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Soliton Dynamics Analysis of Peyrard-Bishop-Dauxois DNA Model Using 4th Order Morse Potential Approach

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Abstract

This research has been carried out to analyze the dynamics of the soliton DNA of the Peyrard-Bishop-Dauxois (PBD) model with fourth-order -approximation Morse Potential. The research aims to know the physical changes of the PBD model with 4th-order -approximation Morse Potential on the stable and unstable state in describing the denaturation process of DNA. The process was carried out by finding a numerical solution of the 4th-order NLS $F\left(x_{i,}t_{j+1}\right)$*as stable equation using the finite-difference method. Then, the result was simulated by Matlab. The results show that on the stable state, expanded Morse Potential for 4th-order than for 3th-order rastically increased oscillation amplitude from 1.89 pm to 16 pm. On the first unstable state, the stable equation* $F\left(x_{i,}t_{j+1}\right)$ *was multiplied by (1+ε), where the value of ε= 0.25. On the second unstable state, the stable equation* $F\left(x_{i,}t_{j+1}\right)$*was multiplied two times by (1+ε) where the value of ε= 0.25. On three of them, the amplitude of oscillation decreased from 16 pm, 2.9 pm to 2.5 pm. Compared to the previous order, there is a new addition to the 4th-order Morse Potential coefficient γ, which has the physical meaning that more considerable expansion requires more significant dissociation energy. So it can be concluded that the PBD model of DNA can descriptively explain the biological phenomenon of denaturation in DNA.*

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Abstract

Telah dilakukan penelitian untuk menganalisis dinamika soliton DNA model Peyrard-Bishop-Dauxois (PBD) dengan pendekatan Potensial Morse orde ke-4. Penelitian ini bertujuan untuk mengetahui perubahan fisis model DNA PBD dengan Potensial Morse orde ke-4 pada keadaan stabil dan gangguan. Proses dilakukan dengan mencari solusi numerik dari NLS orde ke-4 $F\left(x_{i,}t_{j+1}\right)$ *sebagai persamaan stabil menggunakan metode beda-hingga. Hasil persamaannya kemudian disimulasikan menggunakan Matlab. Hasil ditemukan bahwa pada keadaan stabil, ekspansi Potensial Morse pada orde ke-4 dibandingkan orde ke-3, mengalami peningkatan amplitudo osilasi secara drastis dari 1,89 pm menjadi 16 pm. Pada keadaan gangguan pertama, persamaan stabil* $F\left(x_{i,}t_{j+1}\right)$ *dikalikan dengan (1+ε) dimana nilai ε = 0.25. Pada keadaan gangguan kedua, persamaan stabil* $F\left(x_{i,}t_{j+1}\right)$ *kembali dikalikan dengan (1+ε) sebanyak dua kali, dimana nilai ε = 0.25. Pada ketiga keadaan, amplitudo osilasi menurun dari 16 pm menjadi 2,9 pm dan 2,5 pm. Dibandingkan orde ke-3 pada orde ke 4 terjadi penambahan baru pada koefision potensial morse orde ke-4 γ yang memiliki makna fisis bahwa ekspansi yang lebih besar membutuhken energi disosiasi yang lebih besar juga. Sehingga dapat disimpulkan bahwa model DNA PBD secara deskriptif mampu menjelaskan fenomena biologis denaturasi di DNA.*

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1. Introduction

The ability to live things to inherit genetic information is a biological phenomenon that can be studied physically. Inheritance requires DNA which is an essential part of the Process of regenerating the traits to be inherited (Wilson, *et al* 2007). The sequence of DNA base pairs is the main factor for forming DNA structures in living things (Peyrard, 2004).

The double helix structure of DNA is very dynamic. Base pairs, seen as moving atoms, are one of the objects of study in biophysics (Englander et al., 1980). The interaction of these base pairs makes protein synthesis into the genetic information code (Williams & Maher, 2010).

