

Effect of the introduction of impurities on the stability properties of multibreathers at low coupling

J Cuevas, JFR Archilla and FR Romero

Nonlinear Physics Group of the University of Sevilla
Departamento de Física Aplicada I, ETSI Informática
Avda Reina Mercedes s/n, 41012 Sevilla, Spain

Abstract. Using a theorem dubbed the *Multibreather Stability Theorem* [Physica D 180 (2003) 235-255] we have obtained the stability properties of multibreathers in systems of coupled oscillators with on-site potentials, and an inhomogeneity. Analytical results are obtained for 2-site, 3-site breathers, multibreathers, phonobreathers and dark breathers. The inhomogeneity is considered both at the on-site potential and at the coupling terms. All the results have been checked numerically with excellent agreement. The main conclusion is that the introduction of an impurity does not alter the stability properties.

PACS numbers: 63.20.Pw, 63.20.Ry, 63.50.+x, 66.90.+r.

E-mail: jcuevas@us.es

Submitted to: *Nonlinearity*

1. Introduction

Discrete breathers (DBs) are periodic, localized solutions that appear in discrete lattices of nonlinear oscillators. For Klein-Gordon lattices, i.e., lattices with an on-site potential, the conditions for their existence at low coupling are very weak. They are based on properties of the lattice at the *anti-continuous* limit, that is, the same lattice with zero coupling and, therefore, with the oscillators isolated. These conditions can be expressed in simple words as: a) For a given frequency ω_b the isolated oscillator is truly nonlinear ($dE/d\omega_b \neq 0$), with E the energy of the isolated oscillator). b) The breather does not resonate with the phonons ($n\omega_b \neq \omega_o$), with n any positive integer and ω_o the frequency of the isolated oscillators) [1]. The stability of one-site breathers has been proved in Refs. [2, 3, 4], whereas the stability of two-site breathers with symmetric potentials was proved in Ref. [5]. Recently, some of the authors developed the *Multibreathers Stability Theorem* (MST) [6], which provides a method for obtaining the stability properties of any multibreather at low-coupling based on the signs of the eigenvalues of a perturbation matrix Q , and applied it to homogeneous lattices. Although the MST applies to any Klein-Gordon lattice, it depends on analytical or numerical calculation of some magnitudes J_{nm} : This calculation becomes less simple and the number of magnitudes larger as the system

becomes more complicated, involving, for example, different linear frequencies, initial phases for the oscillators or impurities.

In this paper we address the application of the MST to Klein-Gordon lattices with an impurity. This impurity can be modelled at the on-site potential or at the coupling. The implementation of it at the masses is equivalent to at the on-site potential. The necessary magnitudes are calculated and the MST applied to 2-site and 3-site breathers, multibreathers, phonobreathers and dark breathers. The theoretical results are also checked numerically to confirm the validity of the calculations with excellent results.

The paper is organized in the following form: in section 2 we describe the details of the model; in section 3 we recall the Multibreathers Stability Theorem, and give some details of its application to the case of a lattice with an impurity; in sections 4 and 5 we calculate explicitly the eigenvalues of the perturbation matrix Q for 2-site and 3-site breathers; in sections 6 and 7 we obtain qualitative results about the signs of the Q -eigenvalues for multibreathers, phonobreathers and dark breathers, synthesizing the results in two theorems. We end with the conclusions. Details of analytical calculations are relegated to the appendix.

2. The model

In this paper, we consider Klein-Gordon chains with linear nearest-neighbours coupling whose dynamical equations are of the form:

$$\ddot{u}_n + V'_n(u_n) + \varepsilon \sum_{m=1}^N C_{nm} u_m = 0 \quad n = 1, \dots, N \quad (1)$$

where the variables u_n are the displacements with respect to the equilibrium positions, $V_n(u_n)$ is the on-site potential at the site n , N is the number of oscillators, C is a coupling matrix which includes the boundary conditions, and ε is the coupling parameter.

The impurity can be introduced in the system through an inhomogeneity at the on-site potential or at the coupling matrix, in a similar fashion as it was done in Ref. [7].

The linear frequencies of the isolated oscillators are $\omega_n = (V''_n(0))^{1/2}$. If the inhomogeneity is implemented at the potential of the n_0 -th particle, we denote $V_0 = V_{n_0}$ and $\omega_o = \omega_{n_0} = (V''_0(0))^{1/2} \forall n \neq n_0$. We can write $\omega_{n_0}^2 = (1 + \alpha \delta_{n,n_0}) \omega_o^2$, where the inhomogeneity parameter α takes values in $(-1, \infty)$, $\alpha = 0$ corresponding to the homogeneous case.

For a system with nearest-neighbour interaction, the dynamical equations Eqs. (1) can be written [7]:

$$\ddot{u}_n + V'_n(u_n) + \varepsilon [k_{n-1,n} (u_n - u_{n-1}) + k_{n,n+1} (u_n - u_{n+1})] = 0. \quad (2)$$

If the system is homogeneous $k_{n,m} = 1, \forall n, m$, except at $m = 1$ or $n = N$. With periodic boundary conditions, the index n is cyclical so as $0 \sim N$ and $N + 1 \sim 1$ and $k_{0,1} = k_{N,N+1} = 1$. With free ends, $k_{0,1} = k_{N,N+1} = 0$. With fixed ends, two extra oscillators have $u_0 = u_{N+1} = 0$ and $k_{0,1} = k_{N,N+1} = 1$.

Therefore, the coupling matrixes, C^0 , for a finite homogeneous system with N oscillators have the following elements:

$$\begin{aligned} \text{Fixed ends:} \quad C_{nm}^0 &= \begin{cases} 2 & \text{if } n = m \\ -1 & \text{if } |n - m| = 1 \\ 0 & \text{otherwise.} \end{cases} \\ \text{Free ends :} \quad C_{11} = C_{NN} &= 1; \quad C_{nm} = C_{nm}^0 && \text{otherwise} \\ \text{Periodic b. c. :} \quad C_{1N} = C_{N1} &= -1; \quad C_{nm} = C_{nm}^0 && \text{otherwise} \end{aligned} \quad (3)$$

We model the impurity at a site n_0 distinct from the lattice boundaries, by changing the constants k_{n_0, n_0+1} and k_{n_0-1, n_0} to $(1 + \beta/2)$, with β being a parameter which takes its values in $(-2, \infty)$, so as the homogeneous case is recovered when $\beta = 0$. $\beta < 0$ means weaker constants than the homogeneous coupling ones and $\beta > 0$ the opposite.

Therefore, the coupling matrix C_{nm} becomes:

$$C_{nm} = \begin{cases} (\beta + 2) & \text{if } n = m = n_0 \\ -(\beta + 2)/2 & \text{if } |n - m| = 1 \text{ and } n = n_0 \text{ or } m = n_0 \\ (\beta + 4)/2 & \text{if } n = m = n_0 \pm 1 \\ C_{nm}^0 & \text{otherwise,} \end{cases} \quad (4)$$

Note that, with these definitions of C , $\varepsilon > 0$ corresponds to an attractive interaction and $\varepsilon < 0$, to a repulsive one.

3. Multibreathers Stability Theorem

3.1. Previous results

In this section we recall the results of the Generalized MST established in theorem 3 of Ref. [6]. This theorem refers to generalized Klein-Gordon systems of the form

$$m_n \ddot{u}_n + V_n'(u_n) + \varepsilon \frac{\partial W(u)}{\partial u_n} = 0, \quad (5)$$

with $u = (u_1, \dots, u_N)$ and $\varepsilon W(u)$ being the coupling potential. Suppose that u^0 is a T -periodic solution at the anti-continuous limit ($\varepsilon = 0$), with p excited oscillators and $N - p$ ones at rest ($u_n^0 = 0$). The nondiagonal elements of the $p \times p$ perturbation matrix Q (in reduced form) are defined as

$$Q_{nm} = \frac{1}{\mu_n \mu_m} \int_{-T/2}^{T/2} \dot{u}_n^0 \frac{\partial^2 W(u^0)}{\partial u_n \partial u_m} \dot{u}_m^0 dt, \quad n \neq m \quad (6)$$

considering only the indexes corresponding to the excited oscillators and renumbering them from 1 to p .

The diagonal elements are given by

$$Q_{nn} = - \sum_{\forall m \neq n} \frac{\mu_m}{\mu_n} Q_{nm}, \quad (7)$$

with $\mu_n = \sqrt{\int_{-T/2}^{T/2} (\dot{u}_n^0)^2 dt}$.

Note that the diagonal terms of C do not appear in Q . A consequence is that the stability properties of a system with next-neighbour, repulsive, dipole-dipole interaction, with dynamical equations:

$$\ddot{u}_n + V_n'(u_n) + \varepsilon' \sum_{m \neq n} u_n u_m \quad (\varepsilon' > 0) \quad (8)$$

are the same as for the system given by Eq. (1), with $\varepsilon = -\varepsilon'$. With this definitions, we reproduce here the generalized multibreather stability theorem:

Generalized MST *Given a generalized Klein–Gordon system Eq. (5), a specific multibreather solution at zero coupling $\{u_n^0\}$, determined by a suitable set of codes $\{\sigma\}_{i=1}^p$, u the corresponding solution at low coupling, $\{\lambda\}_{i=0}^{p-1}$ the eigenvalues of the reduced, perturbation matrix Q , with only one zero, and being the wells corresponding to the excited oscillators sites of the same type, hard or soft, then:*

The solution u is stable if:

- a) *The on-site potentials are soft and there is not any positive value in $\{\varepsilon \lambda_i\}_{i=0}^{p-1}$.*
- b) *The on-site potentials are hard and there is not any negative value in $\{\varepsilon \lambda_i\}_{i=0}^{p-1}$.*

We can summarize the stability properties in the following way. If $S = 1$ means stability and $S = -1$ instability, $H = 1$ corresponds to a hard on-site potential, and $H = -1$ to a soft one, and we define $\text{sign}(Q) = 1$ if all the eigenvalues of Q but a zero one are positive and $\text{sign}(Q) = -1$ if they are negative except for the zero one, then

$$S = H \times \text{sign}(Q) \times \text{sign}(\varepsilon). \quad (9)$$

It there are eigenvalues of different signs, the multibreather is always unstable. It is important to take into account that there is always a zero eigenvalue due to a global phase mode. If there is more than one zero eigenvalue, the stability theorem can only predict the instability in the case that there exists at least one eigenvalue λ that leads to $S = -1$ in the previous equation (changing $\text{sign}(Q)$ for $\text{sign}(\lambda)$), but not the stability, as the 0-eigenvalue is degenerate.

