Moving breathers in a DNA model with competing short and long range dispersive interactions

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Abstract

Moving breathers is a means of transmitting information in DNA. We study the existence and properties of moving breathers in a DNA model with short range interaction, due to the stacking of the base pairs, and long range interaction, due to the finite dipole moment of the bond within each base pair.

In our study, we have found that mobile breathers exist for a wide range of the parameter values, and the mobility of these breathers is hindered by the long range interaction. This fact is manifested by: (a) an increase of the effective mass of the breather with the dipole–dipole coupling parameter; (b) a poor quality of the movement when the dipole–dipole interaction increases; and (c) the existence of a threshold value of the dipole–dipole coupling above which the breather is not movable.

An analytical formula for the boundaries of the regions where breathers are movable is calculated. Concretely, for each value of the breather frequency, it can be obtained the maximum value of the dipole–dipole coupling parameter and the maximum and minimum values of the stacking coupling parameter where breathers are movable. Numerical simulations show that, although the necessary conditions for the mobility are fulfilled, breathers are not always movable.

Finally, the value of the dipole–dipole coupling constant is obtained through quantum chemical calculations. They show that the value of the coupling constant is small enough to allow a good mobility of breathers.

Key words: DNA, Discrete breathers, Mobile breathers, Intrinsic localized modes, Long range interaction
PACS: 63.20.Pw, 63.20.Ry, 66.90.+r, 87.10.+e

1 Introduction

Discrete breathers (DBs) are periodic localized oscillations that arise in discrete nonlinear systems. Their existence was proven by MacKay and Aubry [1], and ever since discrete breathers have been widely studied in systems with short range interactions (for a review, see, e.g., [2,3]). Energy and decay properties of DBs in systems with long range interactions have also been studied in the framework of the Klein–Gordon [4,5] and the Discrete Nonlinear Schrödinger equations [6].

These localized oscillations can be static, but, under certain conditions can move along the system. They are usually called *moving breathers* (MBs). In contrast to static breathers, which are exact numerical solutions, moving breathers cannot be obtained by continuation methods and there are no existence theorems for them. However, they have been obtained by simulation methods in models for systems like muskovite mica [7,8] and cuprate–like lattices [9], and there exist methods to obtain moving breathers systematically [10–12] which will be explained in section 5.2.

Among the systems that can be studied through discrete nonlinear models is DNA (for a review see, e.g. [13]). A phenomenon for which the study of discrete breathers can provide information is DNA denaturation. Peyrard and Bishop introduced a model for the study of this phenomenon in 1989 [14] and, later on, in 1992, Dauxois, Peyrard and Willis suggested that breathers could appear in DNA models [15]. Afterwards, numerical simulations performed by Dauxois, Peyrard and Bishop suggested that localized oscillations can be precursors of the bubbles that appear in thermal denaturation of DNA [16–18]. Moving breathers can be a means of transmitting information along the double strand. The transmission must exist due to the fact that the promoter and the transcription regions are situated hundreds or thousands of base pairs apart. Also, experiments in irradiated DNA suggest that a localized entity travels from the primary breaks hit by the radiation to points where secondary breaks take place [19].

These models take into account short range interactions, due to the stacking coupling. Other DNA models ignore this kind of interaction and only consider long range interactions, whose origin lies in the dipole moments that characterize the hydrogen bonds between the nucleotides within each base pair of the DNA strand. These models have been studied by Gaididei et al [20] within the framework of the Discrete Nonlinear Schrödinger equations. Breathers in a bent chain with LRI have been studied by the same group in [21,22].

Before obtaining the results presented in this paper, we tried to find moving

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breathers in a DNA model with only dipole–dipole interaction, but we were not able to observe them. This fact suggested us to consider a more realistic DNA model with both stacking and dipole–dipole interactions and study the possibility of obtaining moving breathers.

In this paper we give an affirmative answer to the question of the existence of moving breathers in a DNA model with both stacking and dipole–dipole interactions. The study of static breathers in the parameters space obtains the range of their existence and stability. Moreover, the existence of regions where a change of stability occurs is necessary in order to obtain a moving breather. We have observed the existence of a threshold value of the dipole–dipole interaction above which, the breathers are not movable. Finally, we have also observed that the dipole–dipole interaction hinders the mobility of the breathers

This article is organized as follows. In section 2, the model object of our study is introduced. It is a modification of the Peyrard-Bishop model, augmented with a long range interaction term due to dipole–dipole interactions.

In section 3, we summarize the methods for obtaining static breathers and determining their stability.

Section 4 describes the regions of existence and stability of static breathers in the parameters space. The values of the parameters where the breathers change their stability, i.e., the bifurcation loci, are specially relevant for obtaining moving breathers.

Some properties of moving breathers, such as their effective mass, velocity and domain of existence are studied in section 5.

In section 6 we relate our results with DNA parameters.

Finally, we pose the conclusions of our work in section 7.

2 The model

We consider a modification of the Peyrard-Bishop model [14], which consists in the addition of an energy term that takes into account the long range interaction due to dipole–dipole forces. Thus, the Hamiltonian can be written as:

$$H = H_{PB} + U_{DD} \tag{1}$$

where H_{PB} is the hamiltonian of the Peyrard–Bishop model and H_{DD} is the dipole–dipole energy term.

Let us explain both terms in more detail:

2.1 The Peyrard–Bishop model

The Peyrard–Bishop model only considers short range interactions due to the stacking of base pairs. The hamiltonian is [14]:

$$H_{PB} = T + U_{BP} + U_{ST}, \tag{2}$$

where T is the kinetic energy:

$$T = \frac{1}{2} m \sum_n \dot{u}_n^2, \tag{3}$$

being u_n the transverse stretching of the hydrogen bonds connecting the two bases and m the mass of a nucleotide.

The term U_{BP} represents the interaction energy due to the hydrogen bonds within each base pair:

$$U_{BP} = \sum_n V(u_n), \tag{4}$$

where $V(u)$ is the Morse potential, i.e., $V(u) = D(e^{-b\,u} - 1)^2$. D is the well depth and represents the dissociation energy of a base pair, and b is a spatial scale factor of the Morse potential.

U_{ST} is the short range interaction term, representing the stacking energy between base pairs:

$$U_{ST} = \frac{1}{2} C \sum_n (u_{n+1} - u_n)^2, \tag{5}$$

where C is the stacking coupling constant.

2.2 The dipole–dipole energy

The hydrogen bonds responsible for the interbase coupling has a finite dipole moment, which cause a long range interaction decaying as r^{-3} [20].

The dipole–dipole interaction energy is [23]:

$$U_{DD} = \sum_n \sum_{i \neq n} \frac{1}{4\pi\varepsilon_o} \frac{1}{|\vec{r}_{in}|^3} [\vec{p}_n \cdot \vec{p}_i - 3(\vec{p}_n \cdot \hat{r}_{ni})(\vec{p}_i \cdot \hat{r}_{in})], \tag{6}$$

where $\vec{p}_n$ and $\vec{p}_i$ are, respectively, the dipole moments of the base pairs situated in the n-th and i-th site, and $\vec{r}_{in}$ is a vector that connects the centres of the dipole moments.

In our model the bending, twisting and inhomogeneity of the DNA are not taken into account. Thus the dipole moments are parallel and oriented in the same sense. Therefore, $\vec{p}_n$ and $\vec{p}_i$ will be perpendicular to $\hat{r}_{in}$ and the last equation can be written as:

$$U_{DD} = \sum_n \sum_{i \neq n} \frac{1}{4\pi\varepsilon_o} \frac{1}{|d(n-i)|^3} p_n p_i, \tag{7}$$

where d is the distance between neighbouring base pairs. In equilibrium, all the dipole moments have the same value, $p_n \equiv p_o, \ \forall n$, and, therefore, the equilibrium interaction energy is:

$$U^o_{DD} = \sum_n \sum_{i \neq n} \frac{1}{2} \frac{1}{4\pi\varepsilon_o} \frac{1}{|d(n-i)|^3} p_o^2, \tag{8}$$

