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The influence of energy changes in breathers

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Abstract. This work studies the dynamical behavior of breathers in a single nonlinear lattice under the influence of energy changes. To create the breather we used the anti-continuous limit and studied its stability through the Floquet theory. Using the information entropy we calculated the effective number of oscillators with significant energy and determined if there is or not the formation of a spatially localized structure.

1. Introduction
Breathers are time periodic and spatially localized solutions [1]. This kind of solution is generated by the combination of two factors: the discreteness and nonlinearity [2]. The first one makes the dispersion relation (linear spectrum) limited and discrete, while the second one makes the frequency of vibration dependent on the amplitude motion. Mackay and Aubry [3] proved the existence of breathers in the one-dimensional lattice when the system is composed by weakly coupled nonlinear solutions. Their proof was based on the anti-continuous limit and showed that the solution persists in a space of periodic solutions with a fixed period and decays exponentially in space.

In the last two decades many studies have been done to study this kind of solution [4,5]. They analyze both numeric and analytic ways to create the breather and study its stability for numerous discrete systems. Besides, there are some works [6, 7] that study the behavior of breathers interacting one to another and with some impurity of the lattice, like collisions and trapping. Another works try to apply this knowledge in some phenomenon of nature. In particular, some of them are intended to understand some biological aspects, like DNA transcription [8].

Here, we follow the numeric proceedings suggested by Marin and Aubry [9] to create the breather and use the Floquet theory to analyze its stability [10]. This study gives us solutions with different coupling parameter that can be stable or not. However, the energies involved are fixed and dependent to the breather frequency and coupling. In this work, we verify the influence of energy changes in the dynamic behavior of a breather. In order to do this, we use a stable solution and vary its energy by increasing or decreasing its amplitude. Based on the information entropy [11] we calculate the number of oscillators with significant energy and use it like a criteria to energy localization. The main idea is to know if despite of the energy variation we get a localized solution or not.

2. Prescription to create the breather
The Lagrangian of the system is:
and represents a chain of harmonic oscillators with an additional nonlinear on site potential $V(y_j)$. Here $V(y_j)$ is the Morse potential written, in a simplified way, as:

$$V(y_j) = \left( e^{-\gamma_j} - 1 \right)^2.$$  

The equations of motion obtained from Lagrangian (1) are:

$$m \ddot{y}_j + k(2y_j - y_{j+1} - y_{j-1}) + e^{-\gamma_j}(1 - e^{-\gamma_j}) = 0 \quad (3)$$

The breather can be created using the principle of the anti-continuous limit suggested by MacKay and Aubry [3] and implemented by Marin and Aubry [9] and Cuevas [12]. So, at the beginning we considered the uncoupled system, i.e. $k = 0$. With this limit the system is composed of isolated oscillators under the influence of the nonlinear on site potential.

Because we are looking for periodic solutions, they can be written in terms of a Fourier cosine series:

$$y_j(t) = z_j^0 + 2 \sum_{l=1}^{lm} z_j^l \cos(l\omega_l t), \quad (4)$$

where $\omega_l$ is the breather frequency. Thus, the equation of motion can be changed through substitutions of a set of algebraic equations to obtain the $lm+1$ coefficients of $z_j^l$ parameters (4), these equations can be solved by the Newton method.

Once we found the breather profile for the uncoupled system, $k = 0$, we introduced the coupling into the system by small increments on $k$, $\delta k$. The next step is to find the numerical solution for $k = \delta k$ by using the Newton method and the original profile obtained from $k = 0$. This new solution is used like a seed for the case $k = 2\delta k$ and so on until we reach the desirable value of $k$.

3. Breather stability

Here we use the Floquet theory to study the stability of the breathers, where the Floquet operator ($F$) determines the evolution of the system in a period $T$ and it can be expressed by:

$$\Omega(T) = F\Omega(0) \quad (5)$$

with $\Omega(t)$ equal to the matrix form of the Hill’s equation.

Through this theory the system is linearly stable if none of the eigenvalues of $F$ have a module greater than 1. Hence a necessary condition to linear stability is that all Floquet multipliers are on the unit circle in the complex plane. In other words, $\theta$ must be real. In order to have instability, one or more pairs of eigenvalues must go out of the unit circle. If the eigenvalues go out of the unit circle in the complex plane in $\theta = 0$, we obtain an harmonic bifurcation. If they go out in $\theta = \pi$, we get a sub-harmonic bifurcation. Finally, if the eigenvalues go out of the unit circle in $\theta \neq 0, \pi$, then the bifurcation is called oscillatory.