In the rest of the paper we will often limit ourselves to the calculation of the eigenvalues of Q , the stability of the multibreathers being given by Eq. (9). In this way we avoid considering each time the different signs of ε and the hardness/softness of the on-site potential.

3.2. Application to systems with an impurity

For the system with linear coupling in Eq. (1) we have

$$\frac{\partial^2 W(u^0)}{\partial u_n \partial u_m} = C_{nm}. \quad (10)$$

Therefore the nondiagonal elements of Q are given by

$$Q_{nm} = \frac{C_{nm}}{\mu_n \mu_m} \int_{-T/2}^{T/2} \dot{u}_n^0 \dot{u}_m^0 dt, \quad n \neq m. \quad (11)$$

The diagonal elements are given by Eq. (7). The functions $u_n^0(t)$ are the solutions of the isolated oscillators submitted to the potentials $V(u_n)$, i.e. the solutions of the equations:

$$\ddot{u}_n + V_n'(u_n) = 0, \quad (12)$$

In this paper we limit ourselves to time-reversible solutions, i.e., the excited oscillators at the anti-continuous limit can only have phase 0 or π , or, in other words, if $u_n^0(t)$ is a time-reversible solution of Eq. (12), $u_n^0(t) = u_n^0(-t)$, then $u_n^0(t + T/2)$ is the only possible time-reversible solution apart from $u_n^0(t)$. Therefore, the state of the system at the anti-continuous limit can be described by a code $\sigma = (\sigma_1, \dots, \sigma_N)$,

where $\sigma_n = 0, +1, -1$ means that the corresponding oscillator is at rest, with phase 0, or with phase π , respectively, at $t = 0$ [2].

Let J_{nm} and J'_{nm} be defined as:

$$J_{nm} = \int_{-T/2}^{T/2} \dot{u}_n^0(t) \dot{u}_m^0(t) dt, \quad J'_{nm} = \int_{-T/2}^{T/2} \dot{u}_n^0(t) \dot{u}_m^0(t + T/2) dt, \quad (13)$$

and the parameters η_{nm} , γ_{nm} and φ_{nm} as:

$$\eta_{nm} = \frac{J_{nm}}{\sqrt{J_{nn}J_{mm}}} > 0, \quad \gamma_{nm} = -\frac{J'_{nm}}{\sqrt{J_{nn}J_{mm}}} > 0, \quad \varphi_{nm} = \sqrt{\frac{J_{nm}}{J_{nn}}} > 0, \quad (14)$$

Then, the matrix elements Q_{nm} can be written as:

$$Q_{nm} = \begin{cases} \eta_{nm} C_{nm} & \text{if } \sigma_n \sigma_m = 1 \\ -\gamma_{nm} C_{nm} & \text{if } \sigma_n \sigma_m = -1 \end{cases} \quad (15)$$

$$Q_{nn} = - \sum_{\forall m \neq n} \varphi_{nm} Q_{nm}, \quad (16)$$

where we have taken into account that $\mu_n^2 = J_{nn}$. We have calculated analytically these parameters for several potentials in Appendix A, although only the case of the Morse on-site potential leads to relatively simple expressions.

Some properties of the parameters η_{nm} , γ_{nm} and φ_{nm} can be easily deduced. In the case of symmetric potentials, $J_{nm} = -J'_{nm}$, as $\dot{u}_n^0(t) = -\dot{u}_n^0(t + T/2)$, and, in consequence, $\gamma_{nm} = \eta_{nm}$. Other property is that, for the homogeneous case, $\eta_{nm} = 1$, $\varphi_{nm} = 1$ and $\gamma_{nm} = \gamma_0$, where γ_0 is the symmetry parameter [6] in that case (which is the unity for a symmetric potential).

In order to simplify the notation, as we are considering a single impurity, we define the parameters $\eta \equiv \eta_{nh}$, $\gamma \equiv \gamma_{nh}$, $\varphi \equiv \varphi_{nh}$, where the index n indicates the impurity site and h another one.

In the following two sections we calculate explicitly the eigenvalues of the perturbation matrices for 2-site and 3-site breathers. Sections 6 and 7 deal with multibreathers, phonobreathers and dark breathers, for which we cannot calculate the eigenvalues but only their signs.

Note that the stability properties of 2-site and 3-site breathers are also included in Theorem 1 of Section 6 as they are particular cases of multibreathers.

4. 2-site breathers with an impurity

A 2-site breather is a breather obtained from the anti-continuous limit when two contiguous sites are excited. The boundary conditions are irrelevant as long as the sites are not close to the boundaries. Without loss of generality, let us rename the two indexes so as the impurity is located at $n = 1$, and the corresponding oscillator has phase zero ($\sigma_1 = 1$). The other oscillator is located at $n = 2$. When dealing with the code σ it is enough to consider the codes of these two oscillators, as the other are zero, thus, $\sigma = (\sigma_1, \sigma_2)$. Two cases are possible, in-phase oscillators, $\sigma = (1, 1)$, and out-of-phase oscillators, $\sigma = (1, -1)$.

4.1. Inhomogeneity at the on-site potential

First of all, we consider the in-phase case. Taking into account Eqs. (14-16) and the notation introduced in Section 3, the matrix Q is given by:

$$Q = \begin{bmatrix} \eta\varphi & -\eta \\ -\eta & \eta/\varphi \end{bmatrix}, \quad (17)$$

with eigenvalues $\{\lambda_0, \lambda_1\} = \{0, \eta(\varphi + 1/\varphi)\}$. Then, $\lambda_1 > 0$.

For the out-of-phase case, the perturbation matrix is:

$$Q = \begin{bmatrix} -\gamma\varphi & \gamma \\ \gamma & -\gamma/\varphi \end{bmatrix}, \quad (18)$$

with eigenvalues $\{\lambda_0, \lambda_1\} = \{0, -\gamma(\varphi + 1/\varphi)\}$. Thus, $\lambda_1 < 0$.

If the system is homogeneous $\{\lambda_0, \lambda_1\} = \{0, 2\}$ and $\{\lambda_0, \lambda_1\} = \{0, -2\gamma_0\}$ for the in-phase and out-of-phase cases, respectively [6]. In consequence, the sign of λ_1 does not change when an impurity is introduced in the on-site potential, and the stability properties are not altered.

Figs. 1 and 2 show the dependence of $E = \varepsilon\lambda_1$ with respect to ε calculated numerically and analytically (see Appendix A). The agreement between both calculations is excellent for fairly large values of the coupling constant.

4.2. Inhomogeneity at the coupling constant

For the $\sigma = (1, 1)$ 2-site breathers:

$$Q = \frac{\beta + 2}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} = \frac{\beta + 2}{2} Q_0, \quad (19)$$

where Q_0 is the perturbation matrix of the homogeneous chain. Thus, $\lambda_1 = \beta + 2$. The relation $Q = (\beta + 2)/2 Q_0$ also holds for the code $\sigma = (1, -1)$, and, in consequence, $\lambda_1 = -(\beta + 2)/2\gamma_0$ in this case. As $\beta > -2$, the conclusion is that the stability properties are the same as in the homogeneous system.

Fig. 3 compares this result with the numerically obtained.

4.3. Summary of the stability properties for 2-site breathers

The calculation of the eigenvalues of Q for 2-site breathers with an impurity, either at the on-site potential or the coupling constant, show that their stability properties are the same as in the homogenous case. These properties are included in theorem 1 in section 6 (although for 2-site breathers the only possible patters are in-phase or out-of-phase).

5. 3-site breathers with an impurity

They consist of breathers derived from three contiguous, excited oscillators at the anti-continuous limit. There are seven non-equivalent possibilities, taking into account the position of the impurity and the phases of the oscillators. Let us rename the excited sites as 1, 2, 3, suppose that $\sigma_2 = 1$, and denote with boldface the position of the impurity. Then the three-index codes corresponding to the three excited oscillators are $(1, \mathbf{1}, 1)$, $(1, 1, \mathbf{1})$, $(-1, \mathbf{1}, -1)$, $(-1, 1, \mathbf{-1})$, $(\mathbf{1}, 1, -1)$, $(1, \mathbf{1}, -1)$, $(1, 1, \mathbf{-1})$.

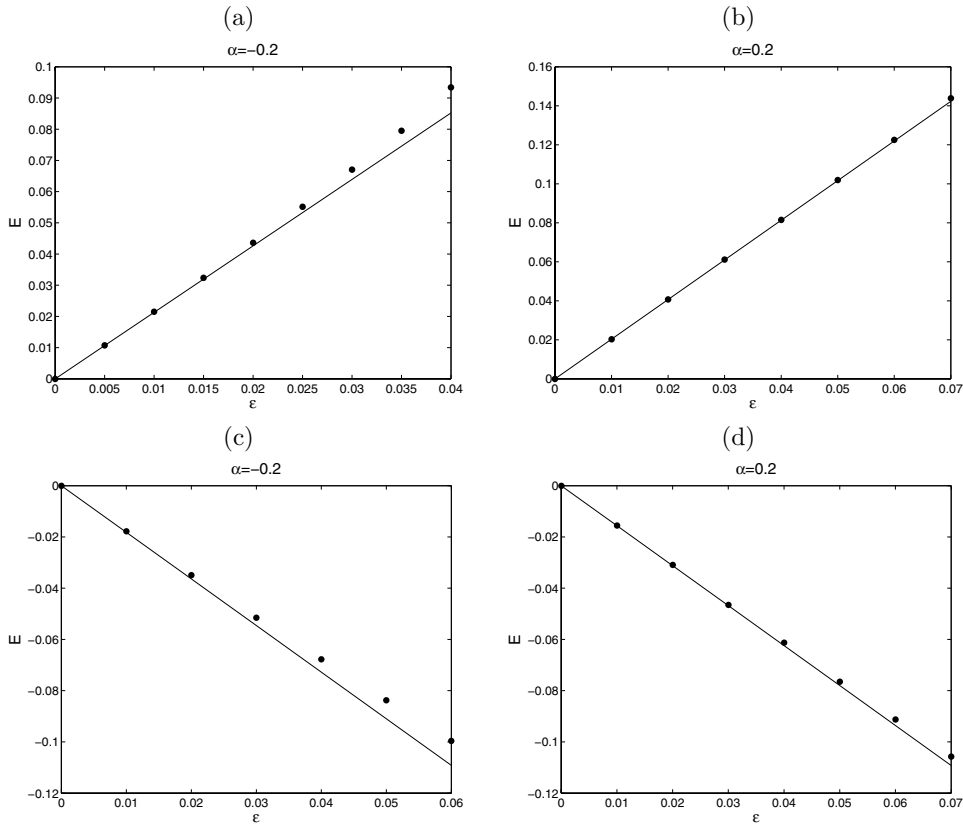


Figure 1. Dependence of $E = \varepsilon\lambda_1$ with respect to ε for two different values of α . (a,b) correspond to in-phase 2-site breathers and (c,d) to out-of-phase 2-site breathers. All the solutions stand for a Morse potential and $\omega_b = 0.8$. Dots represent numerical solutions and lines analytical ones.

