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Numerically exact mobile breathers in Peyrard-Bishop DNA model

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Discrete breathers are spatially localized, time periodic oscillations. They appear in discrete nonlinear systems, particularly in the quasi-linear molecular chains. An interesting example of such objects is the Peyrard-Bishop model of deoxyribonucleic acid molecule (DNA) and its modifications. In the models, discrete breathers precede denaturation bubbles (the regions of separation of complementary chains in the course of the DNA melting). Under certain conditions, such localized oscillations can move and they are known as mobile breathers. There is a systematic method for finding solutions of nonlinear discrete systems in the form of approximate mobile breathers. Approximate mobile breathers have quite a long lifetime, but they move slowly losing energy due to the emission of phonons. However, in nonlinear discrete lattices numerical studies show the existence of so-called numerically exact mobile breathers, moving without loss of energy and changing its shape. The present article deals with these numerically exact mobile breathers in the Peyrard-Bishop model of DNA. A method for finding numerically exact mobile breather is considered. After several oscillation periods, these solutions repeat the same profile but displaced by several lattice sites. Numerically exact mobile breather can be obtained only at certain values of the interparticle interaction describing stacking interaction of DNA.

Keywords: (p/q)-resonant mobile discrete breathers, Peyrard-Bishop DNA model.

1. Introduction

DNA is an interesting object for studies of mobile breathers (MBs). The MBs are responsible for the energy transfer in molecular systems and can be interpreted as precursors of replication and transcription in the DNA molecule [1].

Most articles deal with MB's solutions obtained by adding small perturbations to velocity part of the stationary discrete breathers. These solutions have quite a long lifetime, but they move slowly losing energy due to the emission of phonons and finally stay pinned to the lattice. However, in nonlinear discrete lattices numerical studies show the existence of numerically exact MBs, moving without loss of energy and changing its shape [2-5]. So called (p,q)-resonant numerically exact MBs after qT_b periods ($T_b = 2\pi / \omega_b$ where ω_b – internal frequency of MB) repeat the same profile but displaced by p lattice sites. Numerically exact MBs are the exact solution of model's equation of motions. So it is interesting to study such solutions in the framework of DNA model. The present article deals with these numerically exact MBs in Peyrard-Bishop model of DNA [6].

2. Model

The Peyrard-Bishop model considers that the DNA molecule consists of two polynucleotide chains and represents two chains of disks connected with each other by longitudinal and transverse springs (Fig. 1).

The interaction between the neighboring sites of one chain is described by the harmonic potential $k(u_n - u_{n-1})^2/2$ for the upper chain and $k(v_n - v_{n-1})^2/2$ for the lower chain, respectively, where k is the interaction constant along the chain, u_n and v_n are displacements of nucleotides having mass m from the equilibrium position in directions indicated by arrows. The interaction constant k and the nucleotide mass m in the PB model remain unchanged along the DNA chain. The interaction between sites of different chains is modeled by the Morse potential imitating hydrogen bonds connecting bases of complementary pairs, where D is the dissociation energy of polynucleotide chains and a is the inverse length (the spatial scale of the potential).

The Hamiltonian of the Peyrard-Bishop model has the form:

$$H = \sum_n \left\{ \frac{m}{2}\left(\dot{u}_n^2 + \dot{v}_n^2\right) + \frac{k}{2}\left(\left(u_n - u_{n-1}\right)^2 + \left(v_n - v_{n-1}\right)^2\right) + D\left[1 - \exp\left(-a\left(u_n - v_n\right)\right)\right]^2 \right\}.$$

Here the first term describe the kinetic energy of n-th base pairs. The second term describes nearest-neighbor-range stacking interactions. The third term in Hamiltonian is the Morse potential, which represents the hydrogen bonding of complementary base pair. Let us make the substitution of

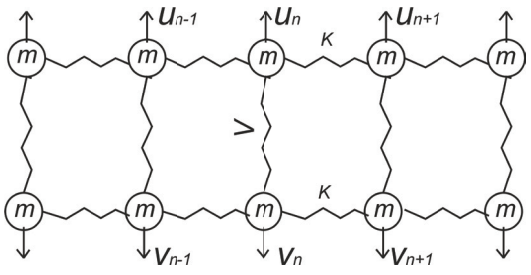

Fig. 1. The Peyrard-Bishop model of DNA.

