Moving breathers in a bent DNA model

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Abstract

We study the properties of moving breathers in a bent 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 bonds within each base pair. We show that the movement of a breather is hindered by the bending of the chain analogously to a particle in a potential barrier.

Key words: Discrete breathers, Mobile breathers, Intrinsic localized modes, DNA
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1 Introduction

Discrete breathers are localised oscillations that appear in nonlinear discrete systems. Their existence and stability, under some rather relaxed conditions, was proven by MacKay and Aubry and, ever since, they have been widely studied [1–3]. These localized excitations, under certain conditions, can move and transport energy along the system and they are usually called moving breathers [4–8].

A particularly interesting discrete system is the Deoxyribonucleic acid, or DNA. In this system, localization of energy has been suggested as a precursor of the transcription bubble [9–11], and moving localized oscillations as a method of transport of information along the double strand [12].

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In order to explain some aspects of DNA dynamics, a great number of mathematical models have been proposed [13]. An interesting approach has been followed by Peyrard and Bishop (PB model) [9], who proposed a model in order to study the dynamics and the thermodinamics of base pairs opening in DNA denaturation and transcription. In this model, the double strand is equivalent to a Klein-Gordon chain, the variables are the distances between nucleotides within each base pair, and only short range interactions due to the stacking coupling are considered. 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 [14,15]. Nevertheless, we have shown that the existence of stacking interaction is a necessary condition to obtain moving breathers in these last kind of models [16].

In the framework of the Peyrard-Bishop model, the bending of the molecule is not relevant, because only nearest neighbour interaction is considered. However, when long range interactions are taken into account, the bending becomes relevant, and it can modify the dynamics of the system. Bending of DNA has been studied as an inhomogeneity in a chain with only nearest neighbour interaction [17,18], and long range interaction has been taken into account in homogeneous bent DNA models using the nonlinear Schrödinger equation (NLS) [19,20]. The relationship between static breathers and bending has also been studied in the framework of the Klein–Gordon equation [21,22].

In this paper, we study the properties of moving breathers in a bent DNA chain with short and long range interactions in a modified Peyrard-Bishop model [16]. The origin of the interactions lies, respectively, in the stacking of the base pairs and the finite dipole moment of the hydrogen bonds within each base pair.

We have found that the bending of the chain can drastically change the properties of moving breathers. They can cross the bent region or be reflected, a behaviour which resembles the movement of a particle in a potential barrier. A similar phenomenon has been recently observed in a two–dimensional FPU model for rigid biopolymers [23,24].

Another important result is that the moving breather behaves as a quasiparticle with constant mass provided that the phonon radiation is small enough. Under these conditions, we have developed a method for calculating the instantaneous translational kinetic energy of the moving breather.

2 The model

We consider a modification of the Peyrard-Bishop model, which consists in the addition of an energy term to the Hamiltonian, that takes into account the long range interaction due to the dipole–dipole forces [16].

The Peyrard–Bishop model has been studied assuming that the double strand has a planar geometry, i.e., the DNA chain lies in a plane. In order to study the influence on the dynamics of a different geometry, we suppose that the plane has been bent and adapted to a parabola of curvature κ (that is, the location of the n-th base pair is determined by the equation $y_n = \kappa x_n^2/2)$ [22]. All the dipole moments are perpendicular to the parabola and parallel among them.

Thus, the hamiltonian of the system can be written as:

$$H = T + U_{BP} + U_{ST} + U_{DD} \tag{1}$$

where T is the kinetic energy:

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

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

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

$$U_{BP} = \sum_n V(u_n), \tag{3}$$

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

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

$$U_{ST} = \frac{1}{2} k \sum_n (u_{n+1} - u_n)^2, \tag{4}$$

where k is the stacking coupling constant.

U_{DD} is the long range interaction term, due to the dipole–dipole interaction. It can be expressed as [16]:

$$U_{DD} = \frac{1}{2}\sum_{n,i} J^*_{ni} u_n u_i, \tag{5}$$

where,

$$J^*_{ni} = \begin{cases} \dfrac{J^*}{|\vec{r}_n - \vec{r}_i|^3} & \text{for } i \neq n \\ 0 & \text{for } i = n. \end{cases} \tag{6}$$

The vector $\vec{r}_n$ describes the position of the n-th base pair. We assume that the chain is inextensible, so that the distance between neighbouring sites remains constant: $|\vec{r}_n - \vec{r}_{n+1}| \equiv d$.