The stretching interaction between base pairs/nucleotides can be seen as the internal movement of DNA. If examined physically, it will produce a nonlinear effect accompanied by the appearance of a soliton wave (Sulaiman *et al.,* 2012). The Peryrad-Bishop-Dauxois model, which will be shortened to the PBD model, is intended to describe the process of stretching DNA nucleotide pairs, known as the denaturation process (Zdar v Kovic and Sataric, 2001). Solitons in the PBD model DNA will be represented by Morse potentials so that the stretching of hydrogen bonds as binding bonds in different chains can be appropriately described (Gao *et al,* 1984).

Switenia's research (2012) analyzed the PBD model numerically on the third order, resulting in a wave amplitude of 1.89 pm with a decreasing disturbance state. Hermanudin's (2011) research analytically on the fourth-order PBD model resulted in an increase in the Morse Potential Order coefficient due to the nonlinearity effect. Although the two studies produced differences in the physical meaning, they could still describe the phenomenon of denaturation in DNA. Therefore, this study was conducted to look at the physical results of the fourth-order PBD model numerically and describe the denaturation process that occurs in the PBD model.

2. Research methods

The tool used in this research is *Matlab software* to simulate the derivative of the fourth-order NLS equation of the PBD model that has been derived by the finite difference method. The finite difference method used is the main difference.

2.1 Finite-difference method

Before simulating in the *MATLAB program*, the derivation of **Equation (1)** as a general equation of the 4th-order PBD model with the finite difference method becomes **Equation (2**). **Equation 1** was obtained through Hermanudin's (2012) research on the fourth-order PBD model, which was carried out analytically. Q and R are the PBD model's nonlinear coefficient, and P is the dispersive coefficient because the wave passes through the dispersion medium.

$$i\frac{\partial F}{\partial t} + P\frac{\partial^2 F}{\partial x} + Q|F|^2F + R|F|^4F = 0 \tag{1}$$

$$\begin{aligned} F(x_i, t_{j+1}) &= 2i\frac{\Delta t}{\Delta x^2}P\big(F(x_{i+1}, t_j) - 2F(x_i, t_j) + F(x_{i-1,}t_j)\big) \\ &+ Q\left|F((x_{i,}t_j)\right|^2 Fx_it_j + F(x_{i,}t_{j-1}) + R\left|F((x_{i,}t_j)\right|^4 Fx_it_j = 0 \end{aligned} \tag{2}$$

Then, in **Equation (1),** the parameters are re-scaled to make the first disturbance state with the second disturbance state. **Equation (3)** becomes the Equation that will be simulated as the first disturbance state, while **Equation (4**) will be simulated as the second disturbance state. Scoreψ and φrepresented as the value of the relationship function of the nucleotide position from one order to another. The four equations are then written in *the Matlab program* with input parameters according to the PBD model literacy. The input parameters can be seen in **Table 1.** These are obtained by combining the input parameters of the research of Switenia (2011) and Zdravkovic and Sataric (2009) in selecting the geometric parameters.

$$F(x_i\, t_j) = \frac{\sqrt{2}}{\psi}\operatorname{sech}\left(\frac{x}{\sqrt{\varphi}}\right)(1+\varepsilon) \tag{3}$$

$$F(x_i\, t_j) = \frac{\sqrt{2}}{\psi}\operatorname{sech}\left(\frac{x}{\sqrt{\varphi}}\right)(1+\varepsilon)\frac{x}{\sqrt{\varphi}}(1+\varepsilon) \tag{4}$$

3. Results and Discussions

Three conditions was similated and analyzed are stable state, first disturbance state, and second disturbance state. All those three have been expanded to Morse Potential up to the fourth order.

Table 1. 4th order PBD model input parameters.

