

Stability of breathers in simple mechanical models for DNA

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2010 J. Phys.: Conf. Ser. 246 012039

(<http://iopscience.iop.org/1742-6596/246/1/012039>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 200.145.3.40

The article was downloaded on 18/07/2013 at 21:38

Please note that [terms and conditions apply](#).

Stability of breathers in simple mechanical models for DNA

G G Slade, E Drigo Filho and J R Ruggiero

UNESP – Universidade Estadual Paulista, Instituto de Biociências, Letras e Ciências Exatas, Departamento de Física, Rua Cristóvão Colombo 2265, 15054-000, São José do Rio Preto, Brazil.

Email: ggslade@hotmail.com

Abstract. This work studies through the Floquet theory the stability of breathers generated by the anti-continuous limit. We used the Peyrard-Bishop model for DNA and two kinds of non-linear potential: the Morse potential and a potential with a hump. The comparison of their stability was done in function of the coupling parameter. We also investigate the dynamic behaviour of the system in stable and unstable regions. Qualitatively, the dynamic of mobile breathers resembles DNA.

1. Introduction

The DNA molecule contains genetic information and is responsible for the transmission of hereditary information [1]. The discovery of the double helix structure [2] is considered a landmark for the development of molecular biology. However studies in the last four decades have been revealing that the DNA dynamic is complex and essential for its function. The base pairs hold the genetic information and they stay “hidden” in the helix interior. The sequences that codify the proteins must be read. This requires the display of the bases to the solution, necessitating movements of great amplitude. This implies a nonlinear dynamic.

Experiments with proton exchanges [3,4] show that the macromolecule presents fluctuations highly localized with the possibility of opening even a single base pair. They are also very dynamic because the lifetime of a base pair (the average time that the base pairs remains closed) is estimated in milliseconds. This data indicates that the DNA dynamic, in particular the study of vibrational modes that are localized in a few base pairs, is important for the comprehension of these aspects.

In nonlinear systems, breathers are solutions that are both spatially localized and time periodic [5,6]. This kind of solution is generated by the combination of two factors: the discreteness and the nonlinearity of the system [7]. 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 [8] proved the existence of breathers in the one dimensional lattice when the system is composed by weakly coupled nonlinear oscillators. 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 this paper, we study the stability and dynamic of breathers in a simple mechanical model for DNA. The model used reduces the problem to the one-dimensional harmonic lattice with an additional non-linear potential on site, which simulates the H bond in DNA. Two kinds of non-linear potential were used: the original Morse potential and a potential with a hump. The anti-continuous limit was used to generate the breather in the lattices and the Floquet theory permits the study of its stability.

The Floquet multipliers and the energetic dynamics of the system are used to analyze the results. Tests for different frequencies of the breather and coupling constants are done in order to determine the range of stability for the breathers; these parameters are intrinsically related to the system's energy.

2. The Peyrard-Bishop (PB) model

There are several models to describe the DNA molecule [9]. Here we are interested in the localized energy structures that are provided by large amplitude movements, so we need a model whose main characteristic is to describe the base pairs separation of the nucleotides. The Peyrard-Bishop (PB) model [10] fills, in a minimalistic view, these conditions. In this model, a harmonic chain simulates each ribbon of DNA macromolecule and the interaction between them is simulated by a nonlinear potential. The three dimensional aspects of the helical structure are not considered and the motion analyzed is perpendicular to the ribbon. The positions of the nucleotides are denoted by u_j and v_j , respectively; with $j = 1, \dots, N$. For simplicity, it is assumed that the chains are homogeneous, i.e., the masses and the elastic coupling constants are the same.

The Lagrangian of the PB model for a homogeneous chain is given by:

$$L_{PB} = \sum_{j=1}^N \left\{ \frac{m}{2} (\dot{u}_j^2 + \dot{v}_j^2) - \frac{k}{2} (u_{j+1} - u_j)^2 - \frac{k}{2} (v_{j+1} - v_j)^2 - V(u_j - v_j) \right\}. \quad (1)$$

By changing the variables to $x_j = \frac{(u_j + v_j)}{\sqrt{2}}$ and $y_j = \frac{(u_j - v_j)}{\sqrt{2}}$ it is possible to rewrite the Lagrangian as the sum of two terms, each one depending only on one coordinate, x or y . The part of the Lagrangian depending on x represents a chain of harmonic oscillators and is unimportant here. The term depending on y is written as

$$L_y = \sum_{j=1}^N \left\{ \frac{m}{2} \dot{y}_j^2 - \frac{k}{2} (y_{j+1} - y_j)^2 - V(\sqrt{2}y_j) \right\}, \quad (2)$$

and represents a chain of harmonic oscillators with an additional potential on site.

The equations of motion obtained from Lagrangian (2) are:

$$m\ddot{y}_j + k(2y_j - y_{j+1} - y_{j-1}) + V'(\sqrt{2}y_j) = 0, \text{ with } j = 1, 2, \dots, N. \quad (3)$$

For the numerical calculation we used the periodic boundary conditions, that is, $y_0 = y_N$ and $y_{N+1} = y_1$.