variables $x_n = (u_n + v_n)/\sqrt{2}$ and $y_n = (u_n - v_n)/\sqrt{2}$ in Hamiltonian. The coordinate x_n describes positions of the center of mass for the pair of bases, and the coordinate y_n describes stretching of hydrogen bonds of the bases:

$$H = \sum_n \left\{ \frac{1}{2}\dot{y}_n^2 + \frac{1}{2}S(y_n - y_{n-1}) + \left[1 - \exp(-\sqrt{2}y_n)\right] \right\} + \\ + \sum_n \left\{ \frac{1}{2}\dot{x}_n^2 + \frac{1}{2}S(x_n - x_{n-1}) \right\},$$

where we introduce dimensionless time $\tau = t\sqrt{Da^2/m}$ and displacement $u_n = ay_n$ and employ original variables $u \to y$ and $\tau \to t$. $S = k/(Da^2)$ is the dimensionless parameter that characterizes the coupling of the oscillators.

The equations of motion corresponding to dimensionless Hamiltonian is:

$$\begin{cases} \dfrac{d^2x_n}{dt^2} = (x_{n-1} - 2x_n + x_{n+1}), \\ \dfrac{d^2y_n}{dt^2} = S(y_{n-1} - 2y_n + y_{n+1}) - \\ -2\sqrt{2}\exp(-\sqrt{2}y_n)\left[1 - \exp(-\sqrt{2}y_n)\right]. \end{cases}$$

Let us focus our attention on a solution of the nonlinear equation of motions for y_n:

$$\ddot{y}_n = S(y_{n-1} - 2y_n + y_{n+1}) - \\ -2\sqrt{2}\exp(-\sqrt{2}y_n)\left[1 - \exp(-\sqrt{2}y_n)\right]. \quad (1)$$

Different values of the parameters are used in different works $D = 0.33$ eV, $a = 1.8$ Å^{-1}, $k = 0.003$ eV/Å^2 [6], $D = 0.1$ eV, $a = 2$ Å^{-1}, $k = 1.5$ eV/Å^2 [7]. The parameter of the stacking interaction is varied in a wide range ($k = 0.003$-4.8 eV/Å^2 [8]). In this case, dimensionless parameter S ranges from 0.002 to 3.75.

3. Methodology

There are two stages to obtaining a numerically exact MB's solutions. Firstly, it is finding the good initial conditions for Newton method and secondly using Newton method with these initial conditions.

Let us consider the first stage of the method: finding the initial conditions for numerically exact MB moving with velocity $v_b = p/(qT_b)$:

1) For a given value of the parameter S and ω_b stationary discrete breather solution $y_n^{st}(0)$ is obtained [9,10];

2) velocity part of this discrete breather is calculated as $\dot{y}_n(0) = -\mu\left(y_{n+1}^{st}(0) - y_{n-1}^{st}(0)\right)/2$, where μ is small parameter;

3) the equations of motion is integrated until time $t = qT_b$;

4) The norm of difference between position of the MB and DB solution shifted by p sites is calculated;

5) Parameter $\mu = \mu_{\min}$, that minimize norm used as perturbation parameter for initial condition for Newton method for finding numerically exact MBs.

4. Results

In this section we introduce obtained numerically exact stable MB's solution for values $\omega_b = 1.8$, $S = 0.6$ numerically exact unstable MB's solution for value $S = 0.44$. Fig. 2 illustrates the initial position profile for the solution, and Fig. 3 shows the initial velocity profile of the solution. The velocity of the solution is $v_b = 1/(12T_b)$.

Specific feature of these solutions is the presence of extended small oscillating tails (Fig. 4,5).