Considering excited states of the system, we assume that

$$p_n = p_o + q \ u_n \ , \tag{9}$$

with u_n being the deviations from the equilibrium, i.e., the stretching of the hydrogen bonds, and q the charge transfer due to their formation. Inserting the expression (9) into equation (7) we obtain the dipole–dipole contribution to the potential energy of the system. It has the form:

$$U_{DD} = U^o_{DD} + U^1_{DD} + \sum_n \sum_{i \neq n} \frac{1}{2} \frac{q^2}{4\pi\varepsilon_o} \frac{1}{|d(n-i)|^3} u_n u_i, \tag{10}$$

where U^o_{DD} and U^1_{DD} stand for the constant and linear terms on $\{u_n\}$. It is worth noting that this terms do not appear in the Hamiltonian (1) because, in accordance with the definition of equilibrium, the first order terms in the Taylor expansion of the total potential energy of the system should vanish in equilibrium, where the variables u_n are zero. Therefore, we can write the dipole–dipole interaction contribution to the Hamiltonian as:

$$H_{DD} = \sum_n \sum_{i \neq n} \frac{1}{2} \frac{q^2}{4\pi\varepsilon_o} \frac{1}{|d(n-i)|^3} u_n u_i \ . \tag{11}$$

This formula provides an expression for the dipole–dipole coupling constant:

$$J = \frac{q^2}{4\pi\varepsilon_o d^3}, \tag{12}$$

and the dipole–dipole Hamiltonian can be written as:

$$H_{DD} = \frac{1}{2} \sum_{n,i} J_i u_{n+i} u_n, \tag{13}$$

where,

$$J_m = \begin{cases} \frac{J}{|i|^3} \text{ for } 1 \leq |i| \leq (N-1)/2 \\ 0 \quad \text{otherwise,} \end{cases} \tag{14}$$

being $|i|$ is the normalized distance between base pairs. In practice, if N is the size of the system, we limit the long range interaction to $(N-1)/2$, if N is odd, or $(N-2)/2$, if N is even, in each direction to keep the spatial homogeneity in a finite system with periodic boundary conditions [4].

2.3 Dimensionless equations

The Hamiltonian can be written as:

$$H = \sum_{n=1}^{N} \left(\frac{1}{2} m \dot{u}_n^2 + D(e^{-b\,u_n} - 1)^2 + \frac{1}{2} C(u_{n+1} - u_n)^2 + \frac{1}{2} \sum_n \sum_{i \neq n} J_i u_{n+i} u_n \right), \tag{15}$$

and the dynamical equations are:

$$F(\{u_n\}) \equiv m\ddot{u}_n + 2Db(e^{-b\,u_n} - e^{-2b\,u_n}) + C(2u_n - u_{n+1} - u_{n-1}) + \sum_{i\neq n} J_i u_{n+i} = 0. \tag{16}$$

The following changes of variables are introduced:

$$t \to \omega_o t, \quad u_n \to b u_n, \quad C \to \frac{C}{m\omega_o^2}, \quad J \to \frac{J}{m\omega_o^2}, \tag{17}$$

where

$$\omega_o = \sqrt{\frac{2b^2 D}{m}}, \tag{18}$$

is the frequency of the oscillators in the harmonic limit.

With these changes the dynamical equations become:

$$F(\{u_n\}) \equiv \ddot{u}_n + (e^{-u_n} - e^{-2u_n}) + C(2u_n - u_{n+1} - u_{n-1}) + \sum_{i\neq n} J_i u_{n+i} = 0. \tag{19}$$

2.4 Discussion

Although the dipole interaction manifests as a long range force, it also includes nearest–neighbour terms, due to the form of the potential. So, it is interesting to write apart the terms that involve nearest–neighbour interactions from the rest. Thus, the dynamical equations can be written as:

$$F(\{u_n\}) \equiv \ddot{u}_n + (V'(u_n) + 2Cu_n)) + (J - C)(u_{n+1} + u_{n-1}) + \sum_{|i|\geq 2} J_i u_{n+i} = 0. \tag{20}$$

For $J = C$, the nearest–neighbour term vanishes in (20) so, for these values of the parameters, the only interactions that explicitly appear are those due to the second and further neighbours.

3 Numerical methods for obtaining breathers and determining their stability

3.1 Obtaining breathers

In order to obtain a static breather we have used the methods developed in [24–27]. Discrete breathers in Hamiltonian lattices are periodic and time–reversible solutions, i.e., they can be expressed as a Fourier series of the form:

$$u_n(t) = z_o + 2\sum_k z_n^k \cos(k\omega_{\rm b} t). \tag{21}$$

In this paper we choose a frequency with value $\omega_{\rm b} = 0.8\omega_{\rm o}$ and the number of particles is $N = 21$, which proves to be large enough to study breathers as long as they are localized a few particles, and, moreover, the phenomena that we observe are independent on the number of particles. We have also choose periodic boundary conditions.

A static breather can be obtained for given values of the dipole–dipole coupling parameter, J, and the stacking coupling parameter, C. This solution can be continued by varying C and maintaining J constant or vice versa.

In order to study the existence of bifurcations, it is useful to analyze the eigenvalues of the Jacobian operator, $\mathcal{J}(\mathbf{u}) \equiv \partial_{\mathbf{u}} F(\mathbf{u})$. Its domain is the space of functions of t that are time–reversible, with period $T = 2\pi/\omega_{\rm b}$, continuous second derivative, and an appropriate norm, $\mathcal{E}_s^2(\omega_{\rm b})$. When $\mathcal{J}$ acts on a function ξ in this space, the following eigenvalue equations are obtained:

$$(\mathcal{J}(\mathbf{u}).\xi)_n \equiv \ddot{\xi}_n + V''(u_n)\xi_n + C(2\xi_n - \xi_{n+1} - \xi_{n-1}) + \sum_{m\neq n} J_m \xi_{n+m} = \lambda \xi_n. \tag{22}$$

We will refer to this operator, for short, as the *Jacobian*. When it has no zero eigenvalues, the implicit function theorem conditions are satisfied, and there exists a unique branch of solutions in a neighbourhood of $\{u_n\}$. It allows us to continue a solution using the Newton–Raphson method, starting from the anticontinuous limit (i.e., zero coupling). The dependence of the eigenvalues with the parameters will also give us valuable information about the system.

3.2 Breather stability

The same operator can be considered with a different domain, the space of functions with continuous second derivative, without constrictions on time–reversibility and periodicity, $\mathcal{C}^2$. This operator will be referred here as the *Newton operator* and denoted $\mathcal{N}(\mathbf{u})$ [2]. The eigenvalue equation for the Newton operator with $\lambda = 0$ gives the linear evolution of small perturbations of the breather, which allow us to study its stability [2]. Hereafter it will be referred to as the stability equation. The functions in $\mathcal{C}^2$, are determined by the initial conditions, $\Omega(0) \equiv (\{\xi_n(0)\}, \{\dot{\xi}_n(0)\})$. Integration of the stability equation until $t = T$, gives $\Omega(T) \equiv (\{\xi_n(T)\}, \{\dot{\xi}_n(T)\})$. As the space is finite and linear, there exists a matrix of dimension $2N$ corresponding to the Floquet operator, which is called the *monodromy*. This operator is thus defined by:

$$\begin{pmatrix} \{\xi_n(T)\} \\ \{\dot{\xi}_n(T)\} \end{pmatrix} = \mathcal{M}_0 \begin{pmatrix} \{\xi_n(0)\} \\ \{\dot{\xi}_n(0)\} \end{pmatrix} \tag{23}$$

The Floquet operator is here a symplectic and real map. As a consequence, if λ is an eigenvalue, then λ^*, $1/\lambda$ and $1/\lambda^*$ are also eigenvalues. Therefore, stability implies that all the eigenvalues have modulus unity. The Floquet operator corresponding to $\lambda \neq 0$, denoted as $\mathcal{M}_\lambda$, will also be used later.

3.3 Linear modes

Static breathers can be continued until that an integer multiple of their frequency does not resonate with any of the frequencies of the linear modes (or phonons), which are given by:

$$\left(\frac{\omega_{ph}}{\omega_{\mathrm{o}}}\right)^2 = 1 + 4C\sin^2\frac{q}{2} + 2J\sum_m \frac{\cos(mq)}{m^3}, \tag{24}$$

where q is the wave vector of the linear modes. The second harmonic of the breather is the responsible for the resonance with the phonon band. Besides, this resonance involves the phonon with vector $q = \pi$ so this phenomena occurs when:

[2] This term is usually used for the two operators, $\mathcal{J}$ and $\mathcal{N}$, but we will use this terminology to distinguish easily between them.

$$C = \left(\frac{\omega_{\rm b}}{\omega_{\rm o}}\right)^2 - \frac{1}{4} - 2J\sum_m \frac{(-1)^m}{m^3}. \tag{25}$$

If we suppose an infinite system [3], the sum can be expressed in terms of the Riemann's zeta function:

$$C = \left(\frac{\omega_{\rm b}}{\omega_{\rm o}}\right)^2 - \frac{1}{4} + \frac{3}{8}\zeta(3)J \tag{26}$$

This equation is an analytical expression for the upper boundary of the existence of static breathers, both 1–site and 2–site.