3. Prescription to create the breather

The breather can be created using the principle of the anti-continuous limit suggested by MacKay and Aubry [8] and implemented by Marin and Aubry [11] and Cuevas [12]. So in 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 potential on site.

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

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

where ω_b is the breather frequency. Thus, the equations 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 , δk . The next step is to find the numerical solution for $k = \delta k$ by using the Newton method and the original profile obtained for $k = 0$. This new solution will be used like a seed for the case $k = 2\delta k$ and so on until we reach the desired value of k .

4. Breather stability

An important question concerning the breather is its stability. Using $y_j(t)$ as a periodic solution of (3) and introducing a perturbation, $\varsigma_j(t)$, it is possible to construct a perturbed solution as $\psi_j(t) =$

$y_j(t) + \zeta_j(t)$. Considering that $\psi_j(t)$ is a solution of the system and by expanding the equations of motion (3) near the solution $y_j(t)$, we find:

$$\ddot{\zeta}_j(t) + k(2\zeta_j(t) - \zeta_{j+1}(t) - \zeta_{j-1}(t)) + V''(\sqrt{2}y_j)\zeta_j(t) = 0, \quad (5)$$

which is a linear equation for the perturbation $\zeta_j(t)$ (Hill's Equation).

The equations (5) can be written like a system of equations by the definition:

$$\pi_j(t) = \dot{\zeta}_j(t) \quad (6)$$

$$\dot{\pi}_j(t) = -k(2\zeta_j(t) - \zeta_{j+1}(t) - \zeta_{j-1}(t)) - V''(\sqrt{2}y_j)\zeta_j(t), \quad (7)$$

or, in a matricial notation: $\Omega(t) = [\zeta(t) \pi(t)]^T$, where $\zeta(t) \equiv \{\zeta_j(t)\}$ and $\pi(t) \equiv \{\pi_j(t)\}$. In the matricial form, $\Omega(t)$ is a column vector with $2N$ dimensions and N is the number of degrees of freedom of the system. In this notation the information contained in the equation (5) can be summarized as:

$$\dot{\Omega}(t) = A(t)\Omega(t), \quad (8)$$

where $A(t) = \begin{bmatrix} 0 & I \\ J & 0 \end{bmatrix}$. Each element of $A(t)$ is a matrix $N \times N$, I is an identity matrix and J has the elements $J_{i,j} = -(2k + V''(\sqrt{2}y_j))\delta_{i,j} + k(\delta_{i+1,j} + \delta_{i-1,j})$ with $\delta_{i,j}$ as the delta of Kronecker. Periodic boundary conditions impose that for $i = 1$ we have $\delta_{i-1,j} = \delta_{N,j}$ and for $i = N$ we have $\delta_{i+1,j} = \delta_{1,j}$.

Since we are working with periodic equations, the system stability can be analyzed using the Floquet theory [13]. In this way, one can consider the matrix $2N \times 2N$ $\phi(t)$, where each column represents a linearly independent solution of the system (8) corresponding to the different initial conditions. Thus, $\phi(t)$ is definite in $t = 0$ as a vector with $2N - 1$ components equal to zero, and with the component in the i th position ($i = 1, 2, \dots, 2N$) equal to 1. This matrix is known as the fundamental matrix and it satisfies the relation:

$$\dot{\phi}(t) = A(t)\phi(t). \quad (9)$$

Since $A(t)$ is a periodic matrix with period T , $\phi(t + T)$ must be a solution of (8) and each column of $\phi(t + T)$ can be written as a linear combination of $\phi(t)$, which means:

$$\phi(t + T) = \phi(t)M, \quad (10)$$

where M is a constant matrix. Since $\phi(0) = I$, we have that $\phi(T) = M$ and M is the monodromy matrix or Floquet operator, F .

The Floquet operator F determines the evolution of the system in a period T and it can be expressed by:

$$\Omega(T) = F\Omega(0). \quad (11)$$

For a system that obey a periodic potential, the Bloch theorem [5] guarantees eigenfunctions in the form of $\zeta(t) = e^{i\theta \frac{t}{T}} v(t)$, where $v(t)$ is a periodic function on time, with period T . These eigenfunctions correspond to eigenvalues of F in the form of $\lambda = e^{i\theta}$, ($\theta \in \mathbb{C}$). These eigenvalues are named Floquet multipliers and θ is named as the Floquet argument. The Floquet operator is real and symplectic, that is, its physical properties are invariant for time translation. It implies that if λ is an eigenvalue, then λ^* , $\frac{1}{\lambda}$ and $\frac{1}{\lambda^*}$ are eigenvalues too.

From the Floquet theory the orbit of $y(t)$ is linearly stable if none of the Floquet multipliers 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, θ 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.