5.1. Inhomogeneity at the on-site potential

Let us suppose that the $\sigma \equiv (\sigma_1, 1, \sigma_3)$. The in-phase breather corresponds to $\sigma_1 = \sigma_3 = 1$, the out-of-phase to $\sigma_1 = \sigma_3 = -1$ and another one to $\sigma_1\sigma_3 = -1$. Table 1 shows the eigenvalues λ_1 and λ_2 for the different configurations ($\lambda_0 = 0$ always). From this table, it can be deduced that $\lambda_1 > 0$ and $\lambda_2 > 0$ for the in-phase solution, $\lambda_1 < 0$ and $\lambda_2 < 0$ for the out-of-phase breather and $\lambda_1 > 0$ and $\lambda_2 < 0$ otherwise. This result coincides with the homogeneous case.

Figs. 4 and 5 show the dependence of $E_1 = \varepsilon\lambda_1$ and $E_2 = \varepsilon\lambda_2$ with respect to ε calculated numerically and analytically. The agreement between both descriptions is again very good even for fairly large values of the coupling constant.

5.2. Inhomogeneity at the coupling constant

If the impurity is located at $n_0 = 2$, the relation $Q = (\beta + 2)/2 Q_0$ is fulfilled again. The only way to obtain a different relation is to suppose the impurity at an edge of the

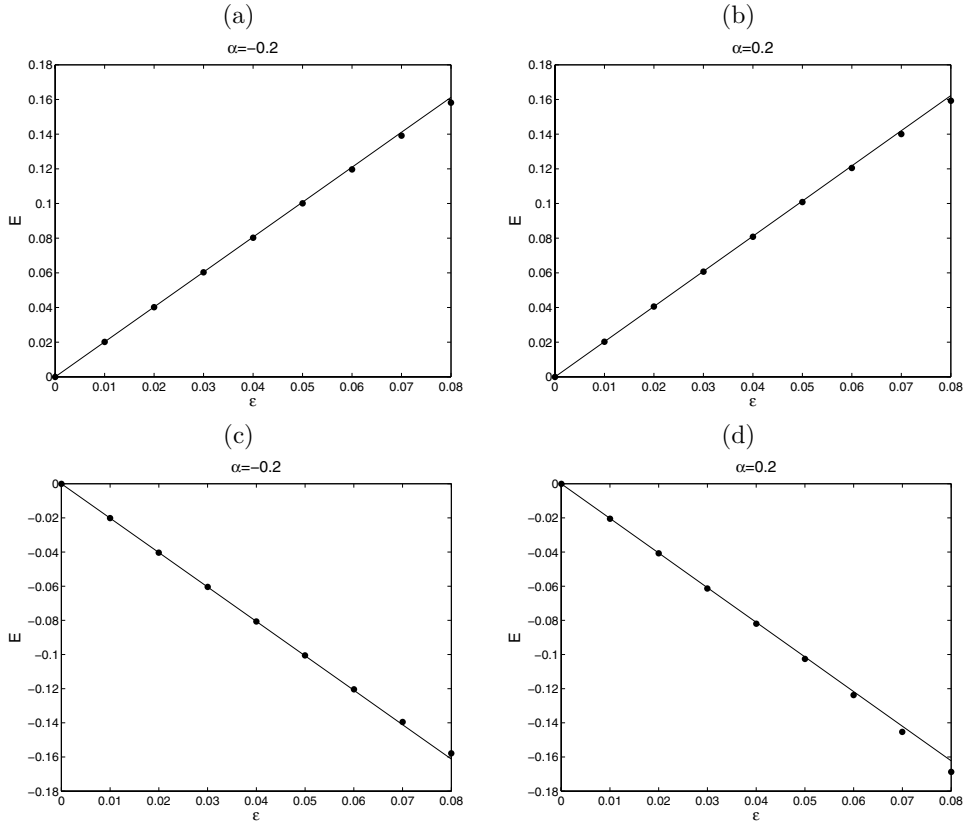


Figure 2. Dependence of $E = \varepsilon\lambda_1$ with respect to ε for two different values of α . (a,b) correspond to in-phase 2-site breathers and (c,d) to out-of-phase 2-site breathers. All the solutions stand for a hard ϕ^4 potential and $\omega_b = 1.3$. Points represent numerical solutions and lines analytical ones.

excited sites, i.e., $n_0 = 1$ or $n_0 = 3$. Table 2 summarizes the different cases. As it can be deduced from the table, the signs of the eigenvalues are the same as in the on-site inhomogeneity case. Fig. 3 compares these results with the numerically obtained ones.

5.3. Summary of the stability properties for 3-site breathers

The calculation of the eigenvalues of Q for 3-site breathers with an impurity, either at the on-site potential or the coupling constant, show that their stability properties are the same as in the homogenous case. These properties are included in theorem 1 in section 6.

6. Multibreathers and phonobreathers with an impurity

A multibreather is obtained from the anti-continuous limit when a number of contiguous oscillators are excited. If all the oscillators are excited it is called a

Table 1. Eigenvalues for a three-site breather with an inhomogeneity at the on-site potential. The impurity site is indicated through a bold font, and, in order to simplify the expressions, we define $\phi = \varphi + 1/\varphi$. γ_0 is the symmetry coefficient for the homogeneous case. Pairs of eigenvalues differing in a sign appear in a single expression with \pm .

Code	λ_1	λ_2
1 1 1	η/φ	$\eta(\varphi + \phi)$
1 1 1	$\frac{1}{2} [2 + \eta\phi \pm (4 - 4\eta\phi + \eta^2\phi^2)^{1/2}]$	
-1 1 -1	$-\gamma/\varphi$	$-\gamma(\varphi + \phi)$
-1 1 -1	$-\gamma_0 - \frac{1}{2} \left\{ \gamma\phi \pm [(\gamma\phi + 2\gamma_0)^2 - 4\gamma\gamma_0(\varphi + \phi)]^{1/2} \right\}$	
1 1 -1	$\frac{1}{2} \left\{ \eta\phi \pm [\eta^2\phi^2 + 4\gamma_0\eta(\varphi + \phi)]^{1/2} \right\}$	
1 1 -1	$\frac{1}{2} \left\{ (\eta - \gamma)\phi \pm [(\eta + \gamma)^2\phi^2 - 4\eta\gamma\varphi^2]^{1/2} \right\}$	
1 1 -1	$\frac{1}{2} [-(\gamma\phi - 2) \pm (\gamma^2\phi^2 + 4 + 4\gamma\varphi)^{1/2}]$	

Table 2. Eigenvalues for a three-site breather with an inhomogeneity at the coupling constant. The impurity site is indicated through a bold font, and, in order to simplify the expressions, we define $\phi = \varphi + 1/\varphi$. γ_0 is the symmetry coefficient for the homogeneous case. Pairs of eigenvalues differing in a sign appear in a single expression with \pm .

Code	λ_1	λ_2
1 1 1	$1 + \beta/2$	$3(1 + \beta/2)$
1 1 1	$\frac{1}{2} [\beta + 4 \pm (\beta^2 + 4)^{1/2}]$	
-1 1 -1	$-\gamma_0(1 + \beta/2)$	$-3\gamma_0(1 + \beta/2)$
-1 1 -1	$-\frac{1}{2}\gamma_0 [\beta + 4 \pm (\beta^2 + 4)^{1/2}]$	
1 1 -1	$1 - \gamma_0 + \frac{1}{2} \left\{ \beta \pm [\gamma_0^2\beta^2 + 2\gamma_0(2\gamma_0 + 1)\beta + 4(\gamma_0^2 + \gamma_0 + 1)]^{1/2} \right\}$	
1 1 -1	$(1 + \beta/2) [1 - \gamma_0 \pm (\gamma_0^2 + \gamma_0 + 1)^{1/2}]$	
1 1 -1	$1 - \gamma_0 + \frac{1}{2} \left\{ \beta \pm [\gamma_0^2\beta^2 + 2\gamma_0(2\gamma_0 + 1)\beta + 4(\gamma_0^2 + \gamma_0 + 1)]^{1/2} \right\}$	

phonobreather. We suppose that a multibreather does not include the sites at the boundaries and that the impurity is not located at the boundaries. With these conditions the coupling matrices Eqs. (3, 4) for multibreathers and phonobreathers with fixed or free ends differ only in the diagonal terms and, therefore, the perturbation matrices are identical and both cases can be studied simultaneously. For phonobreathers with periodic boundary conditions the elements of the coupling matrix $C_{1N} = C_{N1}$ are equal to -1 and it is necessary to treat this case separately from the free / fixed ends case.

We have not been able to obtain analytical expressions for the eigenvalues of the perturbation matrices, but we have demonstrated their stability properties. When the number of oscillators of a multibreather increases, the degree of the characteristic polynomial also increases and an analytical evaluation of its roots is not possible for systems with an impurity. However, in the case of an homogenous

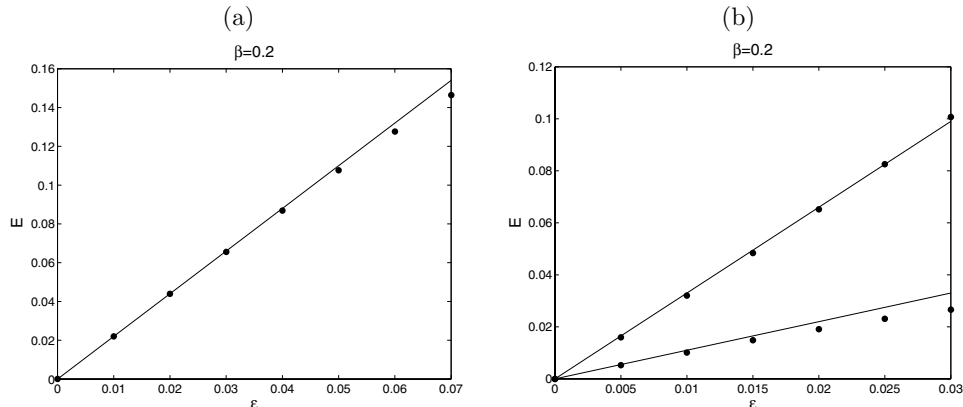


Figure 3. Dependence of $E = \varepsilon\lambda$ for a 2-site (a) and a 3-site breather (b) with an impurity at the coupling located at the edge. All the solutions stand for a Morse potential and $\omega_b = 0.8$. Points correspond to numerical solutions and lines to analytical ones.

system, the eigenvalues can be calculated because the eigenvectors equation of the system is equivalent to the dynamical equations of a linear lattice of oscillators. In Ref. [6] it is demonstrated that in homogeneous systems the Q -eigenvalues for an in-phase and out-of-phase multibreather are $\lambda_m = 4 \sin^2(m\pi/(2N))$ and $\lambda_m = -4\gamma_0 \sin^2(m\pi/(2N))$ (with $m = 0, \dots, N-1$), respectively. They are all positive or all negative, except for a single zero, the stability being given by Eq. (9). It was also suggested that any other multibreather pattern would be unstable. We will demonstrate in the following subsection that the last statement is actually true.