4. Results and discussion

The results reported below were obtained using chains with 21 oscillators ($N = 21$) and the number of coefficients in the Fourier series was $lm = 17$. For numerical simulations we used periodic boundary conditions.
Figure 1. The absolute value of the Floquet multiplier versus coupling parameter $k$.

In figure 1 we present the results for the absolute value of the Floquet multipliers in function of the coupling parameter $k$ with breather frequency $\omega_b = 0.8$. For small values of $k$ all the Floquet multipliers have module equal one, so the stability is guarantee. After a certain value of $k$ ($k = 0.1297$), some bifurcations starts to occur and the stability is lost.

The dynamical behavior of a stable solution is the formation of a spatially localized structure in the chain, and it persists for all time. The Floquet analysis allows knowing the behavior of the system as function of the coupling parameter, but does not give directly any information about the influence of energy changes in the breather. To test this we used a stable solution, $k = 0.1$, and changed its energy by decreasing or increasing all the initial positions of this solution. So, we got one of these new solutions and used it like an initial condition in a dynamic simulation, where we used a Runge-Kutta Nystron of tenth order method [13] to integrate the equations of motion (3). The criterion to analyze the behavior of the system relative to the energy localization is based on the information entropy and measures the number of oscillators with significant energy of the system, $n_{osc}$. This parameter is used as criteria for energy localization [14, 15] and it is given by the following expression:

$$n_{osc} = \frac{e^S}{N},$$

(6)

where $S = -\sum_{j=1}^{N} e_j \ln e_j$ is the information entropy and $e_j = \frac{E_j}{\sum_{j=1}^{N} E_j}$ represents the normalized instant energies.

The figure 2 shows the average of the $n_{osc}$ values in function of the energy. We note the existence of a minimum value of $n_{osc}$ that is equivalent to the energy of the created stable breather ($E = 0.645$). If we look carefully the values of energy near the breather one, we note that the $n_{osc}$ values are lower than 0.2 in the range of energy equivalent to 0.291 – 1.203. It means that for the observable time ($t = 10000$ a.u.) the energy did not spread out through the lattice and remained localized in a small number of oscillators. This fact could be important for the use of breathers in the study of biological systems, like the DNA [14, 16], where a localized structure is observed [17, 18] and despite of the variation of the energy it remains localized.
Figure 2. a) The number of oscillators with significant energy value in function of the energy.
b) Detail of the figure 2a.

Figure 3. Modulus $G(\omega)$ of the complex Fourier transform of the eleventh oscillator. a) $E = 0.0556$ and $n_{osc} = 0.684$, b) $E = 1.5$ and $n_{osc} = 0.251$, c) The representation of the optical branch and d) The representation of the acoustic branch.
However, for energies outside this range of energy (0.291 – 1.203), the $n_{osc}$ value starts to grow rapidly and the energy localization is lost. In these situations the system presents the behavior of harmonic chains, where the energy diffuses in the lattice. The Fourier analysis allows us to rationalize an explanation for this fact. Figure 3 shows the modulus $G(\omega)$ of the complex Fourier transform of the eleventh oscillator for two energies of the system: (a) $E = 0.0556$ and (b) $E = 1.5$. In the case of low energies, the Fourier analysis (figure 3a) shows that the system presents oscillations inside the optical branch, $1 \leq \omega \leq \sqrt{1+4k}$ (figure 3c). So the localization is lost because the nonlinear modes are not excited. When we deal with high energies, (figure 3b), all frequencies with significant intensity are inside the acoustic branch, $0 \leq \omega \leq \sqrt{4k}$ (figure 3d), so the increase in the $n_{osc}$ value occurs. This happens because some oscillators have sufficient energy to overcome the Morse barrier and the system behaves like a purely harmonic one. These results agree with the conjecture that for the existence of localized modes, the system must oscillate outside the linear spectrum.

5. Conclusion
In this work we study the influence of energy changes in the dynamical behavior of a stable breather solution using a parameter based on the information entropy like a criteria. The variation of energy permits, in some range, the localization of the energy in a small number of oscillators (less than 20%) for the observable time and this fact can be important in the use of breather solution in biological system, where localized phenomena are commonly found. However when the energy of the system decreases from this range of energy, the localization is not found because the nonlinear modes are not excited and the system oscillates in the optical branch. For energy above this range, the system acquires energy sufficient to overcome the barrier of the Morse potential and some oscillators of the lattice lost their connection with the on site potential. So the system acquires a behavior similar to purely harmonic network. These results show the importance of the energy in localized phenomena that involves nonlinearity and discreteness.

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