4 Bifurcations

In this section we study the bifurcation loci of static breathers. It is interesting for three different reasons: a) It gives the range of existence of the static breathers; b) It gives the regions in the parameter space where the breathers are stable (and, therefore, physically observable in real systems) or unstable; c) Finally, but of paramount importance, it gives the values of the parameters where the breathers are movable, as it will be explained in the following section.

In this system there appear two types of bifurcations as C and J are varied:

- Stability bifurcations: they occur when a monodromy eigenvalue corresponding to a localized mode abandons the unit circle. They also correspond to a change of sign of a Jacobian eigenvalue, as it is explained in appendix A. The existence of this type of bifurcation is a necessary condition for the existence of movable breathers (see section 5).
- Breather extinctions: they occur when a Jacobian eigenvalue becomes zero and the breather is not continuable any longer.

The points where these bifurcations occur are independent of the number of particles of the system. This result was established by Aubry in [2], and we have checked it by increasing and decreasing the number of particles during our calculations.

We proceed to explain the bifurcations in the limits of only stacking or dipole–dipole interactions and, finally, in the case where both interactions are present.

[3] This is not our case, although the results for $N = 21$ particles only differs 1% from the results for the infinite system

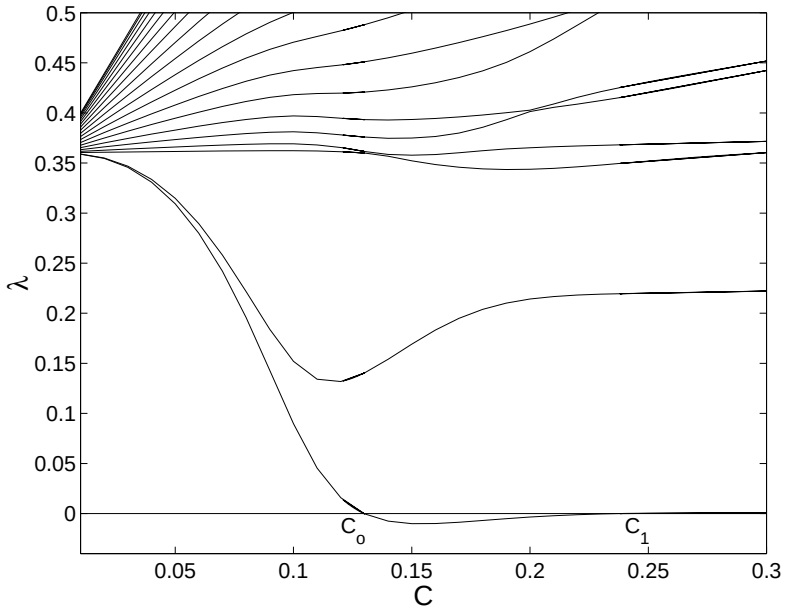

Fig. 1. Jacobian eigenvalues, λ, versus stacking coupling constant, C, when there is only stacking interaction. Note the existence of two zero crossing which correspond to stability bifurcations.

4.1 Bifurcations with only stacking interaction ($J = 0$)

In this case, the only parameter is C. When it is varied, there are only stability bifurcations at two points C_o and C_1. The evolution of the Jacobian eigenvalues with C, for a 1–site breather, is shown in figure 1. Two eigenvalues, which correspond to localized modes [28], detach from the linear modes band, and one of them, change its sign at the values C_o and C_1. In the interval (C_o, C_1) this eigenvalue is negative (see appendix) and, therefore, the breather is unstable, while in the interval $(0, C_o)$ and above C_1, the eigenvalue is positive and the breather is stable.

4.2 Bifurcations with only dipole–dipole interaction ($C = 0$)

In this case, there are no stability bifurcations (and, therefore, *there are no moving breathers with* $C = 0$) [4]. The breather is annihilated when the phonon band expands and one of its eigenvalues becomes zero (figure 2). In other words, the breather resonates with the phonons.

[4] Actually, there exists a change of stability for a high value of J. However, it cannot be used to move a breather because the eigenmode of the Floquet operator which detaches from the unit circle is not localized.

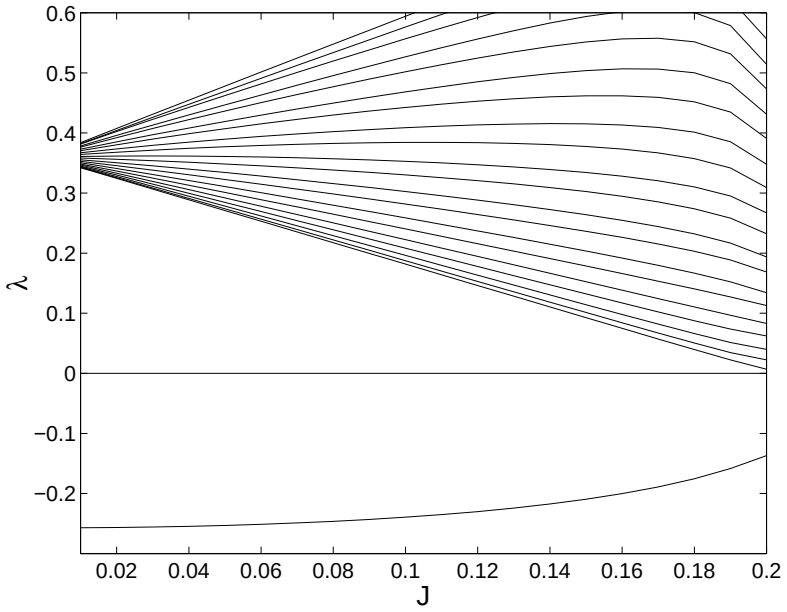

Fig. 2. Jacobian eigenvalues, λ, versus dipole–dipole coupling constant, J, when there is only dipole–dipole interaction. Note that the only bifurcation is due to the crossing of an eigenvalue corresponding to a phonon.

4.3 Bifurcations in the general case

We find the bifurcation loci of the stability bifurcations in the parameter space (C, J), for both the 1–site and the 2-sites breathers. The occurrence of these two bifurcations is a necessary condition for the existence of moving breathers.

4.3.1 Bifurcation study of 1-site breathers

There exists a critical value of the dipole–dipole interaction parameter, J_{c1}, with the following characteristics:

(i) For $J < J_{c1}$, the behaviour is qualitatively similar to the observed for $J = 0$, i.e., there are stability bifurcations at two points, $C = C_o$ and $C = C_1$ (which depend on J), as C is increased.
(ii) For $J > J_{c1}$, there are no stability bifurcations, but only an extinction for some value of C, above which, the breather is not continuable. Therefore, there are no moving breathers.

4.3.2 Bifurcation study of 2-site breathers

For the 2–site breathers there exist two critical values of J: J_{c2}, which is analogous to J_{c1}, and J_o, which is called the *mobility limit*. They define three

intervals of J with the following properties:

(i) $J \in [0, J_{c2})$. The breather is unstable for small values of C. When C increases, there are two stability bifurcations.
(ii) $J \in (J_{c2}, J_o)$. Only the first stability bifurcation appears, thereafter the breather is annihilated. At $J = J_o$, the values of C for the annihilation and the stability bifurcation coincide and turn out to be equal to J_o. This point has the characteristic (cfr. equation (20)) that the nearest–neighbour interaction disappears.
(iii) $J > J_o$. The only bifurcation is a breather extinction.

4.4 Discussion

The bifurcation analysis for the 1–site breathers shows that they can be moved only for $J < J_{c1}$. The study of 2–site breathers shows that they are movable for $J < J_{c2}$ being $J_{c2} > J_{c1}$. They are also movable for $J \in [J_{c2}, J_o)$. Therefore, J_o establishes the maximum value of J (and also the minimum value of C) for which breathers can be movable, i.e., *there are no moving breathers for* $C < J_o$ *and for* $J > J_o$. This is the reason why J_o is called the *mobility limit.*

The bifurcation loci for the stability bifurcations are shown in figure 3. In figure 4 the dependence of the mobility limit on the frequency is shown. This curve fits very well to the equation

$$J_o = A\omega_{\mathrm{b}}^r, \tag{27}$$

where A=0.1921 $\pm$ 0.0002 and r=2.377 $\pm$ 0.005. So the range of existence of moving breathers will be determined, for a given frequency, in the following way:

- The minimum value of C is the mobility limit (equation 27). The maximum value of C is given by the resonance with the phonons (equation 26).
- Clearly, the minimum value of J is 0. The maximum value of J is the mobility limit.