A useful tool to study the stability is the Krein signature (κ), which is defined as the sign of the symplectic product of the real part with the imaginary part of the position-velocity vector [12]. By the

Krein criteria, for a collision between eigenvalues to generate instability, it is necessary that its Krein signature must be different.

$$\kappa(\theta) = \text{sgn}([\text{Re}\{\Omega(t)\}, \text{Im}\{\Omega(t)\}]) = \text{sgn}[i \sum_j (\zeta_j(t) \dot{\zeta}_j^*(t) - \zeta_j^*(t) \dot{\zeta}_j(t))]. \quad (12)$$

5. Results

The results reported below were obtained using chains with 21 oscillators ($N = 21$). The number of coefficients in the Fourier series was $lm = 17$. We have studied two different nonlinear potentials: the Morse potential and a potential with a hump. As stressed above, we have considered periodic boundary conditions. When the dynamical equations were explicitly integrated, the initial conditions were the breather profile taken with the method demonstrated in section 3, with velocities equal to zero.

The analysis were done using the Floquet multipliers and the time evolution of the energy distribution among the oscillators of the chain as a function of the coupling parameter and the frequency of the breather ω_b . These two factors determine the energy of the system calculated from the expression $E = \sum_{j=1}^N E_j$, where

$$E_j = \frac{m}{2} \dot{y}_j^2 + \frac{k}{4} (y_{j+1} - y_j)^2 + \frac{k}{4} (y_j - y_{j-1})^2 + V(\sqrt{2}y_j) \quad (13)$$

is the energy of each oscillator and the elastic interaction energy of each spring is equally distributed between the two adjacent oscillators.

5.1 Morse potential

Originally the potential used to describe the hydrogen bonds in the PB model was the Morse potential, given by:

$$V(y) = D(e^{-ay} - 1)^2, \quad (14)$$

where D is the depth of the potential well and represents the energy of dissociation, a has the dimension of inverse of length and is related to the width of the well, and y represents the displacement of the base pairs from equilibrium position ($y = 0$).

Using the Morse potential (14), the Lagrangian L_y (2) is written as:

$$L_y = \sum_{j=1}^N \left\{ \frac{m}{2} \dot{y}_j^2 - \frac{k}{2} (y_{j+1} - y_j)^2 - D[e^{-\sqrt{2}ay_j} - 1]^2 \right\}. \quad (15)$$

It is convenient for the analytic and computational development to let the equations be depend on smallest number of parameters. Using adimensional variables $\xi_j = a\sqrt{2}y_j$ and $\tau = 2 \left(\frac{Da^2}{m} \right)^{\frac{1}{2}} t$, it is possible to let the equation depend on just one parameter, C , and the Lagrangian can be expressed by

$$L = \sum_{j=1}^N \left\{ \frac{1}{2} \dot{\xi}_j^2 - \frac{1}{2} C (\xi_{j+1} - \xi_j)^2 - \frac{1}{2} (e^{-\xi_j} - 1)^2 \right\}, \quad (16)$$

where $\dot{\xi} = \frac{d\xi}{d\tau}$, $C = \frac{k}{4Da^2}$ and $L_y \equiv 2DL$.

In Figure 1 we present the results for the absolute value of the Floquet multipliers as a function of the coupling parameter C for four different values of frequencies: (a) $\omega_b = 0.6$, (b) $\omega_b = 0.7$, (c) $\omega_b = 0.8$ and (d) $\omega_b = 0.9$.