The coupling constant J is related to the charge transfer due to the formation of the hydrogen bonds (q) and the distance between base pairs (d), in the following way:

$$J^* = \frac{q^2}{4\pi\varepsilon_o d^3}. \tag{7}$$

The Hamiltonian can be written as:

$$H = \sum_{n=1}^{N} \left(\frac{1}{2} m \dot{u}_n^2 + D(e^{-b\,u_n} - 1)^2 + \frac{1}{2} k (u_{n+1} - u_n)^2 + \frac{1}{2} \sum_i J^*_{in} u_i u_n \right), \tag{8}$$

With an appropriate change of variables [16], the distance between neighbouring sites is 1 and the dynamical equations become:

$$F(\{u_n\}) \equiv \ddot{u}_n + (e^{-u_n} - e^{-2u_n}) + C(2u_n - u_{n+1} - u_{n-1}) + \sum_i J_{in} u_i = 0, \tag{9}$$

where $C = k/2Db^2$ and $J_{in} = J^*_{in}/2Db^2$. Furthermore, we define $J = J^*/2Db^2$ as a new dimensionless dipole–dipole coupling constant.

3 Moving breathers and parameter values

Our aim is to study the dynamics of a moving breather travelling through a bent chain. In order to obtain a moving breather, we perturb the velocity of a static breather far from the parabola vertex, launching it to the bent part. Static breathers have been calculated using common methods based on the anticontinuous limit [26–29]. Once a suitable static breather is obtained, it is made movable using the marginal mode method [7,8], which basically consists in adding to the velocities of the static breather a perturbation of magnitude λ colinear to the direction of a linear localized mode, and letting the system evolve in time. In this context, an useful concept for describing the moving breather dynamics is the effective mass [7,8], a measure of the moving breather inertia. If the kinetic energy added to the breather is $E = \lambda^2/2$, it is found that the resulting translational velocity of the breather, v, is proportional to λ [7]. Consequently, moving breathers can be considered as a quasi-particle with mass m^*, which can be defined through the relation:

$$\frac{1}{2}m^*v^2 = \frac{1}{2}\lambda^2 = E. \tag{10}$$

A difficult issue is the choice of appropriate values of the parameters in order to fulfill two different requirements. On the one hand, there is only a small range of them that allows breather mobility. On the other hand, the parameters must be consistent with real DNA. The last aspect is controversial by itself as explained below. The requirement that the breathers can move is our first priority, in agreement with the experimentally observed "breathing" modes in DNA [30,31].

While there exists a general agreement in the literature about the order of magnitude of the parameters D and b, there are not accurate data about the value of the elastic constant k, which oscillates between $0.01eV/\text{Å}^2$ and $10eV/\text{Å}^2$ [10,32]. In their original paper, Peyrard and Bishop [9] used a set of values $D = 0.33$ eV, $b = 1.8$ Å^{-1} and $k = 3.0 \times 10^{-3}$ eV/Å^2. This set of parameters gives a value of $C = 0.014$. Afterwards, Dauxois, Peyrard and Bishop used the values $D = 0.04$ eV, $b = 4.45$ Å^{-1} and $k = 0.06$ eV/Å^2 [11], which imply that $C = 0.038$. Consequently, as C must be greater than 0.12 in order to obtain moving breathers [16], they would not exist in the Peyrard–Bishop model with these values of the parameters.

For a given model, a tuning procedure must be achieved in order to correctly fit the parameters to experimental results. Even the experimental results are controversial as each one refers to different aspect of DNA dynamics (torsion, bending, stretching, ...) [33]. Some recent works propose a generalization of the PB model with different values of the elastic constant k. In [33], the