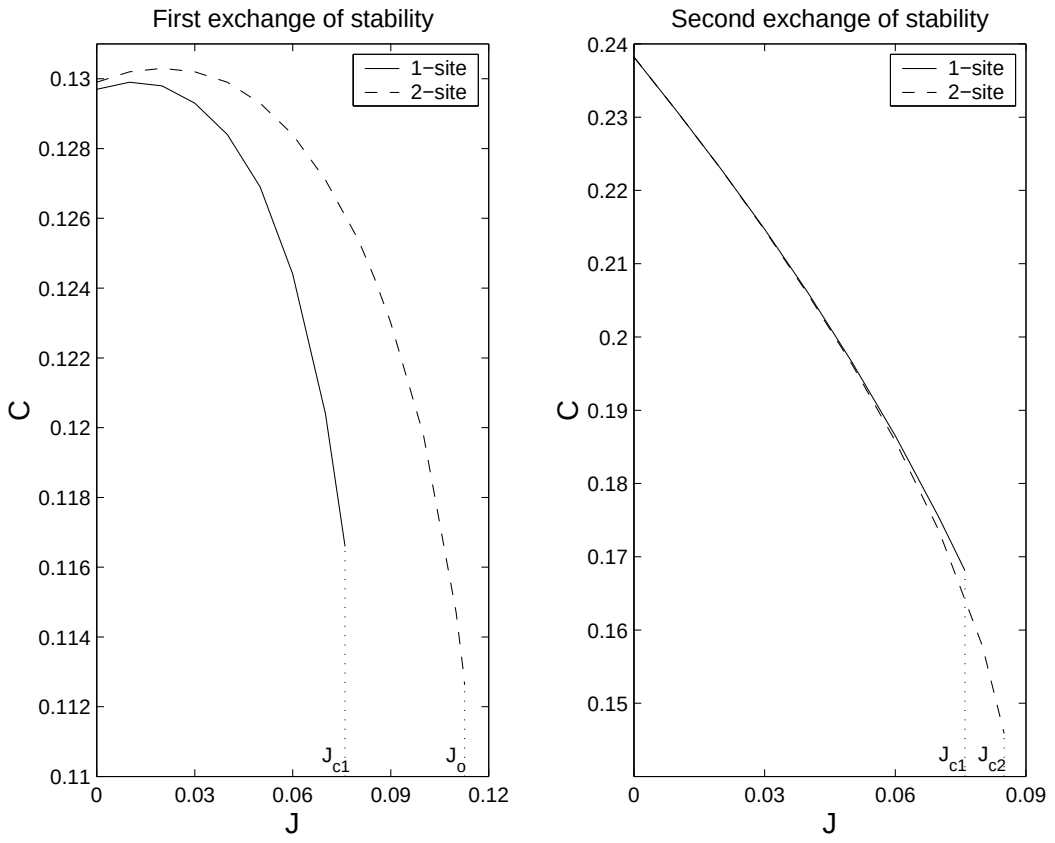

Fig. 3. Bifurcation loci for the first and the second exchange of stability in 1-site and 2-site breathers. The values corresponding to $\omega_{\rm b} = 0.8\omega_{\rm o}$ are: $J_{c1} = 0.076$, $J_{c2} = 0.085$, $J_o = 0.11263$.

5 Moving breathers

5.1 Preliminaries

One of the open fields on the study of localized oscillations is the question of mobility of discrete breathers. There exists a lack of knowledge on this field mainly owing to the fact that moving breathers are not exact solutions [5] of the dynamical equations of the system and, besides, a proof of existence of them has not been found so far.

Many authors [29,11] agree that breathers must be perturbed in the velocity in a similar way to a pendulum overcoming the separatix which separates the oscillating solutions from rotating ones. In the case of discrete breathers we are dealing with a movability separatrix separating static solutions from moving

[5] For exact solutions we mean solutions that can be obtained using continuation methods

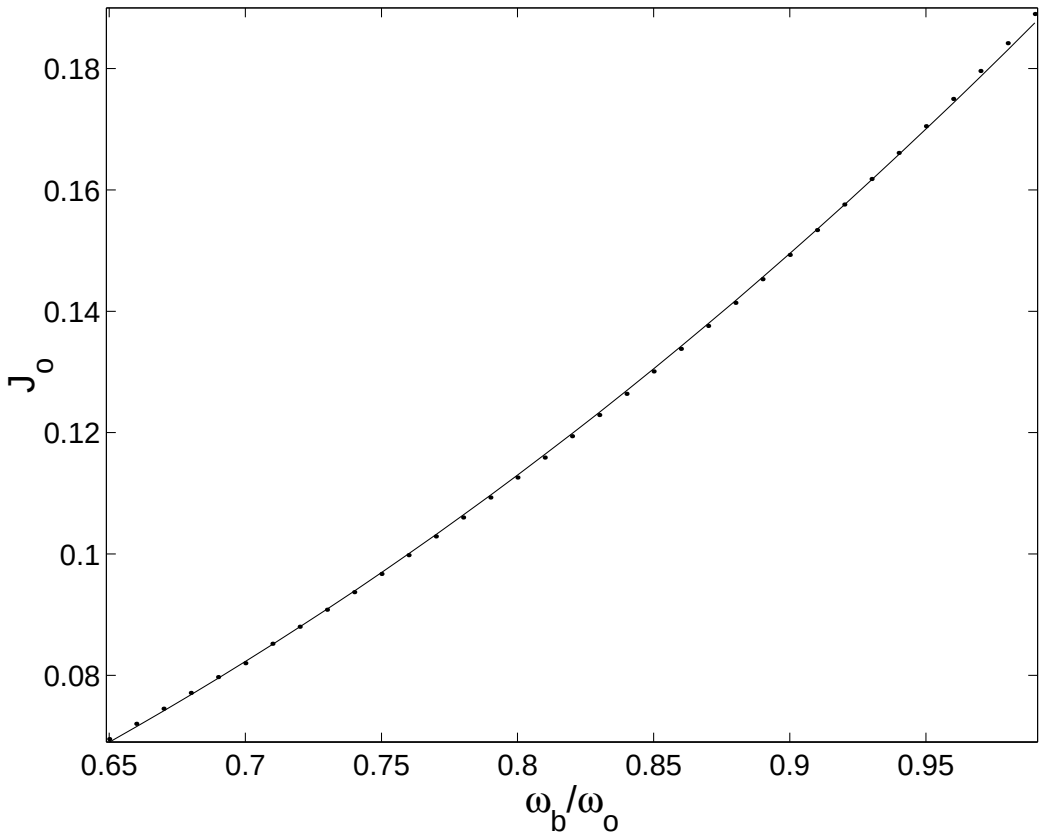

Fig. 4. Dependence of J_o with respect to the breather frequency. This curve fits to $J_o = A\omega_{\mathrm{b}}^r$, where A=0.1921 $\pm$ 0.0002 and r=2.377 $\pm$ 0.005.

ones. The application of this concept is the basis of the marginal mode method for obtaining moving breathers, which has been used in our calculations and is explained below (section 5.2)

Moving breathers can also be seen as a solution that repeats itself after a time shifted by one lattice site [30]. This kind of solutions are called *exact moving breathers* by some authors [11,12] and have certain special features due to the commensurability. However, a perturbation is also needed in order to calculate them.

Another important characteristic of moving breathers is that they have a finite life because they radiate phonons. This fact occurs because a moving breather has two frequencies: one due to the internal vibration and another one due to the periodic translation which is smaller than the first one and is the responsible for the resonance with the phonons, and so, of the emission of them.

5.2 The marginal mode method

A moving breather is obtained by 'kicking' a static breather, i.e., perturbing its velocity components. However, not every breather can be moved, and not every kick can move a breather. Therefore, the problem is to know the conditions that a breather must fulfill in order to be moved and what the characteristics of the perturbation are.

A systematic method used for obtaining moving breathers was proposed by Chen, Aubry and Tsironis [10]. They considered a Klein-Gordon chain of particles with nearest neighbour interactions, modulated by a coupling parameter, and a double well on–site potential. It is observed that a linear mode becomes localized as the coupling parameter in increased and the breather becomes unstable for a critical value of the coupling parameter. The optimum conditions for obtaining a moving breather are satisfied for a range of values close to the critical one. The direction of the perturbation is given by the velocity components of the localized mode.

Later on, Aubry and Cretegny [11,12] have studied the possibility of obtaining moving breathers under more general conditions. They demonstrate that if a conjugate pair of monodromy eigenvalues corresponding to localized linear modes detach from the phonon band, collide at $1+0i$ and abandon the Floquet circle, one of them becomes a *marginal mode* at the collision point, i.e., a perturbation along its direction grows linearly with time and, therefore, is the optimum one to move a breather.