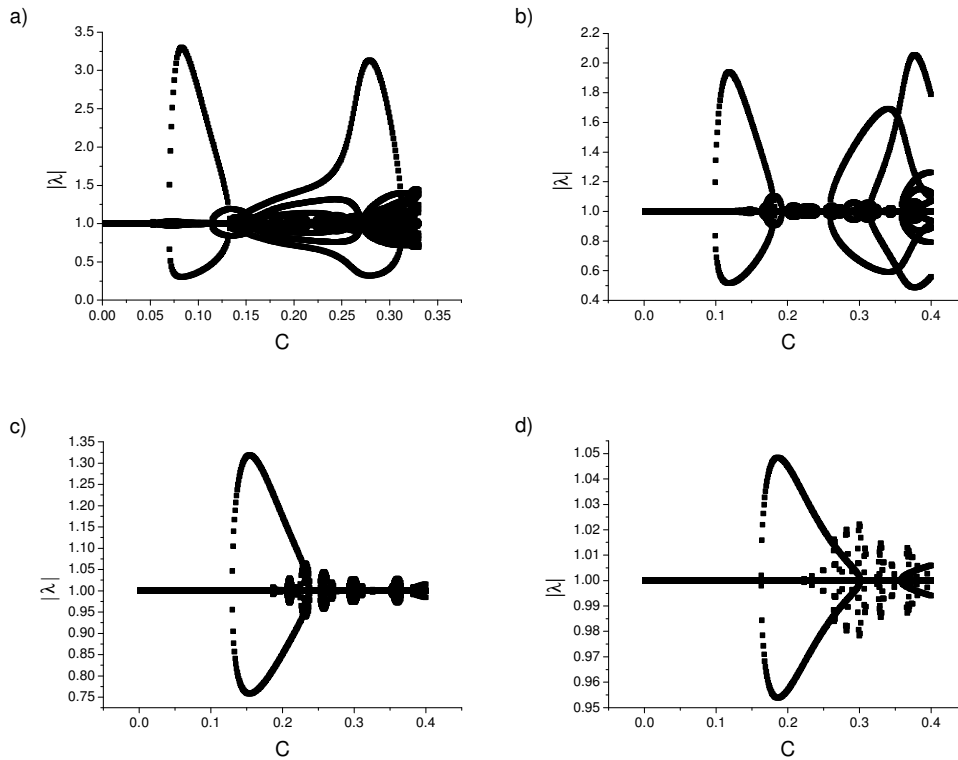


Figure 1. The absolute value of the Floquet multipliers in function of the coupling C for different frequencies of the breathers. (a) $\omega_b = 0.6$, (b) $\omega_b = 0.7$, (c) $\omega_b = 0.8$ and (d) $\omega_b = 0.9$.

A common feature in all cases is that for small values of the coupling parameter C there is not bifurcation and the stability is guaranteed. Interestingly, the range of value of C for which the system presents stability (absence of bifurcation) increases with the frequency of the breather. This behavior could be predicted since small values of C mean that the dynamics of the system are dominated by the non-linear effects. It is possible to demonstrate [12] that the adimensional energy for the system at $t = 0$ is given by $\sqrt{1 - \omega_b^2}$. Therefore, taken $\omega_b \rightarrow 1$ the energy is small and the dynamical behavior is less sensitive to the coupling parameter C . As the values of C increase beyond a threshold depending on ω_b a series of bifurcations happen, meaning that more than one pair of eigenvalues have absolute values greater than one. For some small intervals of values of C the stability is regained, for example, figure 1b around $C \sim 0.25$. For $\omega_b = 0.8$ and $\omega_b = 0.9$ there is stability in several ranges of values of C .

It is interesting to analyze the dynamical behavior of the system, solving explicitly the equations of motion. To do this we used a Runge-Kutta fourth order method [14] to integrate the equations and the profile of the breather in the initial excitation, choosing the velocities of all oscillators equal to zero. In the sequence of figures 2-4 we present the plots in the complex plane of the Floquet multipliers with the respective Krein signature and the time evolution of the energy of each oscillator (in gray pattern) for some values of the coupling parameter C and frequencies ω_b . In figure 2 is shown a typical situation where the system is stable ($C = 0.1$ with $\omega_b = 0.8$). The results show that all Floquet multipliers are in the unit circle (absolute value equal to one) and the energy remains practically in the

initially excited oscillator. In figure 3, on the other hand, we choose a couple of values for C and ω_b at the threshold of bifurcation (a harmonic one) shown in Figure 1c ($C = 0.13$ and $\omega_b = 0.8$). Here a pair of eigenvalues collided and left the unit circle with $\theta = 0$. The energy pattern, on the other hand, still shows the energy essentially localized in one oscillator but running on the chain. Eventually, in figure 4, we show a case where more than one pair of eigenvalues go out of the unit circle ($C = 0.23$ and $\omega_b = 0.8$). The Floquet analysis demonstrates the three kinds of bifurcation and as a result the energy spreads out the chain and the energy localization is lost.

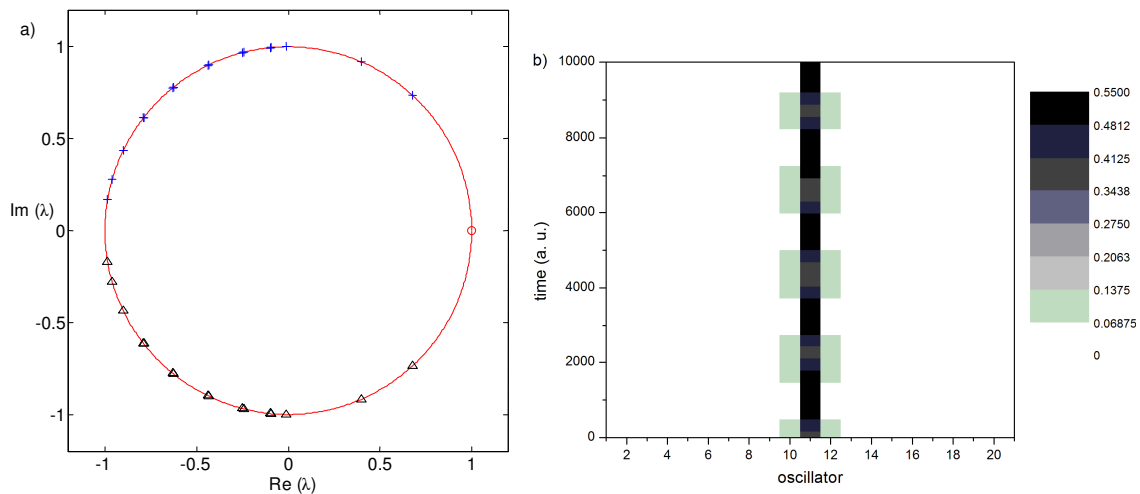


Figure 2. a) Representation of the Floquet multipliers with the respective Krein signature (+ symbol is used for $\kappa = +1$, while Δ is used for $\kappa = -1$ and O for $\kappa = 0$) and b) the energy of each oscillator in function of time. $C = 0.1$ and $\omega_b = 0.8$.

