



# Mean Lyapunov exponent approach for the helicoidal Peyrard–Bishop model

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## ABSTRACT

In this Letter, the ordered and disordered regions of the field variable of an oscillator chain are studied. For this purpose, the mean Lyapunov exponent (*MLE*) theory is applied to the helicoidal Peyrard–Bishop (hPB) model. Applying mean Lyapunov exponent theory introduced by Shibata [H. Shibata, *Physica A* 264 (1999) 226] on the model shows that, the system is very sensitive to the potential parameters. By analyzing the behavior of the *MLE* with respect to the harmonic helicoidal coupling (*K*), it can be found that, it is not possible to set the Morse potential parameters of the hPB model in good qualitative agreement with other experimental and theoretical studies. Furthermore, the results show that the *MLE* is independent of length of the DNA chain. This achievement is important since it can be used to overcome the computational difficulties.

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## 1. Introduction

Fifty eight years after the discovery of DNA double helix structure [1], it is still fascinating for physicists, as well as the biologists, who try to unveil its remarkable properties. The study of nonlinear physics of DNA began in 1980 by the work of Englander et al. [2]. A large group of authors, including Yomosa [3], Takeno [4], Krumhansl et al. [5], Fedyanin and coauthors [6], Yakushevich [7,8], Muto et al. [9], Peyrard and Bishop [10,11] and Barbi [12] made contributions to the development of this field. An overview of these attempts can be found also in Ref. [8].

One of the main contributions was made by Peyrard and Bishop (PB) in 1989 to explain the denaturation process of DNA [10]. Taking into account the helicoidal structure of DNA, the PB model was later improved by Dauxois two years later [13,14] to have a more similar behavior to the real DNA chain. In fact, this model is “helicoidal Peyrard–Bishop” model [15] which is sometimes called Peyrard–Bishop–Dauxois model by Zdravkovic et al. [16–19]. This helicoidal Peyrard–Bishop model will be henceforth referred to as the hPB model. While the asymmetry of the DNA chain is neglected [20], the hPB model describes either the radial opening of strands or the unwinding of the double helix, but not both of them simultaneously [21]. Maybe this is why the hPB model didn't use to describe the experimental phenomena such as denaturation and pre-melting processes of the DNA.

The hPB model can describe a solitonic mode in DNA dynamics [13,16–19]. Although the solitonic solutions can be considered as a success for this model but it has been found that, there are also solitonic and even exact solutions for the Peyrard–Bishop (PB) model and its improved version, the Peyrard–Bishop–Dauxois (PBD) model [22,23]. Also, unlike the original PB and PBD models, the solitonic solutions for the hPB model derived in the range of intrinsic parameters (these parameters describe chemical interactions and geometry of the DNA) which is in conflict with theoretical and experimental reports [24–31]. This may well signal a fundamental difficulty of the hPB model.

The highly nonlinear nature of the hPB model implies the possibility of applying the nonlinear dynamics concepts to study its dynamics [8]. The Lyapunov exponent is one of the most popular concepts of the nonlinear dynamics to measure how stable the systems are [32,33]. In 1999 Hiroshi Shibata introduced mean Lyapunov exponent (*MLE*) in order to characterize the chaos in systems described by partial differential equations (PDE) [34]. The *MLE* theory has attracted researchers' attention and has been successfully applied in several fields [31,35–37].

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In this Letter, the *MLE* theory is used to determine the ordered and disordered regions of the hPB model with respect to the potential parameters and the number of base pairs. It is proved that *MLE* shows independent behavior with respect to the chain length. Also, the variation of the *MLE* with respect to the harmonic helicoidal coupling ( $K$ ) is investigated in detail. The obtained results show that, it is not possible to find a satisfactory approximate method for the parameter selection of the Morse potential in the hPB model. This result is expected because, as mentioned above, the model has encountered some difficulties.

## 2. DNA dynamics

In 1989, Peyrard and Bishop developed a simple theoretical model to describe the thermal separation of a DNA chain [10]. An extended form of the PB model developed by Dauxois two years later [13,14].