Furthermore, at the point where the breather becomes unstable, there is an exchange of stability bifurcation, that is, a solution is stable before reaching the bifurcation point and becomes unstable just after crossing it, whereas another solution does the opposite at a point nearby. These solutions are usually a 1–site and a 2–site breather. The latter is a breather with two neighbouring sites excited and corresponds to a breather centered at the bond.

One of the most important consequences of the results of Aubry and Cretegny's work is that the existence of this bifurcation is a necessary but not a sufficient condition to obtain a moving breather.

Therefore, as indicated in [10–12], the following steps must be performed in order to obtain a moving breather:

1) To look for the existence of the two complementary stability bifurcations for the 1–site breather and the 2–site breather. Their bifurcation loci must have a region where they are fairly close. The static breather to be moved should be obtained for values of the parameters close enough to these bifurcation loci. However, our numerical experiments have shown that breathers are not only

movable in these regions, as we explain in section 5.3

2) To perturb the breather with the velocity components of the marginal mode at the neighbouring bifurcation.

Effective mass

An useful concept used for describing the breather dynamics is its effective mass [10,11]. It is a measure of the breather inertia to external forces.

The breather velocity must be perturbed in a direction colinear to the marginal mode, in order to obtain moving breathers. If the normalized marginal mode is $\mathbf{V}$, the perturbation added to the breather velocities, which are zero at $t = 0$, is given by $\mu\mathbf{V}$, and μ is the magnitude of the perturbation.

Thus, the kinetic energy added to the breather by the initial kick is $1/2\mu^2$. It is found [10] that the resulting translational velocity of the breather, v, is proportional to μ. Then, the concept of effective mass can be defined through the relation $\frac{1}{2}m^*v^2 = \frac{1}{2}\mu^2$. Therefore:

$$m^* = (\mu/v)^2. \tag{28}$$

Nevertheless, this linear relation is fulfilled only for low values of μ. The relation between μ and v for high values of the perturbation is an open question which needs more research [31].

Consequently, moving breathers can be considered as a quasi-particle with mass m^*. The effective mass is a quantitative measure of the breather mobility. Larger mass indicates smaller mobility.

5.3 Study of moving breathers

In this section, we take advantage of the results obtained in the bifurcation study (section 4) in order to know the conditions necessary to move a breather. We have numerically obtained that a breather is not only movable near a stability bifurcation but it is also movable for a wide range of parameters. Moreover, we have observed that, in several cases, breathers could not be moved although the necessary conditions for the movement were fulfilled.

The temporal evolution of the moving breather has been obtained by means of numerical simulations, using the symplectic algorithm developed by Calvo

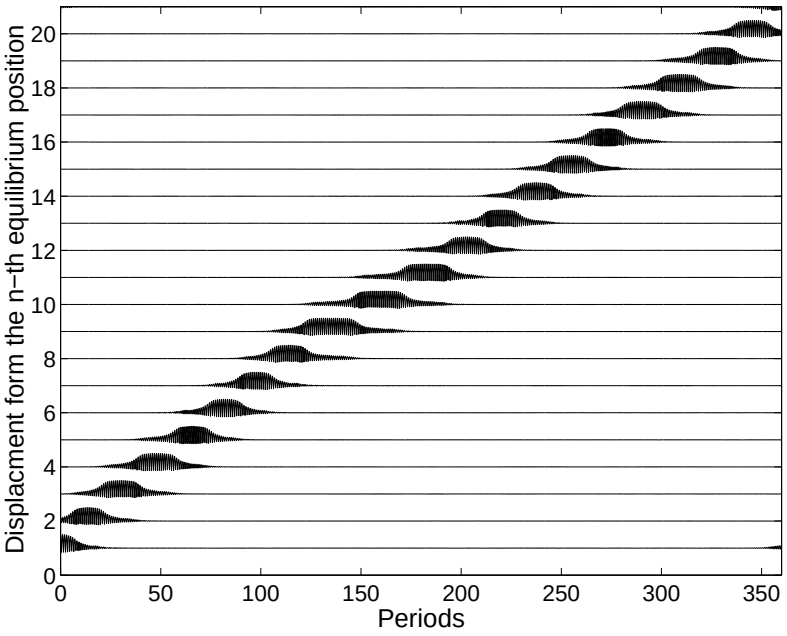

Fig. 5. Evolution of a moving breather for $C = 0.1244$, $J = 0.06$ and an initial 'kick' $\mu = 0.10$. The breather involves basically three sites that oscillate in phase.

[32]. An example of the evolution of a moving breather for certain values of the parameters J and C, is shown in figure 9. We can see that the breather moves uniformly during 350 breather periods with a slight change of shape and emitting a 0.12% of phonon radiation, which is a small value but bigger compared with the emission of only 0.01% for $J = 0$. It can also be seen that the breather is extremely localized with only three sites basically involved and oscillating in phase.

We must remark that all the numerical results of this section have been obtained for a value of the breather frequency $\omega_{\rm b} = 0.8\omega_{\rm o}$.

We summarize our results as follows:

(i) From a bifurcation study of static breathers (section 4), it is obtained the existence of a maximum of the dipole–dipole interaction parameter, J, above which there are no mobile breathers. This value is $J = J_o \approx 0.1162$, but there is a smaller value, $J = J_{c1} \approx 0.076$, above which the 1–site breather cannot be moved. These values have been obtained for a frequency $\omega_{\rm b} = 0.8\omega_{\rm o}$ and are independent of the size of the system.

(ii) For low J, the 1–site and the 2–site breathers can be made mobile for values of C above the first stability bifurcation . These values of J are $J \lesssim 0.5$ and $J \lesssim 0.4$, respectively.

(iii) For high J:

  (a) The 1–site breather can be moved in the proximity of the first stability bifurcation curve, and above the second one.

(b) The 2–site breather can only be moved above the second stability bifurcation curve.

An explanation for these phenomena is that breathers have to be 'metastable' in order to be moved, i.e. their Jacobian eigenvalue responsible for the stability bifurcation must be close to zero. In figure 6 can be seen that for $J = 0$, where mobility is possible for all the values of C above the first stability bifurcation, this eigenvalue is closer to zero than for $J = 0.06$ where breathers are not movable for all of the values of C.

These results demonstrate that the conditions for the mobility posed in section 5.2 are necessary but not sufficient. In figures 7 and 8 a diagram of the range of existence of moving breathers for $\omega_\mathrm{b} = 0.8\omega_\mathrm{o}$ is depicted.

(iv) The dependence of the effective mass with the parameters is not simple. However, two general properties can be established:
   (a) The effective mass has its maximum value in the vicinity of the first stability bifurcation curve. See figure 9.
   (b) This maximum value of the effective mass increases with the dipole–dipole interaction parameter, J. See figure 10

(v) The smoothness of the movement decreases when J increases. In other words, the long range interaction emphasize the discreteness of the system. This can be observed in figure 11, where the temporal evolution of energy the center is plotted. This magnitude is defined as:

$$X_E = \frac{\sum_n n e_n}{\sum_n e_n}, \tag{29}$$

being e_n, the energy of the nth-particle.

6 Application to DNA

The results obtained in the paper are valid for all chains with both short range and long range interactions given by equations (5) and (13). They can be particularized for a DNA model with stacking and dipole–dipole interactions using the transformations (17).

The values for model parameters D, b and m are not well known for DNA. We will use here the proposed in [16,17]. Concretely, they are $D = 0.04$ eV, $b = 4.45$ Å^{-1} and $m = 300$ amu. Thus, with these values, $\omega_\mathrm{o} = 7.05 \cdot 10^{12}$ s^{-1}.

If the breather frequency is chosen so that $\omega_\mathrm{b}/\omega_\mathrm{o} \in (0.67, 1)$ in order to avoid phonon resonances, its value will oscillate between $\omega_\mathrm{b} = 4.5 \cdot 10^{12}$ s^{-1} and $\omega_\mathrm{b} = 7 \cdot 10^{12}$ s^{-1}.