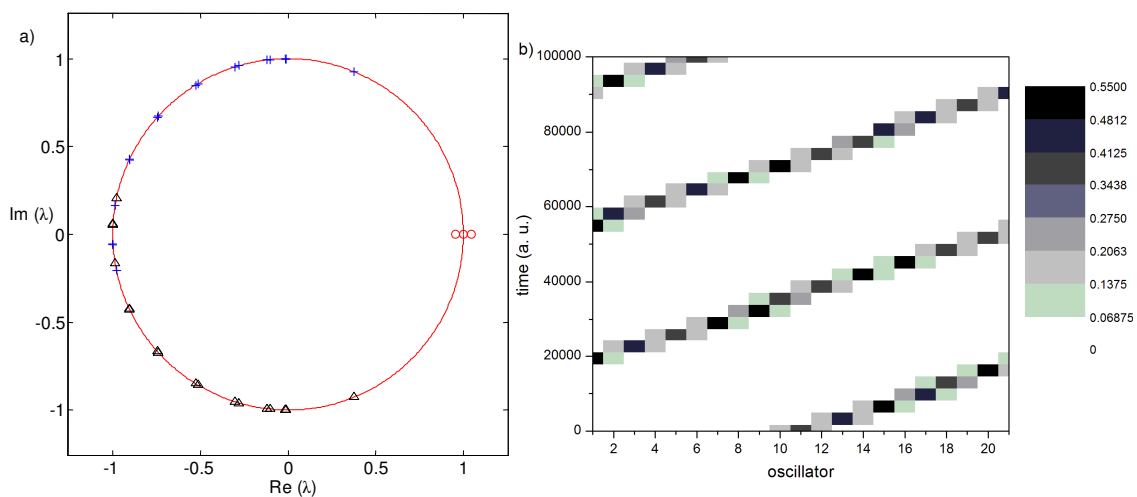


Figure 3. a) Representation of the Floquet multipliers with the respective Krein signature (same convention of figure 2) and b) the energy of each oscillator in function of time. $C = 0.13$ and $\omega_b = 0.8$.

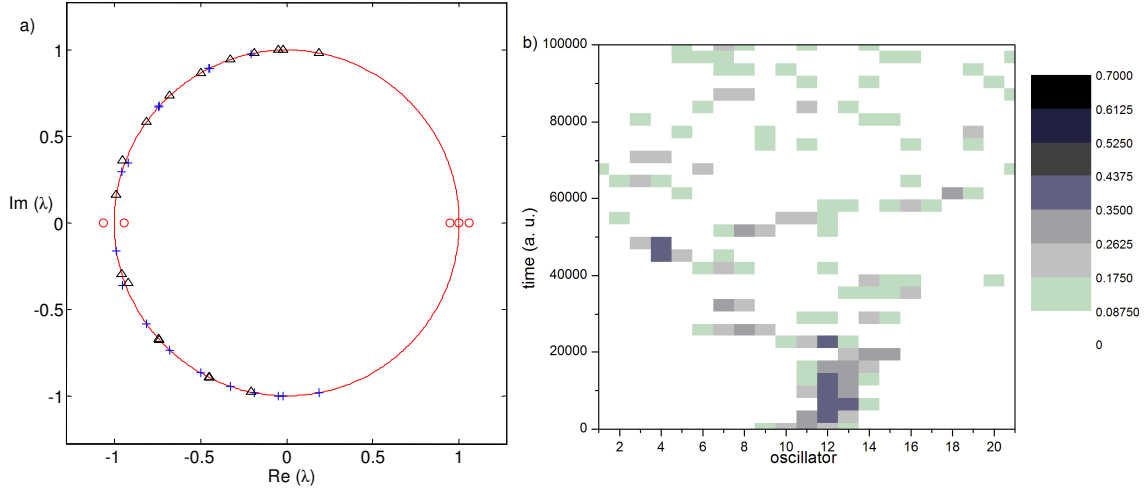


Figure 4. a) Representation of the Floquet multipliers with the respective Krein signature (same convention of figure 2) and b) the energy of each oscillator in function of time. $C = 0.23$ and $\omega_b = 0.8$.

5.2 Potential with a hump

A potential with a hump was introduced by Peyrard and co-workers [15,16], who were trying to establish conditions where the results for the opened and closed states were more compatible with the experimental observations. Essentially, they introduced a barrier of potential for y values around the distance that the hydrogen bonds can be considered broken. This resulted in an increase of time that they, once opened, stayed open. The potential was found by the intersection of the Morse potential ($y < 0$), of one quartic potential (around the origin) and one term that decays exponentially ($y > 1$).