This mechanical model explains DNA dynamics assuming only transversal oscillations of nucleotides. This Letter is within the framework of the hPB model which takes into account the helical structure of the DNA. This structure implies that the nucleotides in the opposite strands become such close that they can interact. Hence the  $n$ th nucleotide of one strand interacts with the both  $(n-h)$ th and  $(n+h)$ th nucleotides of the opposite strand. Indeed, there are about 10 base pairs per turn of the DNA helix, it is common to set  $h=5$  [18].

The Hamiltonian for the hPB model can be written as [16]

$$H = \sum_{n=1}^N \left[ \frac{1}{2} m (\dot{u}_n^2 + \dot{v}_n^2) + \frac{1}{2} k [(u_n - u_{n-1})^2 + (v_n - v_{n-1})^2] + \frac{1}{2} K [(u_n - u_{n-h})^2 + (v_n - v_{n-h})^2 + D(e^{-\alpha(u_n - v_n)} - 1)^2] \right]. \quad (1)$$

Here  $k$  and  $K$  are the harmonic constants of the longitudinal and helicoidal springs, respectively. The last term is the Morse potential with depth  $D$  and the inverse width is  $\alpha$ .

It is more convenient to describe the motion of two strands in terms of the variables

$$x_n = \frac{(u_n + v_n)}{\sqrt{2}}, \quad y_n = \frac{(u_n - v_n)}{\sqrt{2}} \quad (2)$$

which represent the in-phase and out-of-phase motions, respectively. According to Eqs. (1) and (2), one can obtain two perfectly decoupled equations of motion:

$$m\ddot{x} = k(x_{n+1} + x_{n-1} - 2x_n) + K(x_{n+h} + x_{n-h} - 2x_n), \quad (3)$$

$$m\ddot{y} = k(y_{n+1} + y_{n-1} - 2y_n) + K(y_{n+h} + y_{n-h} - 2y_n) + 2\sqrt{2}\alpha D e^{-\sqrt{2}\alpha y_n} (e^{-\sqrt{2}\alpha y_n} - 1)^2. \quad (4)$$

Eq. (3) is only a simple linear dynamical equation of motion while Eq. (4) is nonlinear as it includes the Morse potential. In this work, we are interested in Eq. (4), because it is highly nonlinear.

To stability analysis, it is convenient to transform the second-order differential Eq. (4) into an autonomous system of first-order differential equation of the following form:

$$\begin{cases} \dot{y}_n = w_n; \\ \dot{w}_n = k(y_{n+1} + y_{n-1} - 2y_n) + K(y_{n+h} + y_{n-h} - 2y_n) + 2\sqrt{2}\alpha D e^{-\sqrt{2}\alpha y_n} (e^{-\sqrt{2}\alpha y_n} - 1)^2. \end{cases} \quad (5)$$

If we use the explicit finite difference method, Eq. (5) will take the following form:

$$\begin{cases} y_n^{i+1} = y_n^i + \Delta t w_n^i; \\ w_n^{i+1} = w_n^i + k\Delta t (y_{n+1}^i - 2y_n^i + y_{n-1}^i) + K\Delta t (y_{n+h}^i - 2y_n^i + y_{n-h}^i) + 2\sqrt{2}\alpha D \Delta t e^{-\sqrt{2}\alpha y_n^i} (e^{-\sqrt{2}\alpha y_n^i} - 1). \end{cases} \quad (6)$$

Then we consider the linear stability or the  $2N \times 2N$  Jacobian matrix written as:

$$B_{k,N} = \begin{pmatrix} \frac{\partial y_1^{k+1}}{\partial y_1^k} & \frac{\partial y_1^{k+1}}{\partial y_2^k} & \frac{\partial y_1^{k+1}}{\partial y_3^k} & \dots & \frac{\partial y_1^{k+1}}{\partial y_N^k} & \frac{\partial w_1^{k+1}}{\partial y_1^k} & \frac{\partial w_1^{k+1}}{\partial y_2^k} & \frac{\partial w_1^{k+1}}{\partial y_3^k} & \dots & \frac{\partial w_1^{k+1}}{\partial y_N^k} \\ \frac{\partial y_2^{k+1}}{\partial y_1^k} & \frac{\partial y_2^{k+1}}{\partial y_2^k} & \frac{\partial y_2^{k+1}}{\partial y_3^k} & \dots & \frac{\partial y_2^{k+1}}{\partial y_N^k} & \frac{\partial w_2^{k+1}}{\partial y_1^k} & \frac{\partial w_2^{k+1}}{\partial y_2^k} & \frac{\partial w_2^{k+1}}{\partial y_3^k} & \dots & \frac{\partial w_2^{k+1}}{\partial y_N^k} \\ \vdots & \vdots & \vdots & \dots & \vdots & \vdots & \vdots & \vdots & \dots & \vdots \\ \frac{\partial y_N^{k+1}}{\partial y_1^k} & \frac{\partial y_N^{k+1}}{\partial y_2^k} & \frac{\partial y_N^{k+1}}{\partial y_3^k} & \dots & \frac{\partial y_N^{k+1}}{\partial y_N^k} & \frac{\partial w_N^{k+1}}{\partial y_1^k} & \frac{\partial w_N^{k+1}}{\partial y_2^k} & \frac{\partial w_N^{k+1}}{\partial y_3^k} & \dots & \frac{\partial w_N^{k+1}}{\partial y_N^k} \\ \frac{\partial y_1^{k+1}}{\partial y_1^k} & \frac{\partial y_1^{k+1}}{\partial y_2^k} & \frac{\partial y_1^{k+1}}{\partial y_3^k} & \dots & \frac{\partial y_1^{k+1}}{\partial y_N^k} & \frac{\partial w_1^{k+1}}{\partial y_1^k} & \frac{\partial w_1^{k+1}}{\partial y_2^k} & \frac{\partial w_1^{k+1}}{\partial y_3^k} & \dots & \frac{\partial w_1^{k+1}}{\partial y_N^k} \\ \frac{\partial w_1^{k+1}}{\partial y_1^k} & \frac{\partial w_1^{k+1}}{\partial y_2^k} & \frac{\partial w_1^{k+1}}{\partial y_3^k} & \dots & \frac{\partial w_1^{k+1}}{\partial y_N^k} & \frac{\partial w_1^{k+1}}{\partial y_1^k} & \frac{\partial w_1^{k+1}}{\partial y_2^k} & \frac{\partial w_1^{k+1}}{\partial y_3^k} & \dots & \frac{\partial w_1^{k+1}}{\partial y_N^k} \\ \frac{\partial y_2^{k+1}}{\partial y_1^k} & \frac{\partial y_2^{k+1}}{\partial y_2^k} & \frac{\partial y_2^{k+1}}{\partial y_3^k} & \dots & \frac{\partial y_2^{k+1}}{\partial y_N^k} & \frac{\partial w_2^{k+1}}{\partial y_1^k} & \frac{\partial w_2^{k+1}}{\partial y_2^k} & \frac{\partial w_2^{k+1}}{\partial y_3^k} & \dots & \frac{\partial w_2^{k+1}}{\partial y_N^k} \\ \vdots & \vdots & \vdots & \dots & \vdots & \vdots & \vdots & \vdots & \dots & \vdots \\ \frac{\partial y_N^{k+1}}{\partial y_1^k} & \frac{\partial y_N^{k+1}}{\partial y_2^k} & \frac{\partial y_N^{k+1}}{\partial y_3^k} & \dots & \frac{\partial y_N^{k+1}}{\partial y_N^k} & \frac{\partial w_N^{k+1}}{\partial y_1^k} & \frac{\partial w_N^{k+1}}{\partial y_2^k} & \frac{\partial w_N^{k+1}}{\partial y_3^k} & \dots & \frac{\partial w_N^{k+1}}{\partial y_N^k} \end{pmatrix} \quad (7)$$

the mean Lyapunov exponent is defined as [34]:

$$\lambda_k = \frac{1}{N} \ln |B_{k,N}|, \quad (8)$$

where  $|B_{k,N}|$  means the determinant of matrix  $B_{k,N}$ .

By considering  $B_{k,N}$  for Eq. (6) the *MLE* value can be calculated. In this Letter, we use the *MLE* theory to study the ordered and disordered regions of the hPB model (Eq. (6)) with respect to the parameters:  $\alpha$ ,  $D$ ,  $k$  and  $K$ .

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