For these values of the frequency, the minimum value of C for obtaining moving breathers, which can be calculated from equations (27), oscillates between

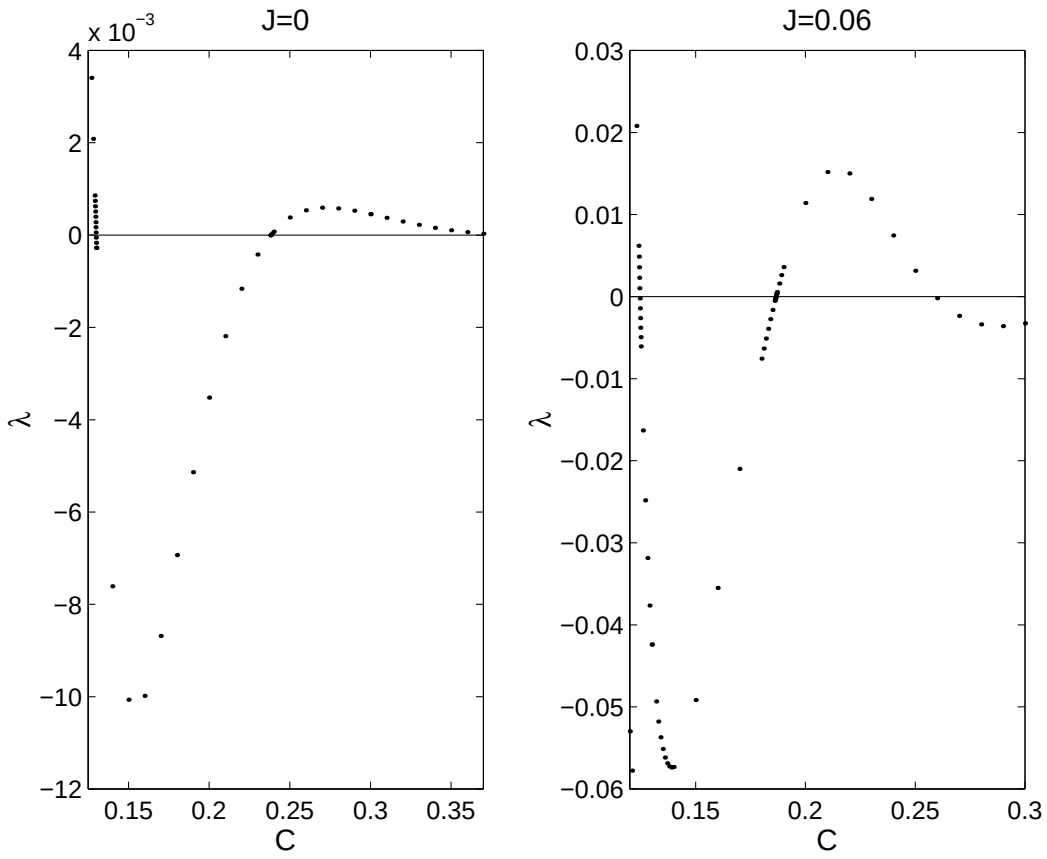

Fig. 6. Jacobian eigenvalue which produces the stability bifurcation versus stacking coupling parameter C for dipole–dipole coupling parameter $J = 0$ (left) and $J = 0.06$ (right). Note that the eigenvalue is closer to zero at $J = 0$ than at $J = 0.06$. In the first case, the breather is mobile for all C greater than the value where the stability bifurcation occurs, but, in the second case, the breather is mobile only at the first stability bifurcation and above the second one.

$C = 0.11$ eV/Å^2 and $C = 0.30$ eV/Å^2 (these values correspond to $C = 0.0690$ and $C = 0.1921$ in dimensionless units). Therefore, for the existence of moving breathers in the Peyrard–Bishop DNA model, C must be greater than 0.11 eV/Å^2. Furthermore, this minimum value of C coincides with the maximum value of J. Thus, in order to exist moving breathers, J must be smaller than 0.30 eV/Å^2 (The minimum value of J is, of course, zero).

From equation (12), the value of the charge transfer q can be calculated. As the distance between base pairs is $d = 3.4$ Å, the maximum value of q for having moving breathers is $q = 0.91\ e$. Quantum chemical calculations (see appendix B) show that $q < 0.062\ e$, which is very much lower than that value. Thus, moving breathers can exist if the dimensionless dipole–dipole coupling parameter, $J < 8.2 \cdot 10^{-4}$, which indicates that the dipole–dipole interaction does not hinder breather mobility in breather mobility.

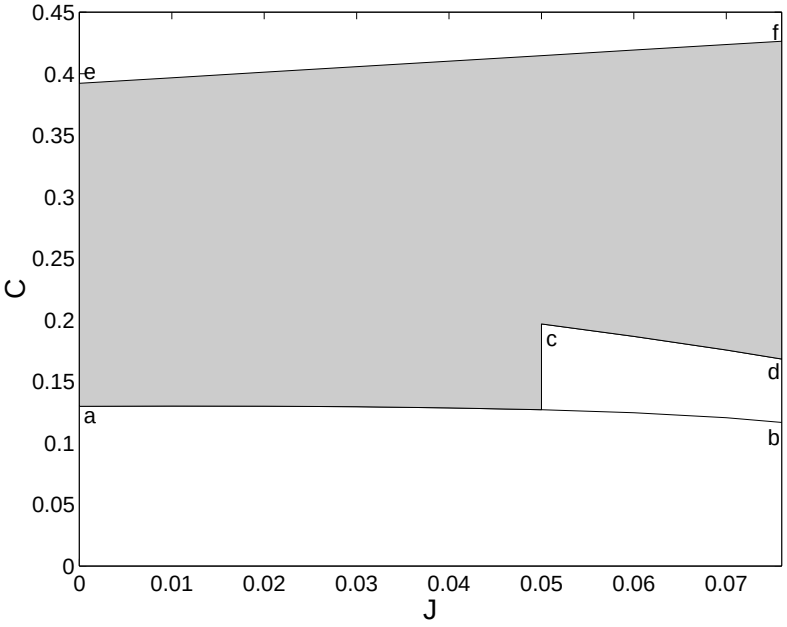

Fig. 7. Range of existence of moving breathers obtained perturbing 1–site breathers. a–b is the first stability bifurcation curve, c–d is the second one, and e–f corresponds to the resonances of the breather with the phonon band. The breather frequency is $\omega_{\mathrm{b}} = 0.8\omega_{\mathrm{o}}$.

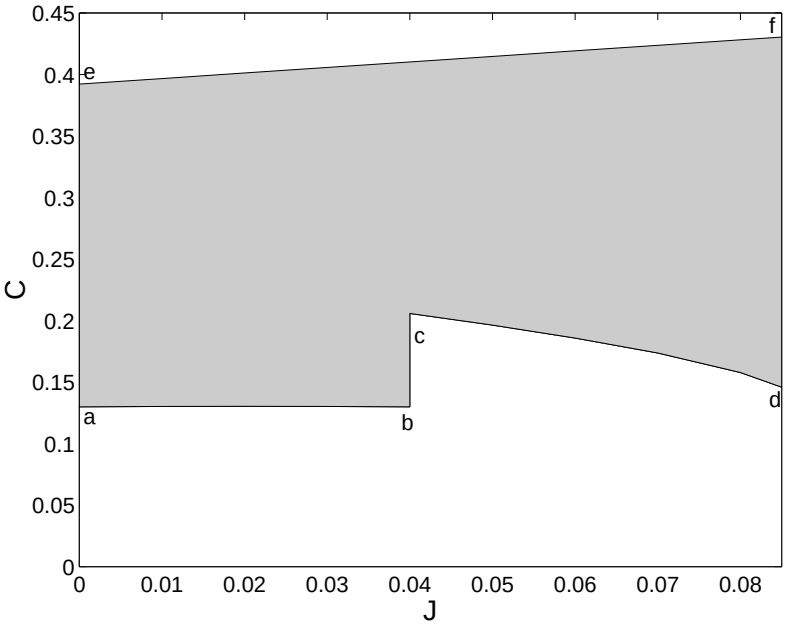

Fig. 8. Range of existence of moving breathers obtained perturbing 2–site breathers. a–b is the first stability bifurcation curve, c–d is the second one, and e–f corresponds to the resonances of the breather with the phonon band. The breather frequency is $\omega_{\mathrm{b}} = 0.8\omega_{\mathrm{o}}$.