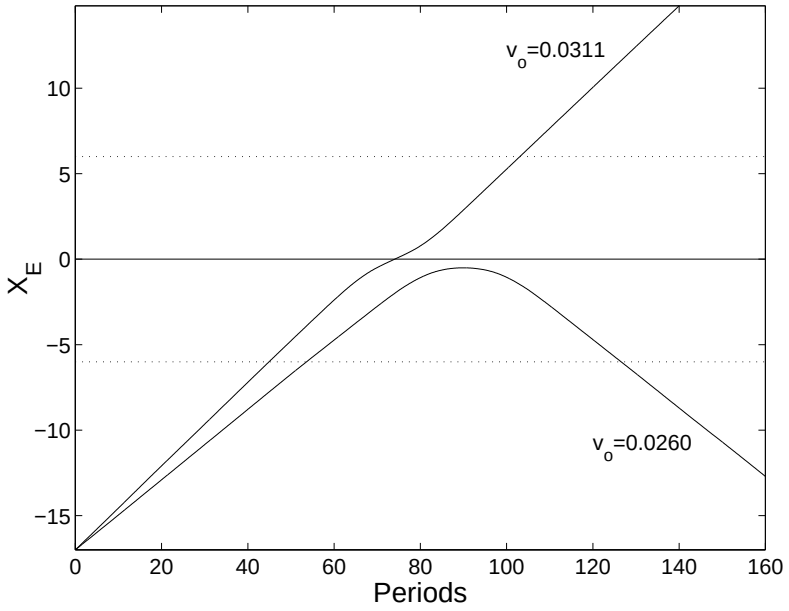

Fig. 1. Evolution of the breather energy centre (X_E) for two different initial velocities. The curvature is $\kappa = 2$.

selected parameter values gives a coupling parameter $C = 0.63$. In [34,32], normal modes corresponding to hydrogen bonds excitations are theoretically investigated, with a range of the coupling parameter $C \in (0.06, 0.31)$ that shows a good agreement with neutron scattering experiments.

In this paper, we have chosen the breather frequency $\omega_b = 0.8$, so that the nonlinear effects are significant but not too strong, as the nonlinearities in DNA are thought to be weak. The stacking and dipole–dipole coupling parameters chosen are, respectively, $C = 0.24$ and $J = 0.02$, which provides with moving breathers with low phonon radiation for small enough values of λ [16]. We have considered different spatial configuration varying the parameter κ.

4 Numerical results

In figure 1 we show the evolution of the energy centre [16] of a moving breather in a bent chain. If the added kinetic energy, $E = \lambda^2/2$ is smaller than a critical value E_c, the breather rebounds, but, if $E > E_c$, the breather passes through the bending point. Figure 2 shows that the critical energy increase monotonically with the curvature.

Bending acts as a hindrance for the movement of breathers. This hindrance reminds to the experimented by a particle in a potential barrier. In this case, breather can be consider as a quasi-particle and this barrier can be calculated by finding the points where breathers rebound (or turning points) for different

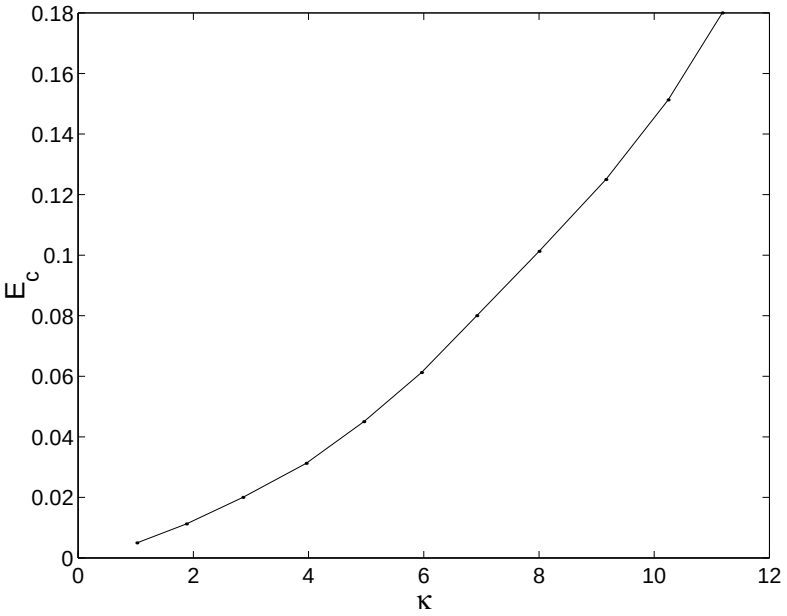

Fig. 2. Critical kinetic energy E_c versus curvature κ.

values of E. Furthermore, if the breather has a constant mass m^*, this potential barrier can be obtained using the expression:

$$E_b = \frac{1}{2}\lambda^2 \left(1 - \left(\frac{v}{v_o}\right)\right) \tag{11}$$

where v is the translational velocity and v_o is its value at $t = 0$. In figure 3 can be observed a good agreement between the barrier calculated using both methods for a given value of κ. The barrier calculated by the second method exhibits an irregular shape, whose origin lies in the non-uniform behaviour of the translational velocity due to the discreteness of the system [35]. This result confirms that, in this case, a moving breather behaves as a particle of constant mass m^*.

