A. Large amplitude breathers

To calculate the PN-barrier, we have to compare the energy between two cases: the breathers is centered on a particle or between particles. In the previous paper [5], we focused our study in the first case, but we can easily extend the method to the second one. The procedure is the following : we look for stationary-mode solutions by putting

\[ u_n = \sum_{i=0}^{\infty} \phi_i^n \cos(i\omega_b t) \],

where \( \omega_b \) is the eigenfrequency of the breather and \( \phi_i^n \) are time independent amplitude oh the \( i^{th} \) mode. Inserting the ansatz (3) in the dimensionless equation of motion, we set the coefficients of \( \cos(i\omega_b t) \) equal to each other, retaining only the first three terms. We obtain:
\[\omega_d^2 \phi_n^0 - [\phi_{n+1}^0 + \phi_{n-1}^0 - 2\phi_n^0] = \omega_d^2 \left[ \phi_n^0 + \frac{\phi_n^1 + \phi_n^2}{2} \right] \tag{4a}\]

\[(\omega_d^2 - \omega_b^2) \phi_n^1 - [\phi_{n+1}^1 + \phi_{n-1}^1 - 2\phi_n^1] = \omega_d^2 \left[ 2\phi_n^0 + \phi_n^2 \right] \phi_n^1 \tag{4b}\]

\[(\omega_d^2 - 4\omega_b^2) \phi_n^2 - [\phi_{n+1}^2 + \phi_{n-1}^2 - 2\phi_n^2] = \omega_d^2 \left[ 2\phi_n^0 \phi_n^2 + \frac{\phi_n^1}{2} \right] \tag{4c}\]

Then, invoking the Green’s functions for the linear left-hand sides, we get a set of simultaneous nonlinear eigenvalue equations determining the eigenfrequency \(\omega_b\) and the eigenfunctions \(\phi_n^i\):

\[\phi_n^0 = \sum_m G(n - m, 0) \left[ \phi_m^0 \phi_m^1 + \phi_m^2 \right] \tag{5a}\]

\[\phi_n^1 = \sum_m G(n - m, \omega_b) \left[ 2\phi_m^0 + \phi_m^2 \right] \phi_m^1 \tag{5b}\]

\[\phi_n^2 = \sum_m G(n - m, 2\omega_b) \left[ 2\phi_m^0 \phi_m^1 + \phi_m^2 \right] \tag{5c}\]

where the Lattice Green’s functions have the following expression:

\[G(n, \omega_b) = \frac{\omega_d^2}{N} \sum_q \frac{e^{i\omega_n}}{\omega_d^2 - \omega_b^2 + 2[1 - \cos(q)]} \tag{6}\]

For solving this system, the procedure requires more care than in the centered case \[5\], to avoid the problem of instability of this mode. Indeed, since the position at the top of the PN barrier is intrinsically unstable, regardless of other possible causes of instability, even starting with a symmetrical initial condition, the results show that in all cases the breather moves so that the center reaches the bottom of the well. \(i.e.\) the solution converges toward the more stable breather. To prevent this tendency we chose to impose the symmetry and calculate the solution for only a half of the chain, the second half being know by symmetry:
thus the position of the breather is fixed. Self-consistently solved, the system (5) give us the values of the breather’s frequency and of the amplitude of the different sites.

In Fig. 2(a), we plot the amplitude versus the frequency for the two modes. At high frequency (i.e. low amplitude), the two curves are very close to each other. As one might expect (see Fig. 1), the amplitude of the mode centered on a particle is larger than when the mode is centered between particles. A comparison of the energies in the two cases reveals a great difference as shown in Fig. 2(b). The solution centered on a particle has a much lower energy. Indeed, as the discreteness effects are important, the substrate energy is the dominant contribution to the total energy. When the breather is centered between particles, two of them participate mainly to the excitation, giving rise to a substantial increase of the energy, in comparison with the previous case, where only one particle has a big amplitude.