With an impurity, we can only obtain qualitative results about the spectrum of the matrix Q for a phonobreather (or N -site multibreather). In particular, we show that the stability properties of the system with an impurity are the same as for an homogeneous system. To this end, we will make use of some congruence properties of symmetric matrices [8].

Two symmetric matrices A and B are congruent if they can be transformed into each other through elementary transformations: $B = PAP^t$, P being any invertible matrix. The inertia of a matrix is defined as $\text{In}(A) = \{i_+(A), i_-(A), i_0(A)\}$ where i_+ , i_- , i_0 denote, respectively, the number of positive, negative and zero eigenvalues of A . Sylvester's inertia law establishes that the inertia of two congruent matrices are the same [9]. In consequence, it is enough to diagonalize a matrix using elementary transformations to obtain its inertia. The diagonal matrix has the structure called first canonical form:

$$D = \left\{ \underbrace{1, \dots, 1}_{i_+ \text{ times}}, \underbrace{-1, \dots, -1}_{i_- \text{ times}}, \underbrace{0, \dots, 0}_{i_0 \text{ times}} \right\} \quad (20)$$

We analyze below the stability properties of phonobreaters with different boundary conditions and an inhomogeneity at the on-site potential or the coupling. In the homogeneous case, the inertia of Q is, for an in-phase breather, $\text{In}(Q) = \{N-1, 0, 1\}$ and, for an out-of-phase (staggered) breather, $\text{In}(Q) = \{0, N-1, 1\}$,

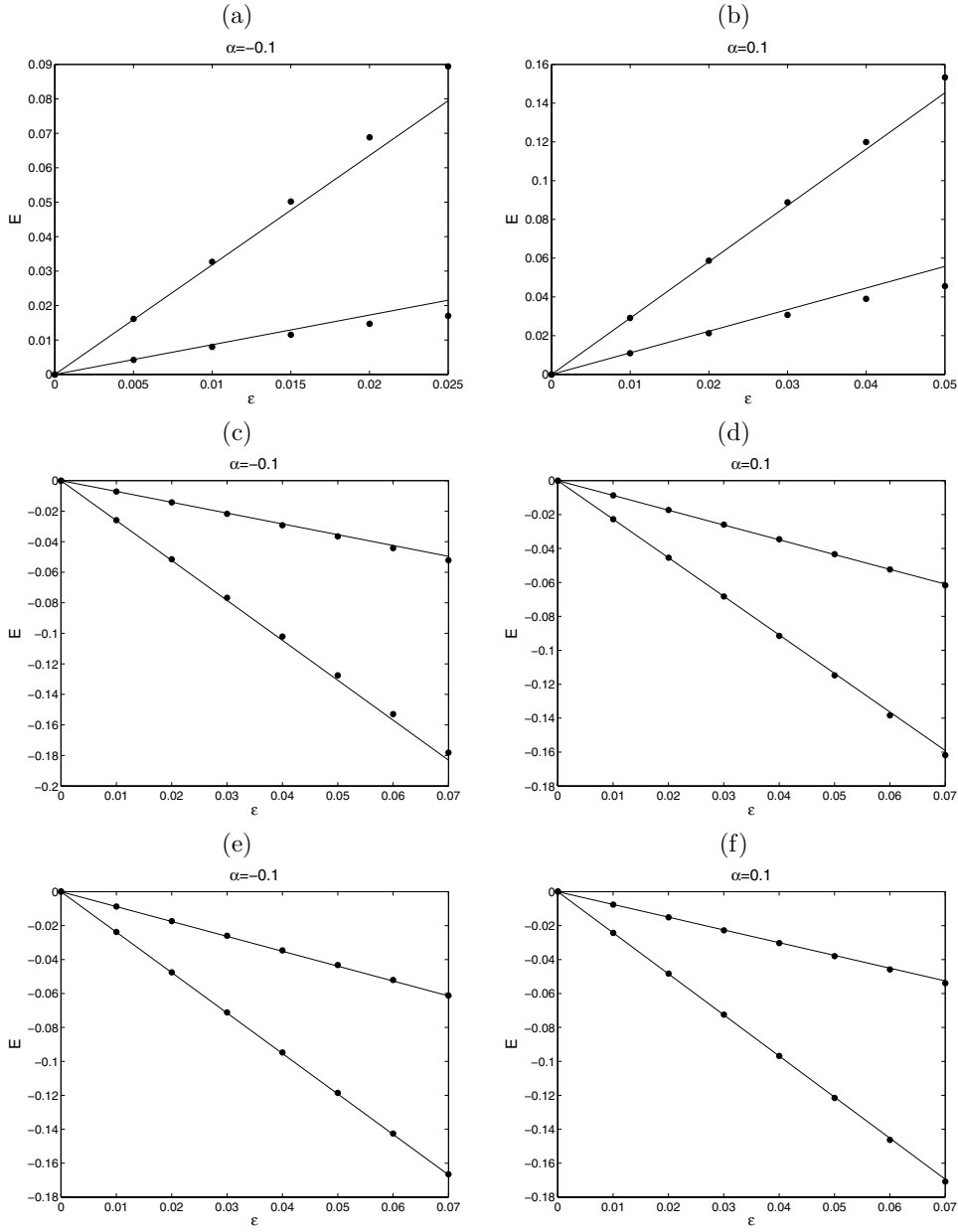


Figure 4. Dependence of $E = \varepsilon\lambda_1$ and $E = \varepsilon\lambda_2$ with respect to ε for two different values of α . (a,b) correspond to in-phase 3-site breathers, (c,d) to out-of-phase 3-site breathers with the impurity at the center and (e,f) to the same as before but with the impurity at the edge. All the solutions stand for a Morse potential and $\omega_b = 0.8$. Points represent numerical solutions and lines analytical ones.

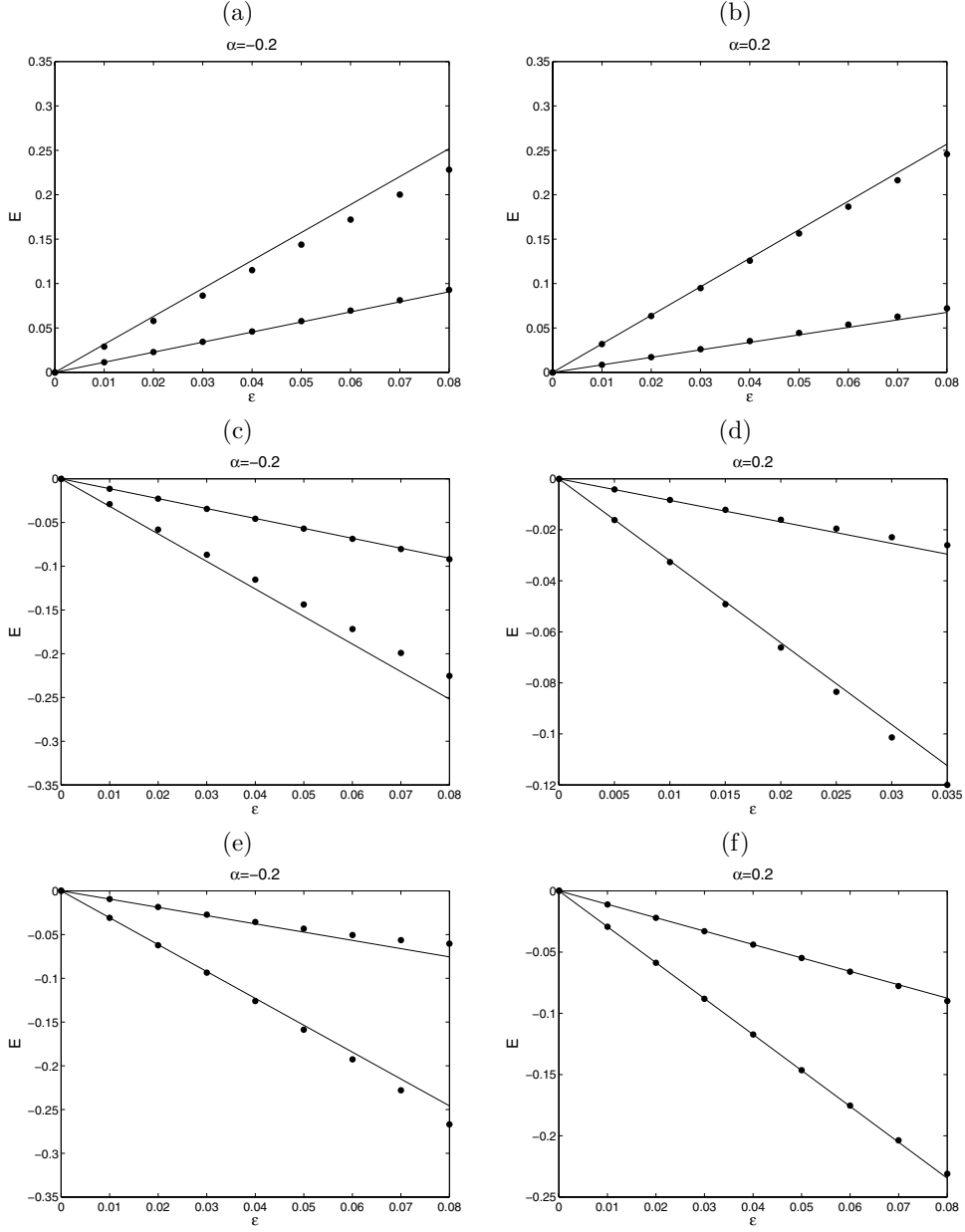


Figure 5. Dependence of $E = \varepsilon\lambda_1$ and $E = \varepsilon\lambda_2$ with respect to ε for two different values of α . (a,b) correspond to in-phase 3-site breathers, (c,d) to out-of-phase 3-site breathers with the impurity at the center and (e,f) to the same as before but with the impurity at the edge. All the solutions stand for a hard ϕ^4 potential and $\omega_b = 1.3$. Points represent numerical solutions and lines analytical ones.

with N being the number of system particles. We will show that the inertia does not change when an impurity is introduced.