For the parameters used in our study, we have observed that the effect of the phonon radiation is not negligible if $E \gtrsim 0.03$, and the properties of the moving breathers change. Thus, in order to have a good agreement between both methods of calculating the potential barrier, the curvature of the parabola must be $\kappa \lesssim 4$ (see figure 2). Otherwise, the value of the energy necessary for a moving breather to cross the bending point will be so high that the phonon radiation will alter the movement.

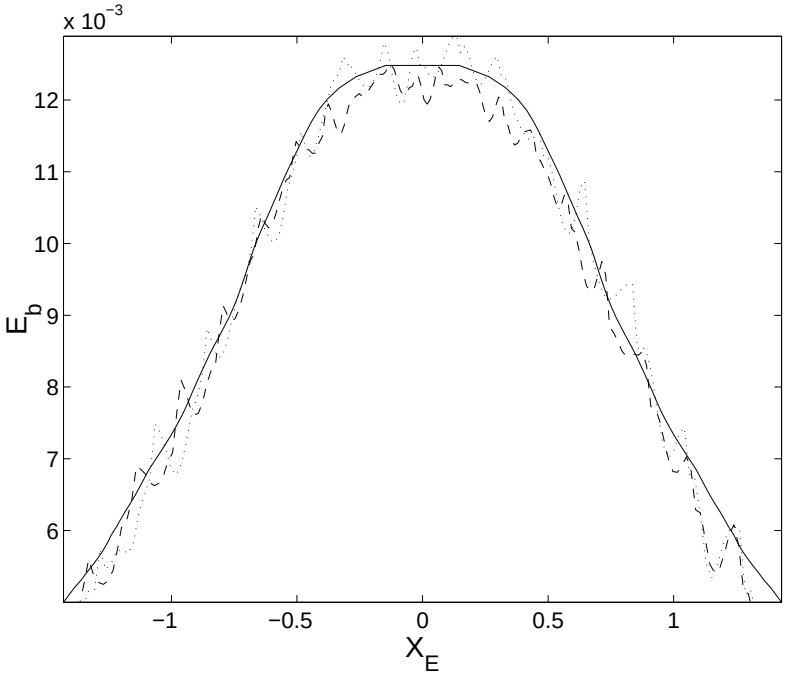

Fig. 3. Potential barrier calculated finding the turning points (solid line) and using Eq. (11) for $E = 0.0162$ (dashed lined) and $E = 0.0200$ (dotted line). The curvature is $\kappa = 2$ and the critical energy is $E_c \approx 0.0126$. The zero value of the energy centre (X_E) represents to the bending point.

5 Conclusions

In this paper, we have studied the behaviour of moving breathers in a bent DNA chain. The movement of a breather is qualitatively similar to the experienced by a particle in a potential barrier. For a given initial velocity, breathers can cross the bending point if the curvature is lower than a critical value. Otherwise, the breather rebounds. This fact suggest that a slight conformational changes in the DNA molecule can modify the dynamic of nonlinear excitations.

Another result is that the breather effective mass remains constant when the breather cross the bending point as long as the curvature is small enough. This fact provides with a method to calculate the instantaneous translational energy, which is given by $E_{\text{trans}} = m^* v^2/2$, being v the translational velocity of the breather. In a recent work, it is proposed a method to calculate the translational energy in a FPU chain based in the asymmetry between the difference between the maxima of the potential and kinetic energies and the total energy of the moving breather [24]. This analysis can be performed because the maximum kinetic and potential energies coincide with the total energy of the static breather, as the interaction potential is spatially symmetric. However, this method cannot be applied in our Klein–Gordon chain because the on–site potential is not spatially symmetric. A further study could consider

a spatially symmetric potential, as the double-well one, in order to find out whether both methods are equivalent.

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