No.	Input Parameters	Information
1.	$dx = 0.001$ m	The position of the nucleotide at the equilibrium
2.	$dt = 0.000025$s	Nucleotide time at equilibrium
3.	$D = 9.6 \times 10^{-9}$ eV	Morse potential depth
4.	$e_1 = 0.0001$	3rd order morse potential expansion value
5.	$m = 5.1 \times 10^{-13}$ kg	Nucleotide mass
6.	$a = 0.9 \times 10^{-9}$ m	The spacing between the nucleotides of the chains differs at equilibrium
7.	$k = 5.370$ N/m	The chained harmonic constants are equal at equilibrium
8.	$K = 1.146$ N/m	The chained harmonic constants differ at equilibrium
9.	$l = 3.4 \times 10^{-13}$ m	The distance between the nucleotides in the same type of chain has been expanded to the fourth order morse potential
10.	know $(\Omega t) = 0$	Angle frequency versus time
11.	$h = 5$ base pairs	The number of base pairs per turn
12.	$e2 = 0.001$	Morse 4th order potential expansion values
13.	$\varphi = 0.001$	The value of the relationship between F_1 and F_0
14.	$\psi = 0.002$	The value of the relationship between F_1 and F_2

3.1 Stable State

Equation (2) was a function of the nucleotide position nl to see how far apart the two nucleotides are when denatured from the equilibrium position. **Equation (5)** became the wave oscillation equation with respect to time $Y_n(t)$for the PBD model made by Dauxois (1993). Then, **Equation (2)** and **Equation (5)** plotted so that the results represent the stable state. In a stable state, these results was compared with the results of the Switenia study (2012), where the research was conducted using the PBD model with third-order Morse Potential with a numerical approach. Then, Hermanudin's research (2011) becomes a reference for analyzing the following research results.

$$Y_n(t) = 2\varepsilon A \sec h\left[\frac{\varepsilon(nl - V_e t)}{L_e}\right] \times \left(\cos(\theta nl - \Omega t) + \varepsilon A \sec h[\varepsilon(nl - V_e t)/L_e] \times \left\{\frac{1}{2}\mu + \delta\cos\big(2(\theta nl - \Omega t)\big)\right\} + O\varepsilon^3\right) \tag{5}$$

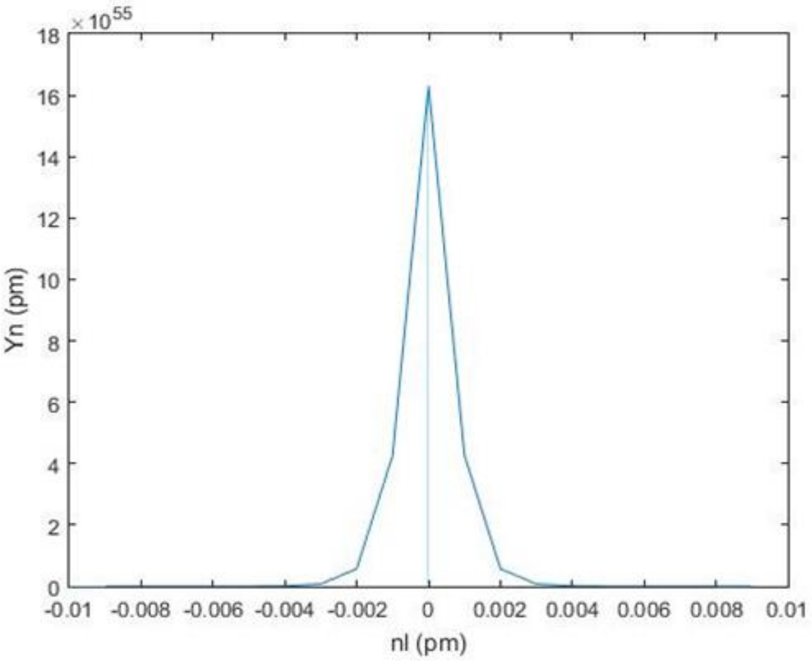

Figure 1. Graph of amplitude and distance relationships between nucleotides in a stable state