Figure 3 illustrates the simulation of the dynamics of the breather with a decentered solution as an initial condition. The numerical scheme for solving the nonlinear equations of motion is a fourth order Runge-Kutta method of a lattice with typically 256 atoms and periodic boundary conditions. Starting with a breather centered between the sites 24 and 25, and with a frequency $\omega_b = 0.93 \omega_d$, the pictures 3(a), 3(b) and 3(c) show the envelop of the oscillations of the particles 24, 26 and 25. It is clear that after about 70 breather’s oscillations, the excitation moves to be centered on particle 25. Although we start with a perfect symmetrical initial condition centered between particles, because of its intrinsic instability, some unavoidable numerical errors have moved the breather down the PN barrier. As the initial condition is clearly not the exact solution at the bottom of the well, a phenomenon of modulation appears: it is a consequence [5] of the combination of the breather’s frequency ($0.88 \omega_d$ after the displacement of the breather) with the mode situated exactly at the bottom of the phonon band, which cannot be radiated away because of its zero group velocity.

Figs. 3(a) and 3(b) show the oscillations of the two nearest neighbors of the center. It is clear that, after the translation of the center, they have a similar evolution, except that a new modulation effect is present: it is due to the combination of the former frequency with
the frequency of the oscillation in the well of the PN barrier. Furthermore the two particles are not in phase, because when one starts with a breather, the shape mode (the derivative with respect to the position of the breather’s center) is odd: so, with the center on a particle, the shape mode is such that the central site does not move, but the two neighboring sites are 90 degrees out of phase.

As the spontaneous evolution of a decentered breather with a frequency \( \omega \) gives a centered breather with a lower frequency, we cannot calculate the PN barrier from such a simulation. Although the energy of the system is conserved during the integration of the equations, it does not stay localized in the excitation since the movement of the breather generates a strong radiation of phonons. The Peierls barrier can be obtained from a calculation of the energy of the solutions given by the Green’s functions method, independently in the two cases. Figure 2(b) shows that the PN barrier is very high; as it is an increasing function of the amplitude of the breather (see Fig. 2(a)), the barrier is a decreasing function of the amplitude. A small amplitude breather will propagate easily the chain along, whereas the large amplitude ones will be trapped on a site because of the additional potential due to the discreteness.

**B. Approximate analytical expression and the PN barrier**

The Green’s function method provides a very accurate expression for the discrete breather modes, but the solution is known only numerically. When the breathers are highly localized, it is possible to derive an approximate analytical solution for the frequency of the mode versus their amplitude in the two cases. First, we consider the centered case where the mode is on a particle which we call \( n = 0 \). As the mode is highly localized, we assume \( |u_n| \ll |u_1| \) for \( |n| > 1 \). We seek an approximate solution of the dimensionless equation of motion, by looking for a solution which is localized over only 3 sites, putting \( u_0 = A + B \cos(\omega_b t) \):
\[ u_1 = u_{-1} = C + D \cos(\omega_b t) . \]  
\[ u_l = 0 \text{ for } |l| \geq 1 . \]  

The dc parts of the ansatz are positive because of the asymmetry of the potential. We insert this ansatz in the dimensionless equation of motion, and set the coefficients of \( \cos(\omega_b t) \) and the constant term equal to each other. We obtain for \( n = 0 \):

\[ 0 = 2(C - A) - \omega_d^2(A - \frac{B^2}{2} - A^2) \]  
\[ - \omega_b^2 B = 2(D - B) - \omega_d^2(B - 2AB) \]  

For \( n = 1 \), it yields:

\[ 0 = A - 2C - \omega_d^2(C - \frac{D^2}{2} - C^2) \]  
\[ - \omega_b^2 D = B - 2D - \omega_d^2(D - 2CD) \]  

As the excitation is rapidly decreasing, we can estimate that \( A \gg C \); equation (10) gives then:

\[ B = \sqrt{2A \left( \frac{2}{\omega_d^2} + 1 - A \right)} , \]  

whereas (11) and (13) gives:

\[ \omega_b^2 = 2 \left( 1 - \frac{D}{B} \right) + \omega_d^2(1 - 2A) \]  
\[ = 2 - \frac{B}{D} + \omega_d^2(1 - 2C) \]  

Neglecting \( C \) in (16), we obtain from these two equations:

\[ \left( \frac{D}{B} \right)^2 + \omega_d^2A \left( \frac{D}{B} \right) - \frac{1}{2} = 0 . \]  