If we introduce local energy at the n-th site of lattice:

$$E_n = \dot{y}_n^2/2 + S\left[(y_{n+1} - y_n)^2 + (y_n - y_{n-1})^2\right]/2 + \\ + \left[1 - \exp(-\sqrt{2}y_n)\right]^2,$$

and center of energy:

$$X_E = \frac{\sum_n (nE_n)}{\sum_n E_n},$$

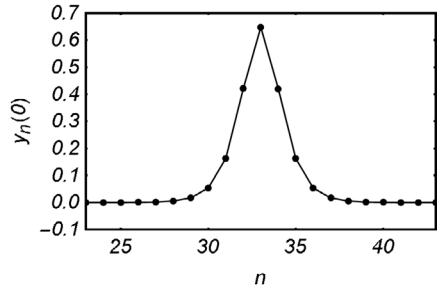

Fig. 2. The initial positions profile of (1,12)-resonant MB.

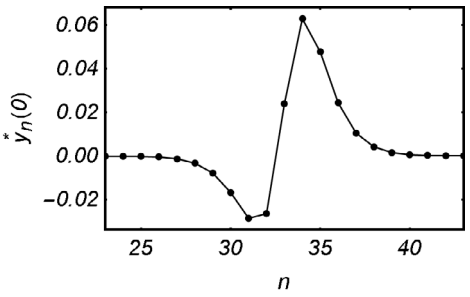

Fig. 3. The initial velocity profile of (1,12)-resonant MB.

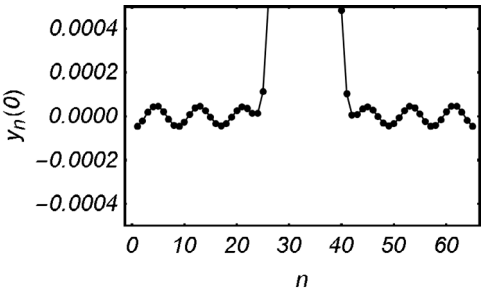

Fig. 4. The tails of initial position profile of (1,12)-resonant MB.

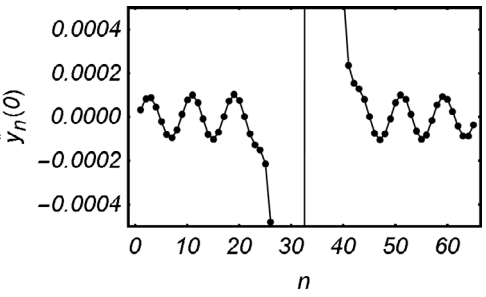

Fig. 5. The tails of initial velocity profile of (1,12)-resonant MB.

then velocity of numerically exact MB may be calculated as:

$$v(t) \approx \frac{X_E(t+\Delta t) - X_E(t)}{\Delta t},$$

where Δt is the short period of time. The velocity of numerically exact MB oscillate about value $v = 1/(12T_b) \approx 0.024$ as shown in the Fig. 6.

The second moment of the energy distribution σ_E is shown in the Fig. 7:

$$\sigma_E = \frac{\sum_n \left\lfloor (n - X_E)^2 E_n \right\rfloor}{\sum_n E_n}.$$

It can be seen that the numerically exact mobile breathers, moving without loss of energy and changing its shape. The total MB's energy was conserved and was approximately equal to $E \approx 0.94$.

Floquet theory can be used to study the linear stability of the obtained solutions. Floquet multipliers λ for the stable (1,12)-resonant MB shown in Fig. 8.

Stable numerically exact MB has a long lifetime and move without radiation Fig.9.

Numerically exact MB can be obtained only at certain values of the interparticle interaction S above some minimal value. For $S < 0.44$ the solutions cannot be obtained. For $0.44 < S < 0.5$ Newton method has very poor convergence, obtained solutions is unstable and have large amplitude tails (Fig. 10, 11).

Such unstable numerically exact MBs (if instability is not so strong) can have quite a lifetime, but finally pinned by lattice and stops Fig 12.

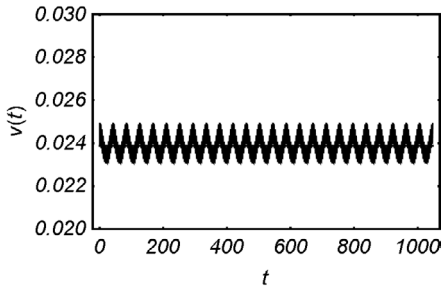

Fig. 6. Velocity evolution of the (1,12)-resonant MB.