Figure 1. showed nl that those who experienced a separation of > 0.002 pm this result was relatively small compared to Switenia's (2011) study, which was separated by 20 pm. In Zdrakovic and Tabi's research (2010), when comparing the two approaches, namely the PBD DNA model with the Jacobian Elliptical Function DNA model to describe denaturation computationally, it was concluded that a directly proportional relationship where a decrease in k causes a decrease in A/nl. Changes in geometric values in each order can be seen in **Table 2.**

At k *values*, a harmonic constant in the same chain directly relates to the degree of separation of nucleotides A/nl moment of denaturation. The changes that occur are not only in nl but also in $Y_n(t)$ that was as nucleotide oscillations. In Siwtenia's study (2011), the wave oscillation obtained in the third order reached 1.89 pm. Whereas in the fourth order shown in **Figure 1. it** is obtained at 16 pm. This value has increased drastically compared to the previous order. However, according to Yakushevich's research (1989) that the standard equilibrium vibration is an amplitude oscillation not exceeding and not less than 0.1 Å so that in this case, the oscillation value obtained is 0.16 Å it can still be stated that the nucleotides are not in equilibrium, so the denaturation process still occurs.

Table 2. Changes in geometric parameters in every order.

Order (Morse Potential)	**Change of Geometric Parameters**			
	a (m)	k (N/m)	K(N/m)	D (eV)
1	$0.9\text{x}10^{-9}$	5.370	1.146	$9.6 \text{ x } 10^{-9}$
2	$0.9\text{x}10^{-9}$	3.112	1.218	$9.784 \text{ x } 10^{-9}$
3	$0.9\text{x}10^{-9}$	2.56	2.67	$9.9321 \text{ x } 10^{-9}$
4	$0.8\text{x}10^{-12}$	1.65	1.65	$10.2 \text{ x } 10^{-9}$

3.2 First Disturbance State

In this situation, it can be seen in **Figure 2.** that the values nl in the stable state are separated by 0.004 pm, while in this state, it reaches > 0.008 pm. Shows that amplitude disturbances also have an impact on the degree to which nucleotides are separated from the equilibrium point. The oscillation amplitude also decreased from 16 pm to 2.9 pm. Let us look more closely at **Figure 2.** for the oscillation amplitude Y_n close to the value of 1 pm. The distance widening reaches > 0.006 pm while in a stable state with a distance of > 0.002 pm. The oscillation amplitude Y_n approaches the value of 2 pm, meaning that Y_n, as a traveling wave in a dispersive medium, experiences inhibition due to interference amplitude.

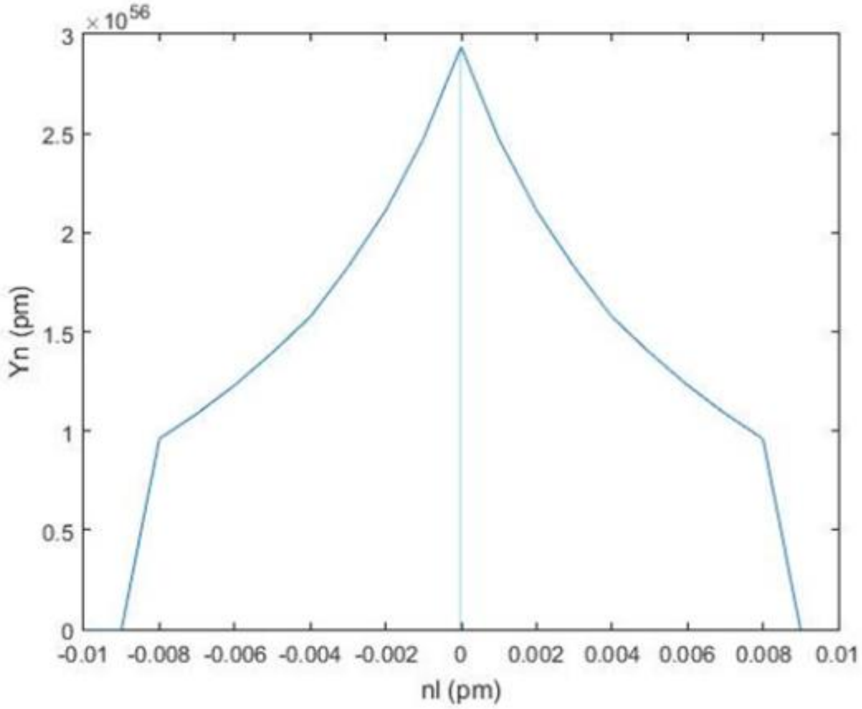

Figure 2. Graph of the relationship between the amplitude and the distance between the nucleotides in the first disturbance state