Furthermore, the only multibreathers that can be stable are those that vibrate in-phase or staggered, as it is demonstrated below.

6.1. Demonstration of the necessity of an in-phase or out-of-phase pattern for the stability of multibreathers

In this subsection we deal first with homogenous systems and secondly with systems with an impurity.

Proposition 1 *In an homogeneous Klein–Gordon system with harmonic, next-neighbour coupling, time-reversible, multibreathers with any code different from the in-phase or out-of-phase ones, the eigenvalues of the perturbation matrix have different signs and, therefore, the multibreathers are unstable for any on-site potential and any sign of ε .*

We use a consequence of Sylvester’s inertia law, called Sylvester’s Theorem [8]. It establishes that, for a positive definite matrix, the principal minors are positive, for a negative definite one, the principal minors alternate their signs when the dimension increases by one and, finally, a matrix is not definite when none of the last conditions are fulfilled.

Let us suppose an homogeneous lattice. If the pattern of vector σ is different from the in-phase or staggered ones, there is always a sequence $\{-1, 1, 1\}$ or $\{1, -1, -1\}$ on it. It is easy to show that in both cases, the perturbation matrix has the form:

$$Q = \begin{bmatrix} \ddots & & & \\ & \ddots & & \\ & & Q_0 & \\ & & & \ddots \end{bmatrix}, \quad (21)$$

with

$$Q^0 = \begin{bmatrix} -\gamma_0 & \gamma_0 & 0 \\ \gamma_0 & 1 - \gamma_0 & 0 \\ 0 & 1 & \bullet \end{bmatrix}, \quad (22)$$

where \bullet is a number that depends on the phase of the particle adjacent to the pattern breaking sequence and γ_0 is the symmetry parameter in the homogeneous case. As the spectrum of Q is invariant under rows/columns exchanges, the block Q^0 can be placed at $Q_{1,1}$, and Sylvester’s theorem can be applied to Q^0 . The 1st order minor is $M^{(1)} = Q_{1,1}^0 = -\gamma_0 < 0$, and the 2nd order one, $M^{(2)} = Q_{1,1}^0 Q_{2,2}^0 - Q_{1,2}^0 Q_{2,1}^0 = -\gamma_0 < 0$. In consequence, the first two principal minors are negative and the matrix is not definite. There are positive and negative eigenvalues and, therefore, the multibreather is unstable. \square

Proposition 2 *Proposition 1 also holds for a system with an impurity.*

Let us suppose now that an impurity is introduced in the pattern breaking sites. The matrices for impurities in the first, second and third sites are (note that we

only consider the first (2×2) submatrix as the result is independent on the third row/column), respectively:

$$Q_1^0 = \begin{bmatrix} -\gamma\varphi & \gamma \\ \gamma & -\gamma/\varphi + 1 \end{bmatrix},$$

$$Q_2^0 = \begin{bmatrix} -\gamma/\varphi & \gamma \\ \gamma & (\eta - \gamma)/\varphi \end{bmatrix}, \quad Q_3^0 = \begin{bmatrix} -\gamma_0 & \gamma_0 \\ \gamma_0 & \eta/\varphi - \gamma_0 \end{bmatrix}, \quad (23)$$

and the corresponding minors are: $\{M_1^{(1)} = -\gamma\varphi, M_1^{(2)} = -\gamma\varphi\}$, $\{M_2^{(1)} = -\gamma/\varphi, M_2^{(2)} = -\gamma\eta\}$, $\{M_3^{(1)} = -\gamma_0, M_3^{(2)} = -\gamma_0\eta/\varphi\}$. In consequence, the first two principal minors are negative and the matrices are not definite. The multibreather is unstable. \square

6.2. In-phase and out-of phase patterns with free/fixed ends boundary conditions and an impurity

The stability of these patterns was calculated in Ref. [6] for an homogeneous system. Here we demonstrate that the same properties hold for a system with an impurity.

Proposition 3 *For multibreathers not including the borders of the system and phonobreathers with free or fixed-end boundary conditions, with or without and impurity, the eigenvalues of the perturbation matrix are positive for the in-phase pattern and negative for the out-of-phase one, except for a nondegenerate zero. The stability is given by Eq. (9).*

Let us consider the in-phase pattern, if the impurity is located at $n = c$, the elements of the perturbation matrix Q^{F0} can be written as:

$$Q_{nm}^{F0} = 2\delta_{n,m}[1 + (\eta\varphi - 1)\delta_{n,c} + (\eta/\varphi - 1)/2\delta_{|n-c|,1} - (\delta_{n,1} + \delta_{n,N})/2] - \delta_{n,m+1}[1 - (\eta + 1)(\delta_{n,c} + \delta_{n,c+1})] - \delta_{n,m-1}[1 - (\eta + 1)(\delta_{n,c} + \delta_{n,c-1})]. \quad (24)$$

This matrix is transformed into a diagonal matrix through $D = P Q P^t$, where

$$P_{nm} = [\delta_{[\frac{m}{c}],0} + \delta_{n,m}][1 + \delta_{[\frac{m}{c}],0}\delta_{n,c-1}(\sqrt{\varphi/\eta} - 1) + \delta_{m,c}\delta_{[\frac{m}{c}],0}/\varphi + \delta_{n,c-1}((\sqrt{\varphi/\eta} - 1)\delta_{[\frac{m}{c}],0} + (1/\sqrt{\varphi\eta} - 1)\delta_{m,c})], \quad (25)$$

where $[\cdot]$ denotes the integer part. $D_{nm} = \delta_{n,m}(1 - \delta_{n,N})$. In consequence, $\text{In}(Q^{F0}) = \{N - 1, 0, 1\}$ and all of the eigenvalues are positive except for one which is zero.

Let us consider now the out-of-phase pattern, the perturbation matrix $Q^{F\pi}$ is given by:

$$Q_{nm}^{F\pi} = -2\gamma_0\delta_{n,m}[1 + (\gamma\varphi - 1)\delta_{n,c} + (\gamma/\varphi - 1)/2\delta_{|n-c|,1} - (\delta_{n,1} + \delta_{n,N})/2] - \gamma_0\delta_{n,m+1}[1 - (\gamma_0 + 1)(\delta_{n,c} + \delta_{n,c+1})] + \gamma_0\delta_{n,m-1}[1 - (\gamma/\gamma_0 + 1)(\delta_{n,c} + \delta_{n,c-1})], \quad (26)$$

which transform into the diagonal matrix $D_{nm} = -\delta_{n,m}(1 - \delta_{n,N})$ through the transformation matrix

$$P_{nm} = [\delta_{[\frac{m}{c}],0} + \delta_{n,m}][1 + \delta_{[\frac{m}{c}],0}\delta_{n,c-1}(\sqrt{\varphi/\gamma} - 1) + \delta_{m,c}\delta_{[\frac{m}{c}],0}/\varphi + \delta_{n,c-1}((\sqrt{\varphi/\gamma} - 1)\delta_{[\frac{m}{c}],0} + (1/\sqrt{\varphi\gamma} - 1)\delta_{m,c})]. \quad (27)$$

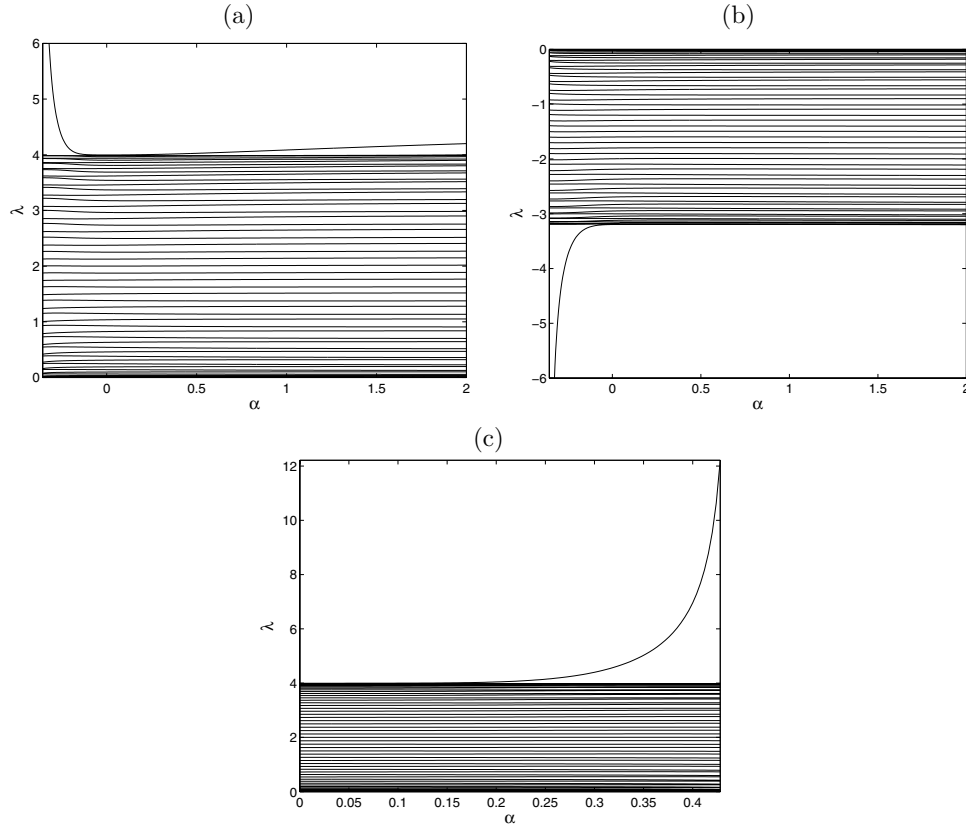


Figure 6. Dependence of the eigenvalues of the perturbation matrix with respect to the impurity parameter α for a phonobreather with free/fixed ends boundary condition. (a) and (b) corresponds to the Morse potential and $\omega_b = 0.8$ while (c) to a hard ϕ^4 potential. (a) and (c) corresponds to a in-phase breather and (b) to a staggered one.

The inertia of the stability matrix is given by $\text{In}(Q^{F\pi}) = \{0, N - 1, 1\}$ and, in consequence, it has all its eigenvalues negative except for the null one. \square

Figure 6 shows the numerical values of the eigenvalues and confirms the results stated previously.

6.3. Phonobreathers with periodic boundary conditions

This subsection refers only to phonobreathers, as we have supposed that the multibreathers do not include the borders. Let us recall the results for homogenous systems [6]: For the in-phase pattern the eigenvalues of the perturbation matrix, except for a single zero, are all positive. For the out-of-phase pattern they are negative if the number of sites is even. If it is odd there appears an extra positive eigenvalue giving rise to the so-called parity instability.