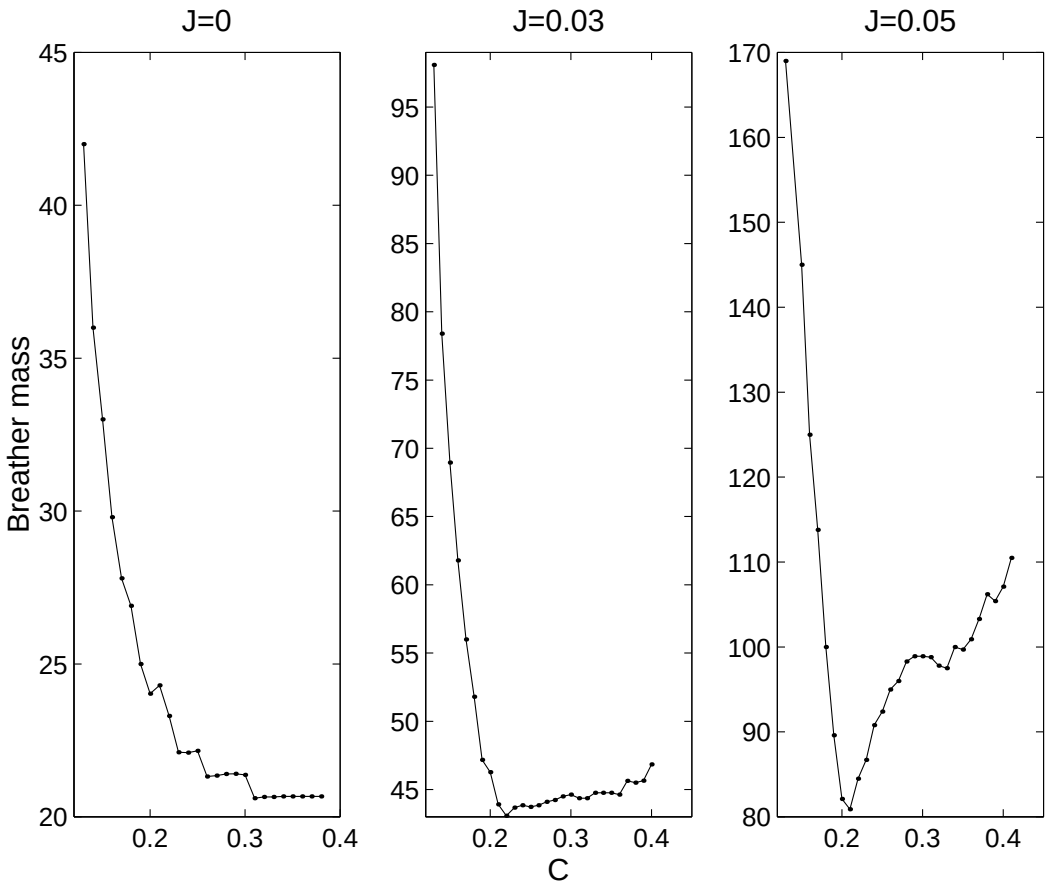

Fig. 9. Breather mass versus stacking coupling parameter C for dipole–dipole coupling parameter $J = 0$ (left), $J = 0.03$ (center) and $J = 0.05$ (right). Note that the maximum value of the mass occurs at the first bifurcation, and that the breather mass for $J = 0.05$ is always greater than the mass for $J = 0$. Note also the different scales at the Y-axis.

7 Conclusions

Up to now, the effect on breather mobility of the interplay between long range and short range interactions had not been considered. However, apart from its theoretical interest, both types of interaction do exist in DNA. This is the reason why we have performed a study of discrete breathers in a modified Peyrard-Bishop model which takes into account long range interactions due to dipole–dipole forces and short range interactions due to stacking forces.

From a bifurcation study of static breathers we have obtained that they cannot be moved if there is no stacking coupling and if the dipole–dipole coupling is larger than a critical value. This critical value of the dipole–dipole coupling coincides, in a 2–site breather, with the value of the stacking coupling parameter where the stability bifurcation occurs, and is also the minimum value for the occurrence of these bifurcations. This point has an important property,

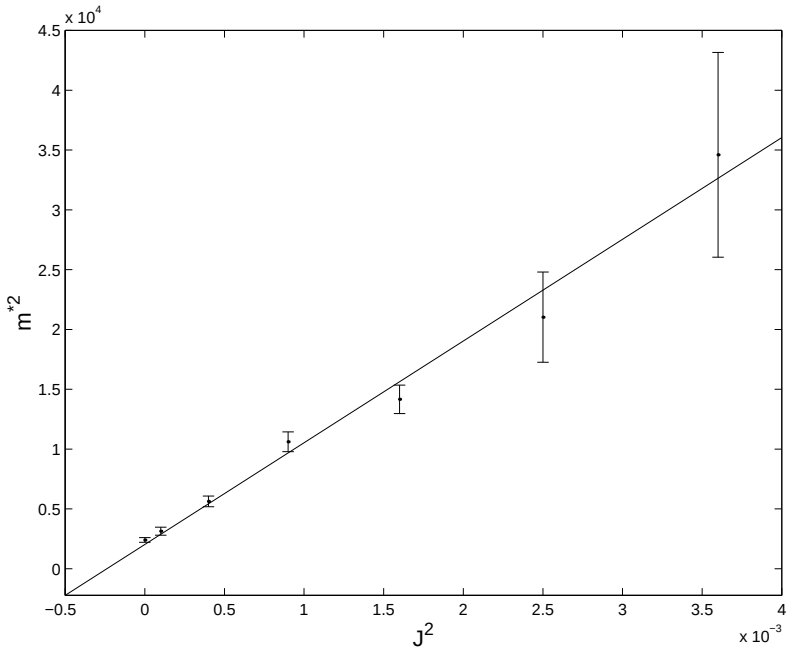

Fig. 10. Dependence of the squared effective mass, m^*, with the squared dipole–dipole interaction parameter, J. The data correspond to the moving 1–site breathers in the vicinity of the first stability bifurcation curve, where $(m^*)^2$ is maximum. Note the almost linear dependence.

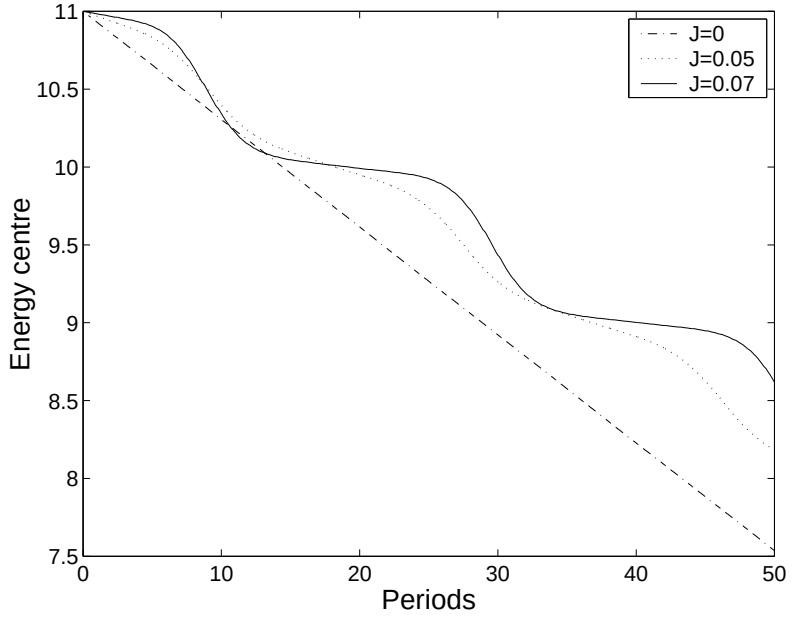

Fig. 11. Moving breather energy centre for different values of the dipole–dipole coupling parameter J, and the values of the stacking coupling parameter C corresponding to the maximum breather mass.

as can be seen in (20), which is that the only interactions which explicitly appear are those due to the second and further neighbours. This could indicate that when the dipole–dipole interaction coupling constant is smaller than the critical value, the stacking interaction dominates and the breathers are movable. However, when the dipole–dipole interaction constant is larger than the critical value, this interaction dominates and breathers are not movable.

The range of existence of moving breathers does not depend on the number of particles of the system, because the bifurcations are due to localized modes, so that the only particles to be taken into account are the central ones [6].

A numerical study of moving breathers show that breather are movable not only at the neighbourhood of the stability bifurcations, but also for all the values of the short range coupling parameter above this bifurcation. However, for high values of the dipole–dipole coupling, this range of existence decreases and, in some cases, it is impossible for the breather to be moved even in the neighbourhood of the stability bifurcations. Another important result is that the dipole–dipole interaction affects to the mobility of the breathers. The study of the dependence of the breather effective mass, shows that the mobility decreases when the dipole–dipole interaction increases.

We have performed some quantum chemical calculations in order to find the value of the dipole–dipole coupling constant. This calculations show that moving breathers in our DNA model are not hindered by the dipole–dipole interaction.

There exists a study performed by Flach and Kladko [30] which relates, for a system with only short range interaction, the moving breather velocity with the localization length of the tails. This study could be done for our model, in order to explain analytically how the long range interaction affects to the mobility. However, this study presents several difficulties, being the main the absence of a definition of localization length in a system with algebraically decaying interaction.

Some extensions of our work, which are underway, consist in performing continuations at constant energy and studying the mobility of breathers in bent DNA.