This kind of potential is expressed by:

$$V_h(y) = \begin{cases} A[e^{-\alpha y} - 1]^2 & y < 0 \\ ay^2 + by^3 + cy^4 & 0 \leq y \leq 1 \\ D + Fe^{-\beta y} \left(y + \frac{1}{\beta}\right) & y > 1 \end{cases} \quad (17)$$

By replacing this potential in the lagrangian L_y and making the follow variable change, $\xi_j = \alpha\sqrt{2}y_j$ and $\tau = 2\left(\frac{A\alpha^2}{m}\right)^{\frac{1}{2}}t$, we find a similar equation to (16) expressed by:

$$L = \sum_{j=1}^N \left\{ \frac{1}{2} \dot{\xi}_j^2 - \frac{1}{2} C (\xi_{j+1} - \xi_j)^2 - \frac{1}{2} V_{hm} \left(\frac{\xi_j}{\alpha} \right) \right\}, \quad (18)$$

$$\text{where } \dot{\xi} = \frac{d\xi}{d\tau}, C = \frac{k}{4A\alpha^2}, L_y \equiv 2AL \text{ and } V_{hm} \left(\frac{\xi_j}{\alpha} \right) = \begin{cases} [e^{-\xi_j} - 1]^2 & \frac{\xi_j}{\alpha} < 0 \\ \frac{a\xi_j^2}{A\alpha^2} + \frac{b\xi_j^3}{A\alpha^3} + \frac{c\xi_j^4}{A\alpha^4} & 0 \leq \frac{\xi_j}{\alpha} \leq 1. \\ \frac{D}{A} + \frac{F}{A} e^{-\beta \frac{\xi_j}{\alpha}} \left(\frac{\xi_j}{\alpha} + \frac{1}{\beta} \right) & \frac{\xi_j}{\alpha} > 1 \end{cases}$$

As the potential function must be continuous, as soon as its first and second derivatives, the number of parameters is reduced to four: α , β , D and F . The other parameters are given by the expressions: $A = \frac{a}{\alpha^2}$, $a = 6D + \frac{1}{2}Fe^{-\beta} \left(\beta^2 + 5\beta + \frac{12}{\beta} + 12 \right)$, $b = -8D - Fe^{-\beta} \left(\beta^2 + 4\beta + \frac{8}{\beta} + 8 \right)$ and $c = 3D + \frac{1}{2}Fe^{-\beta} \left(\beta^2 + 3\beta + \frac{6}{\beta} + 6 \right)$.

The procedure to get the results using this potential required some changes. The number of terms used in the Fourier series increased to $lm = 21$, and in order to study the energetic dynamic of the system we used the Runge-Kutta Nystron of tenth order [17]. We used the same values for the

parameters as Peyrard et al [15,16], which were equivalent to: $\alpha = \beta = F = 4.0 \text{\AA}^{-1}$ and $D = 0.0857 \text{eV}$.