Proposition 4 *The signs of the eigenvalues of the perturbation matrix for a*

phonobreather with an impurity and periodic boundary conditions are the same as with free ends boundary conditions, except for the out-of-phase pattern and an odd number of sites.

The diagonalization of Q is now very difficult. We will make use instead of a theorem due to Weyl [8] to obtain the inertia of the matrix. This theorem establishes that, if the eigenvalues of a matrix are arranged in the following order: $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_N$ then, the k -th eigenvalue of the sum of two matrices holds:

$$\lambda_k(A) + \lambda_1(B) \leq \lambda_k(A + B) \leq \lambda_k(A) + \lambda_N(B). \quad (28)$$

This theorem can be particularized for our case if we denote as Q^{P0} and $Q^{P\pi}$ to the periodic boundary conditions matrices and define $Q^P = Q^F + \Delta$, where Q^F is the perturbation matrix with free boundary conditions. By making $A \equiv Q^F$ and $B \equiv \Delta$ we can apply Weyl's theorem.

For an in-phase phonobreather,

$$Q_{nm}^{P0} = 2\delta_{n,m}[1 + (\eta\varphi - 1)\delta_{n,c} + (\eta/\varphi - 1)/2\delta_{|n-c|,1}] - (\delta_{n,1}\delta_{m,N} + \delta_{n,N}\delta_{m,1}) - \delta_{n,m+1}[1 - (\eta + 1)(\delta_{n,c} + \delta_{n,c+1})] - \delta_{n,m-1}[1 - (\eta + 1)(\delta_{n,c} + \delta_{n,c-1})], \quad (29)$$

and, in consequence,

$$\Delta_{n,m} = \delta_{n,m}(\delta_{n,1} + \delta_{n,N}) - (\delta_{n,1}\delta_{m,N} + \delta_{n,N}\delta_{m,1}). \quad (30)$$

The spectrum of Δ is given by $\text{spec}(\Delta) = \{0, 2\}$ where $\lambda_1(\Delta) = 0$ has multiplicity $N - 1$ and $\lambda_N(\Delta) = 2$ has multiplicity 1. Thus, particularizing Eq. (28) for $k = 1$:

$$\lambda_1(Q^{F0}) + \lambda_1(\Delta) \leq \lambda_1(Q^{P0}) \leq \lambda_1(Q^{F0}) + \lambda_N(\Delta). \quad (31)$$

As $\lambda_1(Q^{F0}) = 0$, then $\lambda_1(Q^{P0}) \in [0, 2]$. If $k = 2$ is taken in Eq. (28), $\lambda_2(Q^{P0}) \geq \lambda_2(Q^{F0}) + \lambda_1(\Delta)$. As $\lambda_2(Q^{F0}) > 0$ then $\lambda_2(Q^{P0}) > 0$. In consequence, Q^{P0} has $N - 1$ positive eigenvalues and one which is equal to zero.

The steps for an out-of-phase multibreather are similar to the in-phase case when N is even. In this case Δ changes to $-\gamma_0\Delta$ and its eigenvalues are a zero one with multiplicity $N - 1$ and $-2\gamma_0$. Taking $k = N$ and $k = N - 1$ in Eq. (28) it is straightforward to show that $Q^{P\pi}$ has all its eigenvalues negative except for one of them which is equal to zero. \square .

Figure 7 shows the numerical values of the eigenvalues and confirms the previously stated results.

Let us remark that for N odd there appear, in a similar fashion to the homogeneous case, parity instabilities due to the breaking of the breather pattern. Figure 8 shows the dependence of the eigenvalues of Q with respect to α in this case. It can be observed the existence of a positive eigenvalue of constant value which corresponds to an eigenvector localized at the boundaries of the lattice. It was demonstrated in Ref. [10] that in a homogeneous lattice, this eigenvalue is $4\gamma_0/3$ in an infinite lattice. This value does not change when an impurity far from the boundaries is introduced as the instability is caused by a border effect.

6.4. Inhomogeneity at the coupling constant

In this case, the perturbation matrix is equivalent to the one corresponding to an inhomogeneity implemented at the on-site potential with the changes $\varphi = 1$ and $\eta = \gamma = 1 + \beta/2$. In consequence, the results are qualitatively the same in both cases.

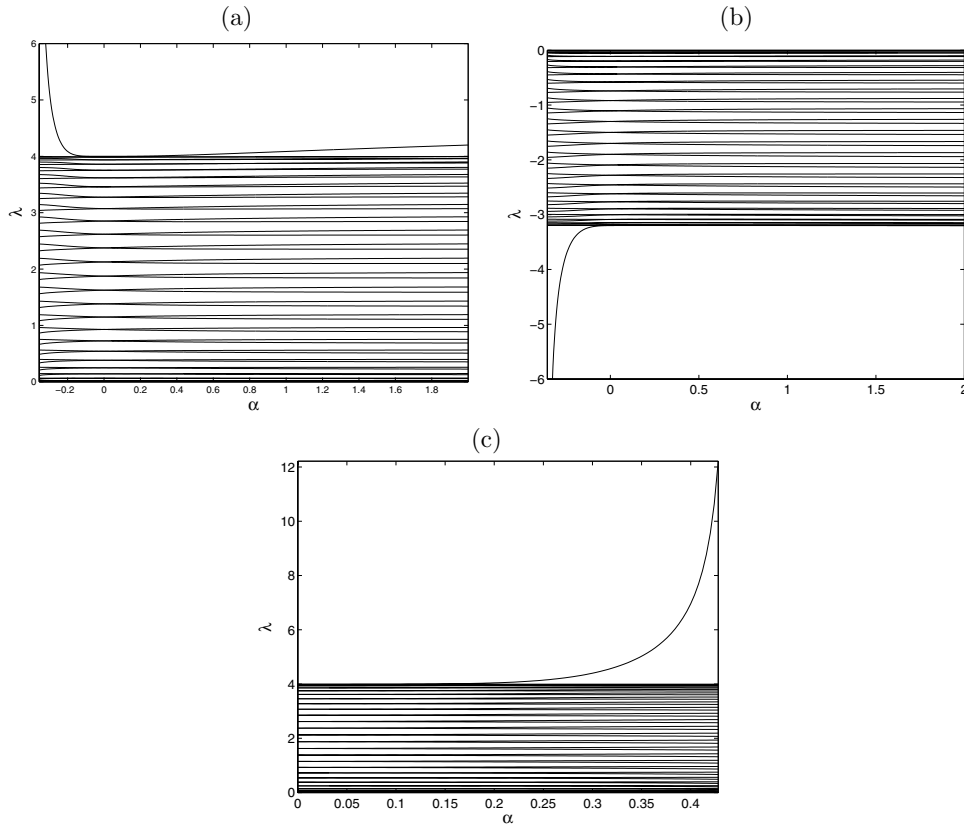


Figure 7. Dependence of the eigenvalues of the perturbation matrix with respect to the impurity parameter α for a phonobreather with periodic boundary condition. (a) and (b) corresponds to Morse potential and $\omega_b = 0.8$ while (c) to a hard ϕ^4 potential. (a) and (c) corresponds to a in-phase breather and (b) to a staggered one.

6.5. Summary of the stability properties for multibreathers and phonobreathers

We can summarize all the results in this section in the following theorem:

Theorem 1 *Time-reversible multibreathers not including the borders of the system and phonobreathers, in Klein-Gordon systems with harmonic, next-neighbour coupling, with or without and impurity, are stable if they have in-phase code, attractive (negative) coupling, and hard (soft) on-site potential. With the out-of-phase pattern, they are stable with attractive (negative) coupling and soft (hard) on-site potential, except for phonobreathers in a system with an odd number of sites, where parity instabilities appear. Any other pattern is always unstable.*

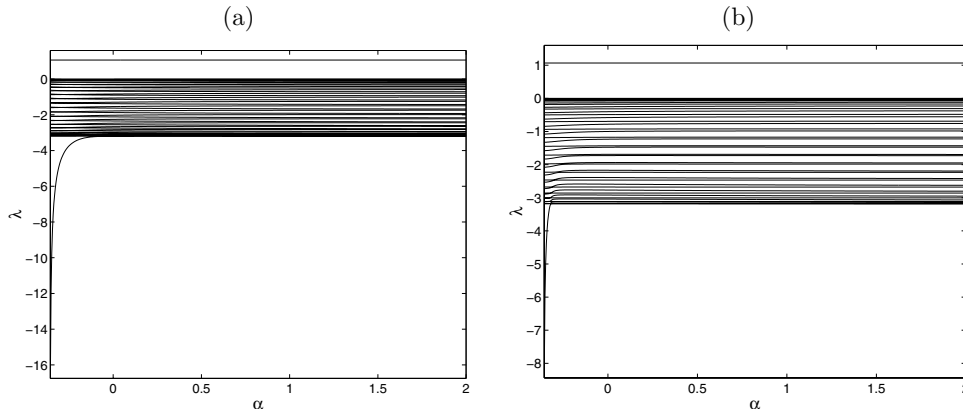


Figure 8. Dependence of the eigenvalues of the perturbation matrix with respect to the impurity parameter α for a Morse potential and $\omega_b = 0.8$ in the case of staggered (a) phonobreathers and (b) dark breathers with periodic boundary conditions. The existence of an isolated positive eigenvalue $\lambda = 4\gamma_0/3 \approx 1.07$ is observed.

7. Dark breathers with an impurity

A particular case of multibreathers in which all the particles of the lattice are excited except for one is called a dark breather [11, 12]. In the case that there are p adjacent sites with no vibration, we deal with a p -site dark breather. As the oscillators at rest at the anti-continuous limit do not appear in the perturbation matrix, the stability properties of p -site dark breathers are the same as for 1-site dark breathers. For simplicity we refer only to the latter.

It is worth noticing that if the impurity is located at the dark site, the perturbation matrix turns into the homogeneous case one. If it is located at another site not adjacent to the dark site, the demonstrations for multibreathers hold and the signs of the Q -eigenvalues are also the same as for the homogenous systems. In consequence, the only possible way for a change in the stability properties is to suppose that the impurity is adjacent to the dark site.

Proposition 5 *The eigenvalues of the perturbation matrix for 1-site dark breathers with an impurity and in-phase pattern are positive, except for a double zero for free ends or fixed boundary conditions and a single one for periodic conditions.*

For the out-of-phase pattern and an even number of sites, the eigenvalues are negative except for the zero ones. If the number of sites is odd there is also a positive eigenvalue, corresponding to a parity instability. Again, the stability is given by Eq. (9).