[6] The phonon resonances do depend on the size of the system but the values where they occur do not change appreciably with it

A Relationship between the Jacobian eigenvalues and the Floquet eigenvalues

A means of determining the bifurcations where a breather changes its stability, is to find the point where a Jacobian eigenvalue changes its sign. Of course, the eigenvalues related to the stability are the Floquet ones, but the relationship between them can be easily understood within the framework of Aubry's band theory [2]. Integrating the equations $\mathcal{N}(u) = \lambda u$ (see section 3.2), we can obtain the monodromy matrices, M_λ. For each λ there are $2N$ eigenvalues. They can be writen as $\exp(j\theta)$, with θ real if their moduli are the unity, and complex otherwise. If $\theta = 0$, the corresponding eigenfunctions are periodic of period T and they will be eigenfunctions of the Jacobian with their corresponding eigenvalues, as they are also time reversible. If the set of points $(\theta_i(\lambda), \lambda)$ is represented, a band structure is obtained. Each band is symmetric with respect to the axis $\theta = 0$, as the Floquet matrices are real and each eigenvalue have a corresponding complex conjugate.

The breather is stable if there are $2N$ crossings at the $\lambda = 0$ axis, i.e., if all the eigenvalues have modulus unity and they are not degenerate, except for a double eigenvalue at $+1$, which is always present. It corresponds to the eigenfunctions $\dot{u}(t)$ and $\partial u/\partial\omega_\mathrm{b}$, which are time antisymmetric.

The stability bifurcations in this paper appear in the following way [7] (see figure A.1):

(i) The breather is stable; a band crosses the $\theta = 0$ axis at $\lambda_o > 0$ and the $\lambda = 0$ axis at $\pm\theta_o$ with $\theta_o \neq 0$. Then λ_o appears as a Jacobian eigenvalue.

(ii) As a parameter changes, the band moves downwards, both λ_o and $|\theta_o|$ diminish, and, eventually, they become zero. This is the bifurcation point and it will appear as a zero of the Jacobian eigenvalues and as another double $+1$ of the Floquet eigenvalues.

(iii) As the band moves further downwards, λ_o becomes negative and $\pm\theta_o$ become non real, as there are no crossings of the $\theta = 0$ axis. The breather is unstable.

Further change of the parameters may cause that the band moves upwards and the stability bifurcation is reversed.

[7] The way how the band changes with the parameters also depends on the convexity of the band

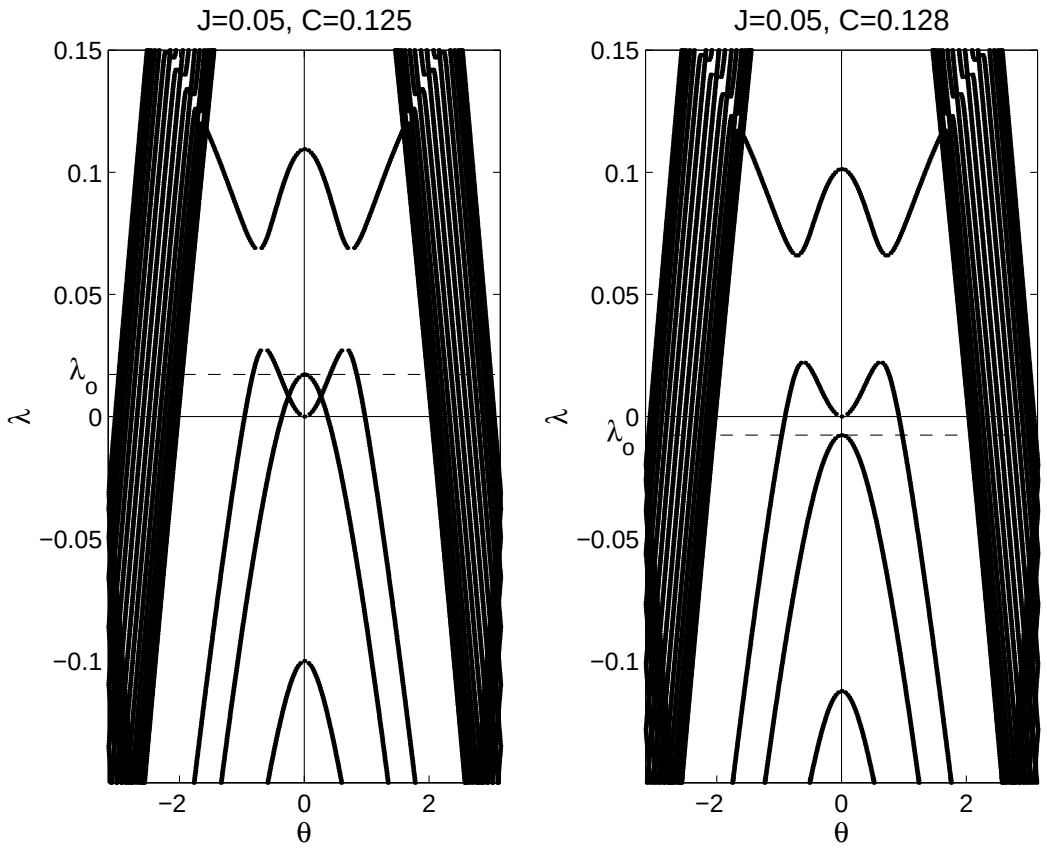

Fig. A.1. Aubry's bands before (left) and after (right) a stability bifurcation. λ_o also appears as a Jacobian eigenvalue.

B Quantum chemical computational details

Ab initio RHF and DFT calculation have been performed using the Gaussian 98 suite of programs [33]. DFT calculations employed either the Perdew and Wang exchange-correlation (PW91) functional [34] or the three parameter hybrid Becke fuctional for the exchange [35] and the Lee-Yang-Parr [36] (B3LYP). In all cases, the standard 6-31G** basis set has been used for all atoms and the geometry of the base pairs has been fully optimized by standard analytical gradient techniques at the theoretical level used. The amount of charge transfer has been estimated from the results of Mulliken population analysis.

Table 1: Computed bond distances and charge transfer for A-T and G-C base pairs

A-T base pair

Method	H bond distance / Å				charge	dipole moment
	C=O ··· H-N	N-H ··· N	C=O	H-C[a)]	transfer[b)]	(Debye)
RHF	2.0571	1.9204	2.9482		-0.0014	6.4420
PW91	1.8900	1.6975	2.6722		-0.0211	5.7547
B3LYP	1.9649	1.7772	2.7381		-0.0183	5.9817

G-C base pair

Method	H bond distance / Å			charge	dipole moment
	N-H ··· O=C	N-H ··· N	C=O ··· H-N	transfer[c)]	(Debye)
RHF	1.8947	2.0115	1.9987	-0.0248	6.4834
PW91	1.8476	1.8249	1.6635	-0.0612	6.0038
B3LYP	1-9026	1.8949	1.7475	-0.0548	6.0935

a) not really a H bond (actually, there is no hydrogen bond but is necessary for the calculation)
b) A is the negative end
c) G is the negative end

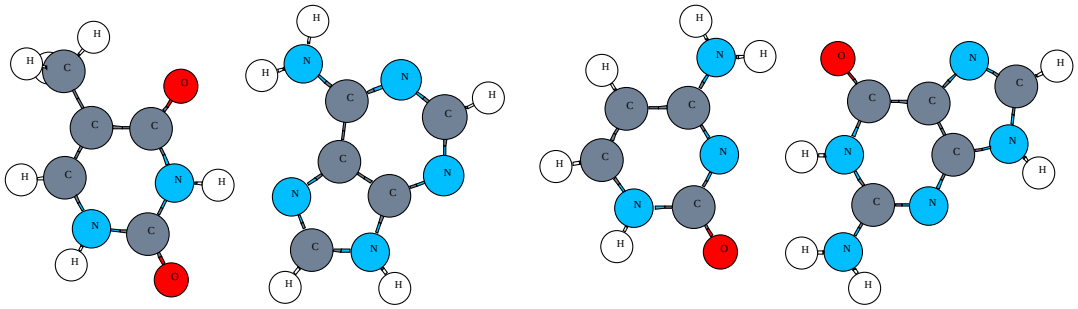

Figure 13: Structure of T-A and C-G base pairs

Acknowledgments

This work has been supported by the European Commission under the RTN project LOCNET, HPRN-CT-1999-00163.

JFR Archilla and Yu B Gaididei acknowledge the hospitality of Professor PL Christiansen and the Department of Informatics and Mathematical Modelling, at the Technical University of Denmark, where this work was started.

We acknowledge Antonio Márquez, of the Department of Chemical Physics of the University of Sevilla, for having provided us with the quantum chemical calculations.

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