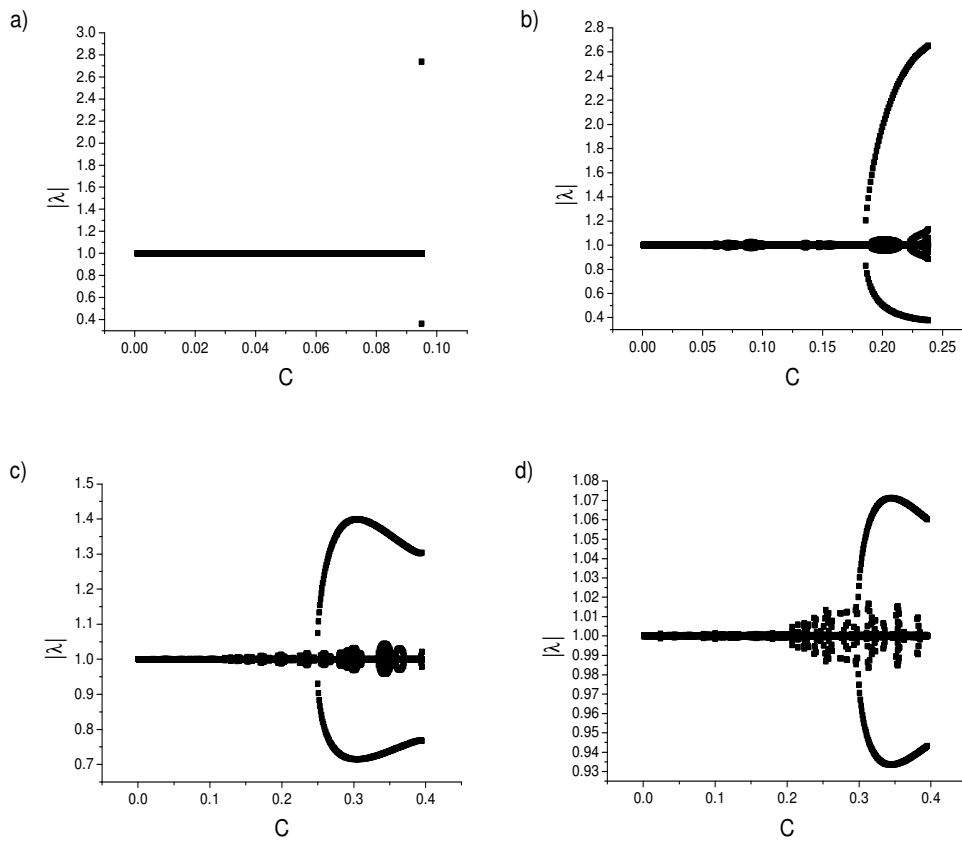


Figure 5. The absolute value of the Floquet multipliers in function of the coupling C for different frequencies of the breathers. (a) $\omega_b = 0.6$, (b) $\omega_b = 0.7$, (c) $\omega_b = 0.8$ and (d) $\omega_b = 0.9$.

In figure 5 it is shown the absolute value of the eigenvalues of the Floquet matrix as function of the coupling C , for four values of the breather frequency ω_b . Compared to the results obtained with the Morse potential the eigenvalues present greater regions of stability. However, in these regions exist some pairs of eigenvalues that have absolute values greater than 1 only by a few hundredths, and we decided to investigate their behavior. In figures 6-7 we show the plots in the complex plane of the Floquet multipliers with the respective Krein signature and the time evolution of the effective number of oscillators with significant energy n_{osc} , calculated from information entropy [18] and used as a criteria for energy localization [19,20].

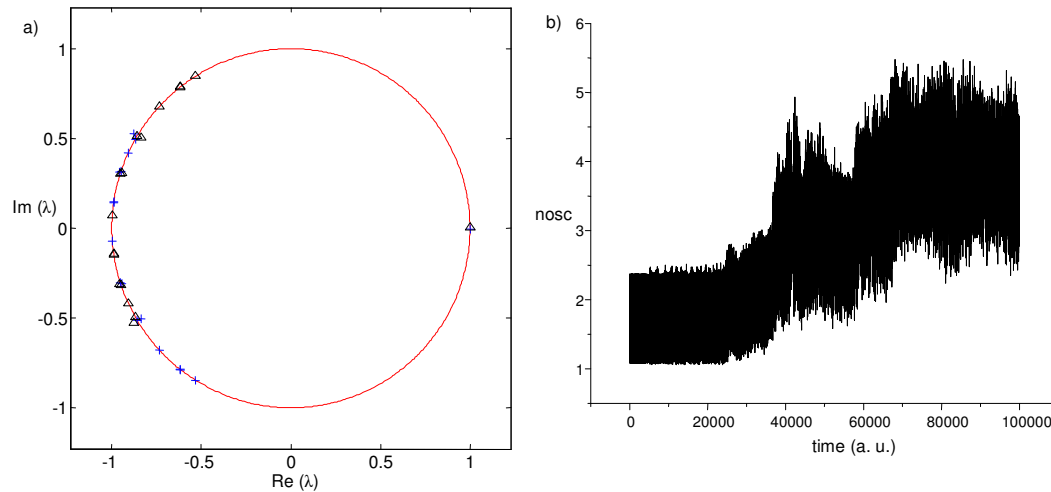


Figure 6. a) Representation of the Floquet multipliers with the respective Krein signature (same convention of figure 2) and b) the energy of each oscillator in function of time. $C = 0.09$ and $\omega_b = 0.7$.

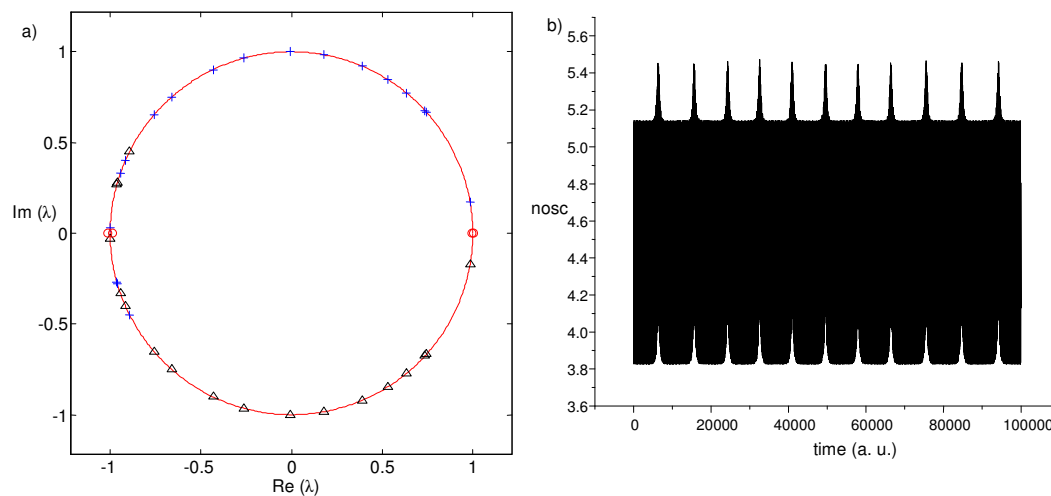


Figure 7. a) Representation of the Floquet multipliers with the respective Krein signature (same convention of figure 2) and b) the energy of each oscillator in function of time. $C = 0.255$ and $\omega_b = 0.9$.