3.3 Second Disturbance State

In this situation, it can be seen in **Figure 3.** which shows that the value nl remains > 0.08 pm so that the representation of nl as a geometric variable separates the nucleotides. In this case, the disturbance does not have a significant impact due to the absence of nl a drastic change in value. Significant changes in this condition occurred $Y_n(t)$ when the amplitude oscillations at the two nucleotides decreased by 2.5 pm. This value, converted to angstroms, becomes 0.025 Å, not close to the 0.1 equilibrium vibration limit value Å according to research by Yakushevich (1989). This means that the disturbance given to the traveling wave oscillations in the DNA model keeps the two nucleotides out of their equilibrium position so that the denaturation process occurs.

In both cases, by comparing the graph in **Figure 2**. and **Figure 3**. at nl the same time > 0.08 pm, the change in the direction of the graph slopes upwards before it hits the value of 1 pm, while in the second disturbance, it occurs in conditions exceeding 1 pm. The difference can be seen in that multiplying twice (1+ ε) to the function $F(x_i\, t_j)$ in Equation (36) does not significantly impact nl but $Y_n(t)$.

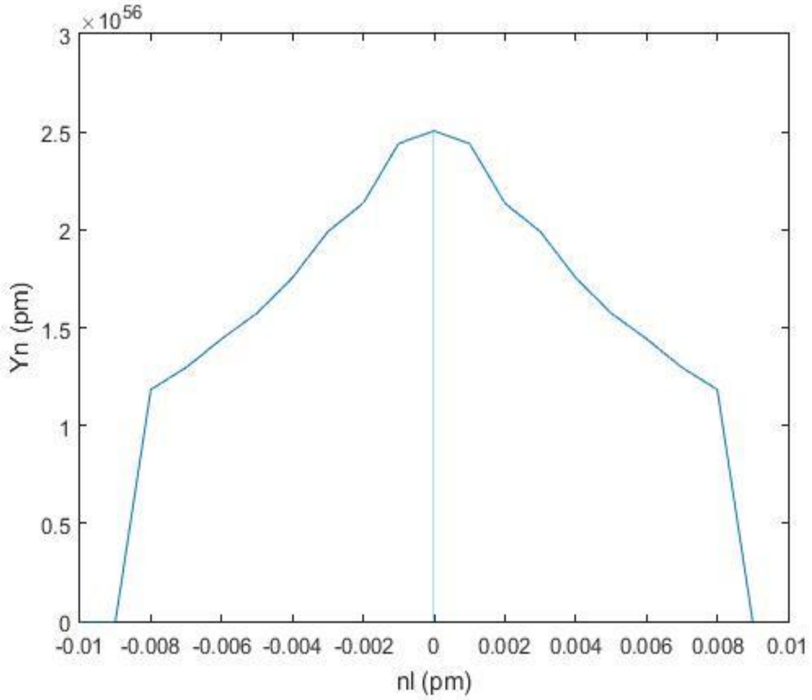

Figure 3. Graph of the relationship between the amplitude and the distance between the nucleotides in the second disturbance state

4. Conclusion

Based on research that has been carried out, changes in physical values such as amplitude oscillations $Y_n(t)$ and nl, those that occur in the fourth-order PBD DNA model, can still describe the denaturation process of DNA well. The disturbance state created also affects the value $Y_n(t)$ and nl in the fourth order PBD model so that it can be found the cause of the separation of the two nucleotides in the denaturation process.

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