For an in-phase breather, the perturbation matrix is given by (notice that the $c + 1$ row and column are removed):

$$Q_{nm}^{D0} = 2\delta_{n,m}[1 + (\eta\varphi - 1)\delta_{n,c} + (\eta/\varphi - 1)/2\delta_{n,c-1} + (b - 1)(\delta_{n,1} + \delta_{n,N})/2] - \delta_{n,m+1}[1 - (\eta + 1)\delta_{n,c-1}] - \delta_{n,m-1}[1 - (\eta + 1)\delta_{n,c-1}] - b(\delta_{1,N} + \delta_{1,N}), \quad (32)$$

where $b = 0$ for fixed/free ends and $b = 1$ for periodic boundary conditions. If $b = 0$ the perturbation matrix is block diagonal, being the lower block the matrix of

a phonobreather with fixed/free ends boundary conditions and $N - (c + 1)$ particles. The upper block is a matrix Q_1 with positive eigenvalues except for a null one. In consequence, the inertia of the perturbation matrix for $b = 0$ is $\{N - 2, 0, 2\}$. The existence of two zero eigenvalues makes it impossible to determine the stability through the theorem as, to first order of the perturbation, the degeneration is not raised. This result was also obtained in the homogeneous case.

For $b = 1$, i.e. periodic boundary conditions, the perturbation matrix can be transformed into Q_1 through row/columns interchange. This transformation lets the characteristic polynomial invariant. In consequence, the matrix has $N - 1$ positive eigenvalues and a null one.

The perturbation matrix of a staggered dark breather is

$$\begin{aligned} Q_{nm}^{D\pi} = & -2\gamma_0\delta_{n,m}[1 + (\gamma\varphi - 1)\delta_{n,c} + (\gamma/\varphi - 1)/2\delta_{n,c-1} + (b - 1)(\delta_{n,1} + \delta_{n,N})/2] - \\ & - \gamma_0\delta_{n,m+1}[1 - (\gamma/\gamma_0 + 1)\delta_{n,c-1}] \\ & - \gamma_0\delta_{n,m-1}[1 - (\gamma/g_0 + 1)\delta_{n,c-1}] - b\gamma_0(\delta_{1,N} + \delta_{1,N}). \end{aligned} \quad (33)$$

It can be shown straightforwardly that $\text{In}(Q^{D\pi}(b = 0)) = \{0, N - 2, 2\}$ and $\text{In}(Q^{D\pi}(b = 1)) = \{0, N - 1, 1\}$. In the case of N odd and $b = 1$, parity instabilities also occur (see Figure 8). \square

If the impurity is modelled at the coupling, the transformations described in subsection 6.4 are also valid and the results do not change qualitatively.

Figure 9 shows the eigenvalues for a dark breather with periodic boundary conditions.

We can summarize the results in this section in the following theorem:

Theorem 2 *Time reversible, one-site dark breathers in Klein-Gordon systems with harmonic, next-neighbour coupling, with or without and impurity, in a lattice with periodic boundary conditions, are stable if they have in-phase code, attractive (negative) coupling, and hard (soft) on-site potential. With the out-of-phase pattern, they are stable with attractive (negative) coupling and soft (hard) on-site potential, except for a system with an odd number of sites, where parity instabilities appear. With fixed or free ends the stability is undefined.*

8. Conclusions

The *Multibreathers Stability Theorem* [6] provides a method for obtaining the perturbation matrix Q from the anti-continuous limit of any multibreather at low coupling in Klein-Gordon systems. The stability depends on the signs of the eigenvalues of the perturbation matrix Q , the hardness/softness of the on-site potential and the sign of the coupling parameter (i.e., the attractiveness or repulsiveness of the coupling), according to Eq. (9).

In this paper we apply the MST to systems with an impurity either at the on-site potential or the coupling constants, the first case being equivalent to an impurity at the masses. Using analytical methods we have been able to obtain explicitly the eigenvalues of Q for 2-site and 3-site breathers and compare them with numerical results showing an excellent agreement. For larger multibreathers, phonobreathers and dark breathers we have obtained analytically the signs of the Q -eigenvalues and checked them numerically. In all cases, although the values of the eigenvalues change, the stability properties of the system with an impurity coincides with the ones of the homogeneous system, a fact which was not at all evident. The necessity of either

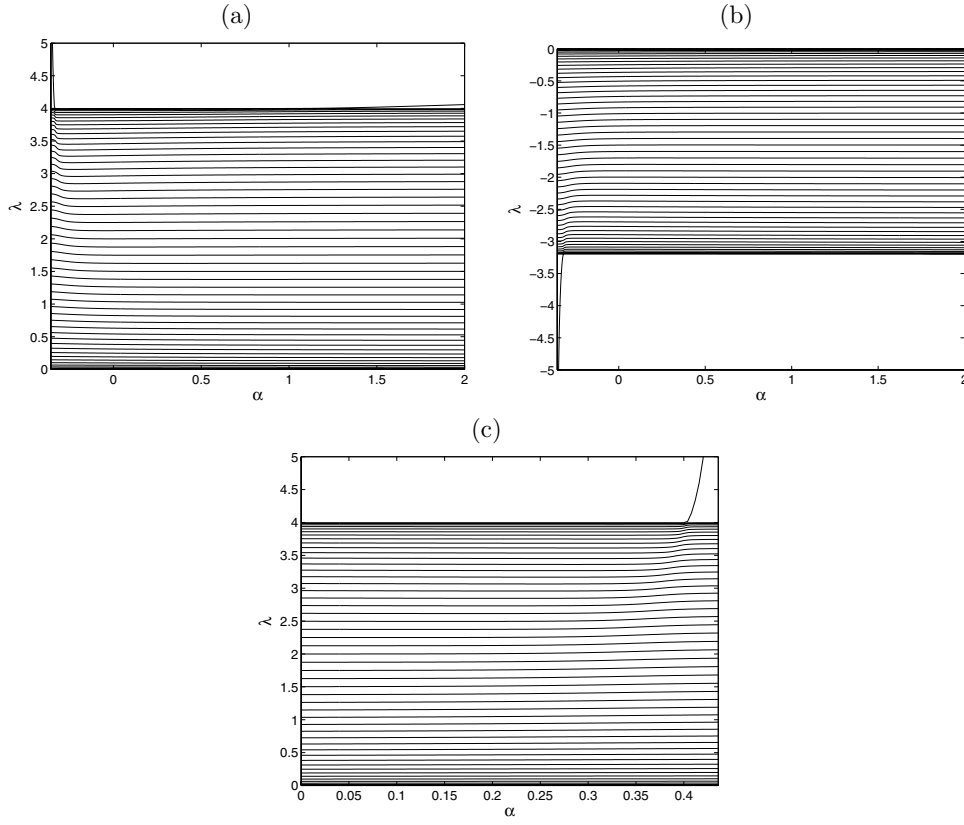


Figure 9. Dependence of the eigenvalues of the perturbation matrix with respect to the impurity parameter α for a dark breather with free/fixed ends boundary condition. (a) and (b) corresponds to Morse potential and $\omega_b = 0.8$ while (c) to a hard ϕ^4 potential. (a) and (c) corresponds to a in-phase breather and (b) to a staggered one.

an in-phase pattern or an out-of-phase one for the stability of a multibreather in the homogenous system, which was conjectured in Ref. [6], has also been demonstrated. Finally, the main results have been summarized in two theorems.

Further applications of the MST are being considered. They consist, among others, in the study of disordered and diatomic lattices, non-time reversible solutions and bistable systems.

Appendix A. Analytical calculation of parameters

The aim of this appendix is to calculate analytically the parameters η_{nm} , γ_{nm} , φ_{nm} defined in Section 3 as:

$$\eta_{nm} = \frac{J_{nm}}{\sqrt{J_{nn}J_{mm}}} > 0, \quad \gamma_{nm} = -\frac{J'_{nm}}{\sqrt{J_{nn}J_{mm}}} > 0, \quad \varphi_{nm} = \sqrt{\frac{J_{mm}}{J_{nn}}} > 0, \quad (\text{A.1})$$

with

$$J_{nm} = \int_{-T/2}^{T/2} \dot{u}_n(t) \dot{u}_m(t) dt, \quad J'_{nm} = \int_{-T/2}^{T/2} \dot{u}_n(t) \dot{u}_m(t + T/2) dt. \quad (\text{A.2})$$

Direct evaluation of these integrals is rather difficult. In order to overcome this difficulty, solutions $u_n(t)$ are expressed as a Fourier series expansion:

$$u_n(t) = z_{0,n} + 2 \sum_{k=1}^{\infty} z_{k,n} \cos(k\omega_b t), \quad (\text{A.3})$$

and the integrals turn into series:

$$J_{nm} = 4\pi\omega_b \sum_{k=1}^{\infty} k^2 z_{k,n} z_{k,m}, \quad J'_{nm} = 4\pi\omega_b \sum_{k=1}^{\infty} (-1)^k k^2 z_{k,n} z_{k,m}. \quad (\text{A.4})$$

In consequence, the theorem parameters can be expressed as a function of the Fourier coefficients of the solution. In the case of the Morse potential, the sum can be performed and a closed expression is obtained.

Appendix A.1. Morse potential

The Morse potential has the expression $V(u_n) = (1 + \alpha_n)\omega_o^2(\exp(-u_n) - 1)^2/2$, and the orbits of the equation $\ddot{u}_n + V'(u_n) = 0$ are given by [6]:

$$u_n(t) = \log \frac{1 \mp \sqrt{1 - (\omega_b/\omega_n)^2} \cos \omega_b t}{(\omega_b/\omega_n)^2}, \quad (\text{A.5})$$

The minus sign corresponds to $u_n(0) > 0$ and the plus sign to $u_n(0) < 0$ with $\omega_n = \sqrt{1 + \alpha_n}\omega_o$. The Fourier coefficients are:

$$z_{0,n} = \log \frac{\omega_n + \omega_b}{2\omega_b^2} \quad ; \quad z_{k,n} = -\frac{\rho_k}{k} \left(\frac{\omega_n - \omega_b}{\omega_n + \omega_b} \right)^{k/2}, \quad (\text{A.6})$$

with $\rho_k = (-1)^{k+1}$ if $u_n(0) > 0$ and $\rho_k = -1$ if $u_n(0) < 0$. Thus,

$$J_{nm} = 4\pi\omega_b \sum_{k=1}^{\infty} \left[\frac{(\omega_n - \omega_b)(\omega_m - \omega_b)}{(\omega_n + \omega_b)(\omega_m + \omega_b)} \right]^{k/2}, \quad (\text{A.7})$$

$$J'_{nm} = 4\pi\omega_b \sum_{k=1}^{\infty} \left[-\frac{(\omega_n - \omega_b)(\omega_m - \omega_b)}{(\omega_n + \omega_b)(\omega_m + \omega_b)} \right]^{k/2}. \quad (\text{A.8})$$