In figure 6, the Floquet analysis shows an oscillatory bifurcation for $C = 0.09$ and $\omega_b = 0.7$. Looking at the dynamic behavior we note a gradual increase in the n_{osc} value passing from approximately 1.7 (average value) in the beginning to 3.5 by the end. In figure 7, we have a sub-harmonic bifurcation case, $C = 0.255$ and $\omega_b = 0.9$, and despite the curious periodic fluctuations in the n_{osc} values, their average value remains around 4.4. So the stability of the breather suffers the influence of these bifurcations although the energy remains localized in a small number of oscillators at least for the time interval considered.

6. Conclusion

In this paper we revisited the problem of 1-site breather formation in homogeneous nonlinear chains described by the Peyrard-Bishop model, using the numeric proceedings suggested by Marin and

Aubry. Two kinds of nonlinear potential were tested: the Morse potential and a potential with a hump. The stability analysis of these structures was done through the Floquet theory and is consistent for the Morse potential, with that found in the work of Cuevas [12].

The dynamic of stable solutions showed a localized structure where the energy is practically in one oscillator, as predicted by the theory. For instable regions, the dynamic suggests some characteristic behavior. When there is a harmonic bifurcation, the energy remains localized but it starts to walk through the chain. This case is known as a mobile breather. In the sub-harmonic bifurcation, the localized structure suffers some periodic changes that affect the effective number of oscillators with significant energy. In the oscillatory case, the energy starts to diffuse slowly through the chain, but remains localized for the time interval observed, that is relevant for the DNA dynamics. When the three bifurcations happen for one condition, their effects are joined and the energy spreads out the chain and the localized structure is completely lost.

The potential with a hump presents greater regions of stability. This fact should be related with the barrier existent in this potential, as it increases the confining region of the potential and this inhibits the loss of stability.

Qualitatively the behavior of the mobile breathers resembles that of the DNA, where a structure of localized energy walks through the chain. However, the values for the DNA amplitudes of movement and life time for open states are not equivalent to that found in our tests. So improvements in the model and the way to analyze the DNA dynamics should be made.

Acknowledgements

The authors are grateful to Capes and CNPq for financial support. The authors also are indebted to Ms. Kaylee Harrison for her assistance with the English of the manuscript.

References

- [1] Alberts B, Johnson A and Lewis J 2004 *Biologia Molecular da Célula* (Porto Alegre: ARTMED)
- [2] Watson G B and Crick F H 1953 *Nature* **171** 737-8
- [3] Englander S W, Kallenbach N R, Heeger A J, Krumhansl J A and Litwin A 1980 *Proc. Natl. Acad. Sci.* **77** 7222-6
- [4] Leroy J L, Kochoyan M, Huynh-Dinh T and Guéron M 1988 *J. Mol. Biol.* **200** 223-38
- [5] Aubry S 1997 *Physica D* **103** 201-50
- [6] Aubry S 2006 *Physica D* **216** 1-30
- [7] Flach S and Willis C R 1998 *Physics Reports* **295** 181-264
- [8] MacKay R and Aubry S 1994 *Nonlinearity* **7** 1623-43
- [9] Yakushevich L 1998 *Nonlinear Physics of DNA* (Chichester: Wiley series in nonlinear science) chapter 1 pp 1-19
- [10] Peyrard M, Bishop A R 1989 *Phys. Rev. Lett.* **62** 2755-8
- [11] Marin J L and Aubry S 1996 *Nonlinearity* **9** 1501-28
- [12] Cuevas J 2003 *Localización y Transferencia de Energía em Redes Anarmónicas No Homogéneas* Phd thesis Universidad de Sevilla
- [13] Hoppensteadt F C 2000 *Analysis and Simulation of Chaotic Systems* (New York: Springer) chapter 1 pp 1-24
- [14] Press W H, Teukolsky S A, Vetterling W T and Flannery B P 1992 *Numerical Recipes* (New York: Cambridge University Press)
- [15] Peyrard M, Cuesta-López S and Angelov D 2009 *J. Phys.: Condensed Matter* **21** 034103
- [16] Peyrard M, Cuesta-López s and James G 2008 *Nonlinearity* **21** T91-T100
- [17] Tsitouras C 1999 *Celest. Mech. Dyn. Astron.* **74** 223-30
- [18] De Luca J, Lichtenberg A J and Lieberman 1995 *Chaos* **5** 283-97
- [19] De Luca J, Drigo Filho E, Ponno A and Ruggiero J R 2004 *Phys. Rev. E* **70** 026213
- [20] Silva J M, Drigo Filho E and Ruggiero J R 2009 *Eur. Phys. J. E* **29** 245-51