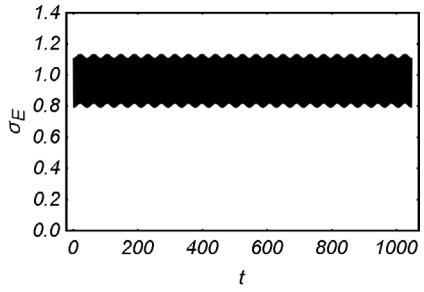

Fig. 7. The second moment of the energy distribution σ_E.

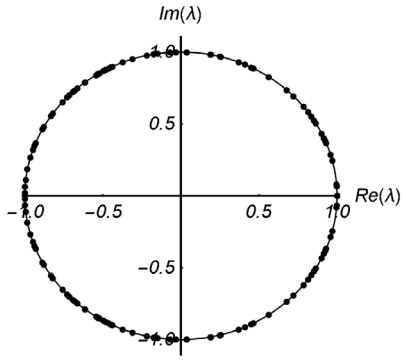

Fig. 8. Floquet eigenvalues of (1,12)-resonant MB.

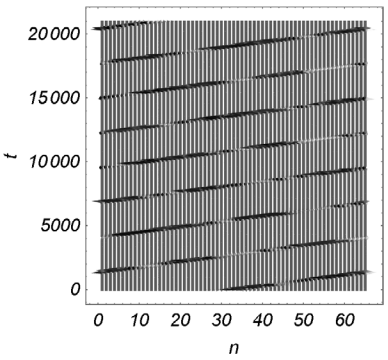

Fig. 9. Time evolution of the of (1,12)-resonant MB in a periodic lattice.

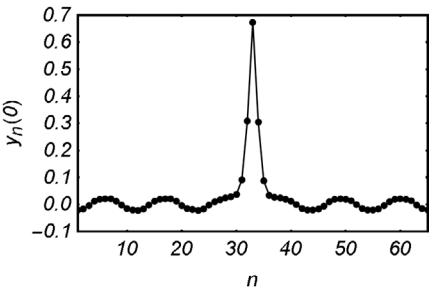

Fig. 10. The initial positions profile of (1,7)-resonant MB.

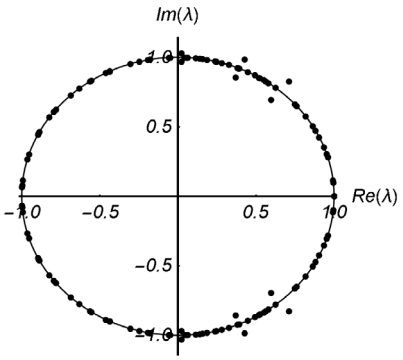

Fig. 11. Floquet eigenvalues of (1,7)-resonant MB.

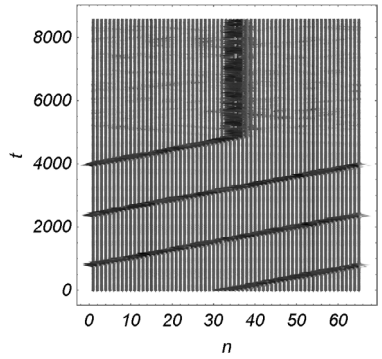

Fig. 12. Time evolution of the of (1,7)-resonant MB in a periodic lattice.

5. Conclusion

In our work numerically exact mobile breathers solutions of equations of motions of Peyrard-Bishop model of DNA are obtained. Such mobile breathers can move along the lattice without loss of energy and change in its shape but for existence of these solutions presence of small oscillating tails is needed. When coupling constant *S* is small the solutions cannot be obtained. When coupling constant *S* grow, highly unstable numerically exact breathers appear and with further growth of the coupling constant the solutions become more stable. It can be expected that the last conclusion is valid for models with other nonlinear interaction potentials.

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