Then, we get:
\[
\frac{D}{B} = \frac{-A\omega_d^2 \pm \sqrt{(A\omega_d^2)^2 + 2}}{2}. \tag{18}
\]

As we are interested in breather modes, the particles should oscillate in phase: the ratio \(D/B\) must be positive and that’s why we keep only the plus sign. Equation (19) gives then:

\[
\frac{\omega_b^2}{\omega_d^2} = \frac{2}{\omega_d^2} + 1 - A - \sqrt{\frac{2}{\omega_d^2} + A^2} \tag{19}
\]

Consider now the case where the center of the excitation is between two particles (in our notation, between the site (-1) and (0)). We take the similar ansatz with two unknown functions \(u_0 = u_{-1}\) and \(u_1 = u_{-2}\). Now we obtain the two following equations for the case \(n = 0\):

\[
0 = (C + A - 2A) - \omega_d^2(A - \frac{B^2}{2} - A^2) \tag{20}
\]

\[
- \omega_b^2 B = (B + D - 2B) - \omega_d^2(B - 2AB) \tag{21}
\]

An analysis similar to that given above, can be carried out and we obtain:

\[
\frac{D}{B} = \frac{-(1 + 2A\omega_d^2) + \sqrt{(1 + 2A\omega_d^2)^2 + 4}}{2}. \tag{22}
\]

and

\[
\frac{\omega_b^2}{\omega_d^2} = \frac{3}{2\omega_d^2} + 1 - A - \sqrt{\frac{1}{2\omega_d^2} + \left(\frac{1}{2\omega_d^2} + A\right)^2} \tag{23}
\]

The comparison of the two equations (19) and (23), with the results of the Green’s functions method is shown in Fig. 2(a). As might be expected at low amplitude, the results tends to the NLS case, with a good agreement. In this domain, as the excitation concern more than three or four particles contrary to the postulate in the ansätze (7) and (8), the present formalism failed and the agreement is poor. But, in the highly localized regime, in which we are essentially interested, the two expressions given by the simple anzätze are valid. Although the method can seem very crude, it provides accurate results in the very discrete cases because the solution are naturally well localized so that the displacements which are ignored here are really very small.
Using these results we can obtain the energy of the mode. The expression for the case centered between particles is

\[ E_c = \frac{1}{2} u_1^2 + (u_1 - u_0)^2 + \omega_d^2 \left( \frac{u_0^2}{2} - \frac{u_0^3}{3} \right) + 2\omega_d^2 \left( \frac{u_1^2}{2} - \frac{u_1^3}{3} \right) \]  

\( (24) \)

and

\[ E_d = E_c + \omega_d^2 \left( \frac{u_0^2}{2} - \frac{u_0^3}{3} \right) \]  

\( (25) \)

in the other case, where the expression of the two displacements \( u_0 \) and \( u_1 \) are easy determined, using \( A, B, C \) and \( D \). The results shown in Fig. 2(b), attest that, despite its simplicity, the calculation gives accurate results especially in the second case.

III. LOCALIZATION BY COLLISIONS

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. Fig. 4 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. [3] 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 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 Nose scheme [11].

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.

IV. CONCLUSION

Discreteness can be viewed as a perturbation of the integrable Nonlinear Schrödinger 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 [12]. 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 [13]. 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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FIGURES

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

FIG. 2. Comparison of the centered and decentered breather. (a) Frequency of the breather modes versus amplitude. The solid line refer to the equation (19), the dotted line to the equation (23) and the dash-dot-dot-dotted to the NLS approximation. (b) Total energy as a function of the frequency. The circles (resp. the plus signs) correspond to the solution obtained with the Green’s function technic when the breather is centered on a particle (resp. between two particles).

FIG. 3. Envelop of the oscillations of the particle 24(a), 25(c) and 26(b), when the breather is centered between the 24 and 25 ones, at the beginning of the simulations. After about 300 breather oscillations, the excitation moves down to the Peierls-Nabarro well.

FIG. 4. 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.

FIG. 5. Time evolution of the energy of the three central particles of the biggest breather in the numerical simulation of fig. 4.