The sums are geometric series whose ratios have absolute values smaller than one. In consequence, they can be easily summed and the resulting values of J and J' are:

$$J_{nm} = 4\pi\omega_b \frac{\sqrt{(\omega_n - \omega_b)(\omega_m - \omega_b)}}{\sqrt{(\omega_n + \omega_b)(\omega_m + \omega_b)} - \sqrt{(\omega_n - \omega_b)(\omega_m - \omega_b)}}, \quad (\text{A.9})$$

$$J'_{nm} = 4\pi\omega_b \frac{\sqrt{(\omega_n - \omega_b)(\omega_m - \omega_b)}}{\sqrt{(\omega_n + \omega_b)(\omega_m + \omega_b)} + \sqrt{(\omega_n - \omega_b)(\omega_m - \omega_b)}}. \quad (\text{A.10})$$

Then, applying equation (A.1), the theorem parameters are:

$$\eta_{nm} = \frac{2\omega_b}{\sqrt{(\omega_n + \omega_b)(\omega_m + \omega_b)} - \sqrt{(\omega_n - \omega_b)(\omega_m - \omega_b)}}, \quad (\text{A.11})$$

$$\gamma_{nm} = \frac{2\omega_b}{\sqrt{(\omega_n + \omega_b)(\omega_m + \omega_b)} + \sqrt{(\omega_n - \omega_b)(\omega_m - \omega_b)}}, \quad (\text{A.12})$$

$$\varphi_{nm} = \sqrt{\frac{\omega_m - \omega_b}{\omega_n - \omega_b}}. \quad (\text{A.13})$$

Appendix A.2. ϕ^4 potential

This potential is given by $V(u_n) = (1 + \alpha_n)\omega_0^2 u_n^2/2 - s u_n^4/4$, with $s = \pm 1$. The sign of s allows us to define two different cases:

Appendix A.2.1. Hard ϕ^4 potential. $s = +1$. The orbit of a hard oscillator is given by:

$$\begin{aligned} u_n(t) &= \pm \omega_n \sqrt{\frac{2\kappa_n^2}{1-2\kappa_n^2}} \operatorname{cn}\left(\frac{\omega_n t}{\sqrt{1-2\kappa_n^2}}, \kappa_n\right) \\ &= \pm \omega_n \sqrt{\frac{2\kappa_n^2}{1-2\kappa_n^2}} \operatorname{cn}\left(\frac{2K(\kappa_n)}{\pi} \omega_b t, \kappa_n\right), \end{aligned} \quad (\text{A.14})$$

where cn is a Jacobi elliptic function of modulus κ_n and $K(\kappa_n)$ is the complete elliptic integral of the first kind defined as:

$$K(\kappa) = \int_0^{\pi/2} \frac{dx}{\sqrt{1 - \kappa^2 \sin^2 x}}. \quad (\text{A.15})$$

The breather frequency ω_b is related to the modulus κ_n through:

$$\omega_b = \frac{\pi \omega_n}{2\sqrt{1-2\kappa_n^2} K(\kappa_n)}. \quad (\text{A.16})$$

The elliptic function can be expanded into a Fourier series and it is obtained [13]:

$$z_{2\nu+1,n} = \pm \frac{\pi}{K(\kappa_n)} \sqrt{\frac{2}{1-2\kappa_n^2}} \frac{q_n^{\nu+1/2}}{1+q_n^{2\nu+1}}, \quad \nu = 0, 1, 2, \dots \quad (\text{A.17})$$

q_n is the Nome and is defined as

$$q_n = \exp(-\pi K(\sqrt{1-\kappa_n^2})/K(\kappa_n)). \quad (\text{A.18})$$

Thus, J_{nm} is given by (note that $J' = -J$ as the potential is even):

$$J_{nm} = \frac{8\pi^3 \omega_b}{K(\kappa_n)K(\kappa_m)} \sqrt{\frac{q_n q_m}{(1-2\kappa_n^2)(1-2\kappa_m^2)}} \sum_{\nu=0}^{\infty} \frac{(2\nu+1)^2 (q_n q_m)^\nu}{(1+q_n^{2\nu+1})(1+q_m^{2\nu+1})}, \quad (\text{A.19})$$

and, in consequence,

$$\eta_{nm} = \frac{\sum_{\nu=0}^{\infty} \frac{(2\nu+1)^2 (q_n q_m)^\nu}{(1+q_n^{2\nu+1})(1+q_m^{2\nu+1})}}{\sqrt{\sum_{\nu=0}^{\infty} \left(\frac{(2\nu+1)q_n^\nu}{1+q_n^{2\nu+1}}\right)^2} \sqrt{\sum_{\nu=0}^{\infty} \left(\frac{(2\nu+1)q_m^\nu}{1+q_m^{2\nu+1}}\right)^2}}, \quad (\text{A.20})$$

$$\varphi_{nm} = \frac{\omega_m K(\kappa_n)}{\omega_n K(\kappa_m)} \sqrt{\frac{(1-2\kappa_n^2) \sum_{\nu=0}^{\infty} \left(\frac{(2\nu+1)q_m^\nu}{1+q_m^{2\nu+1}}\right)^2}{(1-2\kappa_m^2) \sum_{\nu=0}^{\infty} \left(\frac{(2\nu+1)q_n^\nu}{1+q_n^{2\nu+1}}\right)^2}}. \quad (\text{A.21})$$

Appendix A.2.2. Soft ϕ^4 potential. $s = -1$. Now, the orbit of an oscillator is given by:

$$u_n(t) = \pm \omega_n \sqrt{\frac{2\kappa_n^2}{1+\kappa_n^2}} \operatorname{cd} \left(\frac{\omega_n t}{\sqrt{1+\kappa_n^2}}, \kappa_n \right) = \pm \omega_n \sqrt{\frac{2\kappa_n^2}{1+\kappa_n^2}} \operatorname{cd} \left(\frac{2K(\kappa_n)}{\pi} \omega_b t, \kappa_n \right), \quad (\text{A.22})$$

where cd is another elliptic function. Now, the breather frequency ω_b and the modulus κ_n are related through:

$$\omega_b = \frac{\pi \omega_n}{2\sqrt{1+\kappa_n^2} K(\kappa_n)}. \quad (\text{A.23})$$

Following Ref. [13], the Fourier coefficients can be obtained:

$$z_{2\nu+1,n} = \pm \frac{\pi}{K(\kappa_n)} \sqrt{\frac{2}{1+\kappa_n^2}} \frac{q_n^{\nu+1/2}}{1-q_n^{2\nu+1}}, \quad (\text{A.24})$$

and, in consequence,

$$J_{nm} = \frac{8\pi^3 \omega_b}{K(\kappa_n) K(\kappa_m)} \sqrt{\frac{q_n q_m}{(1+\kappa_n^2)(1+\kappa_m^2)}} \sum_{\nu=0}^{\infty} \frac{(2\nu+1)^2 (q_n q_m)^\nu}{(1-q_n^{2\nu+1})(1-q_m^{2\nu+1})}, \quad (\text{A.25})$$

$$\eta_{nm} = \frac{\sum_{\nu=0}^{\infty} \frac{(2\nu+1)^2 (q_n q_m)^\nu}{(1-q_n^{2\nu+1})(1-q_m^{2\nu+1})}}{\sqrt{\sum_{\nu=0}^{\infty} \left(\frac{(2\nu+1)q_n^\nu}{1-q_n^{2\nu+1}} \right)^2} \sqrt{\sum_{\nu=0}^{\infty} \left(\frac{(2\nu+1)q_m^\nu}{1-q_m^{2\nu+1}} \right)^2}}, \quad (\text{A.26})$$

$$\varphi_{nm} = \frac{\omega_m K(\kappa_n)}{\omega_n K(\kappa_m)} \sqrt{\frac{(1+\kappa_n^2) \sum_{\nu=0}^{\infty} \left(\frac{(2\nu+1)q_m^\nu}{1-q_m^{2\nu+1}} \right)^2}{(1+\kappa_m^2) \sum_{\nu=0}^{\infty} \left(\frac{(2\nu+1)q_n^\nu}{1-q_n^{2\nu+1}} \right)^2}}. \quad (\text{A.27})$$

Acknowledgements

This work has been supported by the MCYT/FEDER under the project BMF2003-03015 / FISI. J Cuevas acknowledges an FPDI grant from ‘La Junta de Andalucía’.

- [1] RS MacKay and S Aubry. Proof of existence of breathers for time-reversible or Hamiltonian networks of weakly coupled oscillators. *Nonlinearity*, 7:1623, 1994.
- [2] S Aubry. Breathers in nonlinear lattices: Existence, linear stability and quantization. *Physica D*, 103:201, 1997.
- [3] JL Marín, S Aubry, and LM Floría. Intrinsic Localized Modes: Discrete breathers. Existence and linear stability. *Physica D*, 113:283, 1998.
- [4] RS MacKay and JA Sepulchre. Stability of discrete breathers. *Physica D*, 119:148, 1998.
- [5] JL Marín. *Intrinsic Localized Modes in nonlinear lattices*. PhD Thesis, University of Zaragoza (Spain), June 1997.
- [6] JFR Archilla, J Cuevas, B Sánchez-Rey, and A Álvarez. Demonstration of the stability or instability of multibreathers at low coupling. *Physica D*, 180:235, 2003.
- [7] J Cuevas, F Palmero, J F R Archilla, and F R Romero. Moving discrete breathers in a Klein-Gordon chain with an impurity. *J. Phys. A: Math. and Gen.*, 35:10519, 2002.
- [8] RA Horn and CR Johnson. *Matrix Analysis*. Cambridge University Press, 1985.

- [9] JJ Sylvester. A demonstration of the theorem that every homogeneous quadratic polynomial is reducible by real orthogonal substitutions to the form of a sum of positive and negative squares. *Phil. Mag.*, IV:138, 1852.
- [10] J Cuevas. *Localization and energy transfer in anharmonic inhomogeneous lattices*. PhD Dissertation, Physics Faculty, University of Sevilla (Spain), 2003.
- [11] A Álvarez, JFR Archilla, J Cuevas, and FR Romero. Dark breathers in Klein-Gordon lattices. Band analysis of their stability properties. *New Journal of Physics*, 4:72, 2002.
- [12] AM Morgante, M Johansson, G Kopidakis, and S Aubry. Standing waves instabilities in a chain of nonlinear coupled oscillators. *Physica D*, 162:53, 2002.
- [13] M Abramowitz and IA Stegun. *Handbook of mathematical functions*. Dover, New York, 1965.