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Soliton-like Solution on the Dynamics of Modified Peyrard-Bishop DNA Model in the Thermostat as a Bio-Fluid

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Abstract

The Peyrard-Bishop (PB) DNA model is the most representative model to investigate DNA dynamics because the model is able to answer DNA denaturation processes even though the model has restricted review that DNA assumes without surrounding interaction. In this study, we investigate the dynamics of the modified PB DNA model by considering DNA in the Nosé-Hoover thermostat as a bio-fluid with various viscosities. Viscosity variations are reviewed through temperature variations, namely thermal viscosity. We attain the dynamical equation of DNA in the form of a nonlinear Schrödinger-like (NLS-like) equation by using the perturbation method and continuous approximation. We solve the NLS-like equations by the numerical split-step Fourier method. We obtain a soliton-like solution for the dynamics of this specific DNA model. The behavior of the soliton-like solution fluctuates as the temperature increases, representing the fluctuational openings of DNA, i.e., denaturation bubbles. In addition, that behavior also evolves with variations of the perturbation parameter. Moreover, we obtain soliton-like solutions by balancing the perturbation and the nonlinearity of the DNA system from the bio-fluid interaction. Furthermore, for the specific thermal viscosity of bio-fluid, we gain the denaturation temperature at $370\ K \leq T \leq 380\ K$.

Keywords:

Soliton-like Solutions;
NLS-like Equation;
Peyrard-Bishop DNA Model;
Nosé-Hoover Thermostat;
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1- Introduction

Geneticists may not have to think twice about who discovered DNA for the first time. James Watson and Francis Crick, two scientists who won the Nobel Prize in physiology or medicine in 1962, are recognized figures who have introduced DNA since 1953 [1]. An in-depth study of DNA started about a century and a half ago by a young German biochemist, Frederich Miescher, who revealed that DNA is the smallest component in living cells [1, 2]. At that time, Frederich Miescher's study discovered the chemical structure of DNA in the form of a deoxyribonucleic acid chemical compound known to be different from protein chemical compounds [1, 3, 4]. Nowadays, DNA is obviously recognized as a dynamic biomolecule located in the cell nucleus containing genetic information that determines all cell life forms [5-9]. In Nano-scale dimensions, DNA is a large molecule consisting of several molecules [7, 10]. DNA study is inseparable from the involvement of multidisciplinary sciences because it is a very complex set of problems. One of the sciences that attracts attention to this issue is the branch of biophysics, e.g., the molecular dynamics of DNA.

The use of physics principles in a bio-molecular system such as DNA to discuss the system's process and dynamic properties, wherewith other disciplinary approaches only differ statically [11]. The dynamic processes of DNA were

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expressed for the first time in the 1980s through a nonlinear Hamiltonian model by Englander et al. [7, 12-14]. After that period, the study developed rapidly and attracted the interest of several physicists. Until now, it has become a part of modern biophysical research. Several past studies have succeeded in demonstrating and developing Hamiltonian models of the dynamics of nonlinear DNA [15-21]. The most popular Hamiltonian model and considered successful in explaining DNA dynamics effectively so that the phenomenon of thermal denaturation is the Hamiltonian model introduced by Peyrard and Bishop in 1989 [5, 19-21], also known as the PB DNA model. Dauxois revised the PB DNA model for a more realistic case review [2, 5, 22-25]. The modification of the PB DNA model continues to be carried out under the physical purpose of being deeply studied [11, 20, 21, 26].

The formulation of the Hamiltonian in the DNA model develops by including the kinetic and potential energy of the system, where DNA is reviewed as a system that experiences vibrations through harmonic and anharmonic oscillations [19, 27]. Furthermore, more complexly, this basic concept involves vectors that describe (1) torsional, transverse, and longitudinal displacements; (2) angles of rotation of base pairs around sugar and phosphate chains; (3) the distance between the base pairs; and also (4) DNA radius. Additionally, that concept also involves other quantities such as (1) coupling constants along each DNA strand, (2) nucleotide masses, and (3) the potential function that describes the interaction between the base pairs. Interestingly, the graphical view of a solution to the model DNA dynamics is a soliton phenomenon, representing the local opening of DNA base pairs [7, 12, 28]. Soliton has an essential role in the transcription process in transferring genetic information. Two DNA strands must be separated at least locally to copy genetic information and undergo local opening like a soliton. In this case, solitons arise when DNA is reviewed as a nonlinear system using the rules of physics [7, 11]. Soliton is known as a signal of a wave phenomenon with extraordinary stability symptoms. Solitons may arise from the modulation instability activity of plane waves in the DNA system. The modulation instability leads to delocalization, i.e., in the system wave number excitation, in the momentum space, which is equal in the positional space, thus forming a localized soliton and coherent wave structure [12]. Many researchs suggest that soliton excitation can present conformal soliton in the DNA system [13, 28, 29].

This manuscript is organized from the essential motivation to modify the DNA Hamiltonian by involving the solvent potential. This idea accommodates the interaction effect between DNA dynamics and the surrounding fluid. However, this idea is insufficient enough due to the solvent potential is time-independent. Therefore, we also review the DNA system in an artificial thermostat that depends on time in the form of a Nosé-Hoover thermostat, representing the bio-fluid under realistic DNA conditions. Furthermore, we use the perturbation method and continuous approximation to obtain the equation of motion in the NLS-like equation. After solving the equation using the numerical split-step Fourier method, we obtain a soliton-like solution. The existence of soliton reveals that DNA dynamics occur in a nonlinear realm. In addition, these results also explain how the dynamics of the genetic information transfer process in a DNA system. Furthermore, for a specific viscosity, this DNA model is able to explain the phenomenon of denaturation.

2- Hamiltonian in DNA System

The Hamiltonian of the DNA system represents the energy state of the physical and chemical processes along the DNA chain. The basic structure of the DNA strand consists of nucleotides that link to the others [30-32]. A nucleotide consists of sugar, phosphate, and nitrogenous bases in (1) purines; adenine (A) and guanine (G), and (2) pyrimidines; cytosine (C) and thymine (T), as shown in Figure 1. Each nitrogenous base from the different strands is connected by a weak hydrogen bond, namely base pairs. The connections of two strands form a spiral known as the double helix [31, 32].

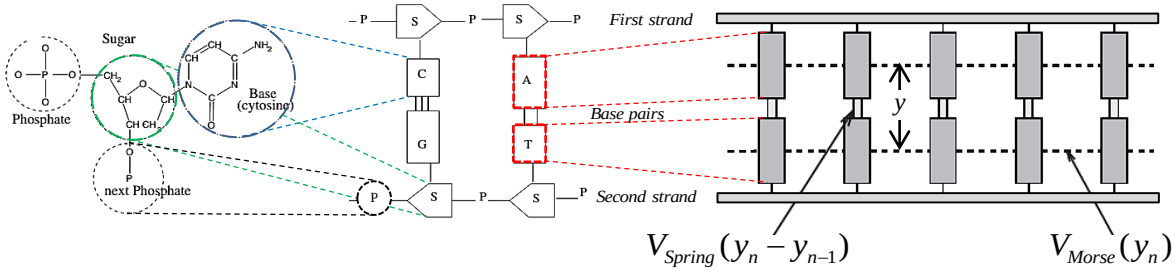

Figure 1. The illustration of nucleotide chemical compounds constructs the mathematical model of DNA double strands [33]

DNA has a structure whose outer side contains sugar and phosphate, forming two long strands of the top and bottom (Figure 1). The possible combination between the two pairs allowed A-T and G-C bases. The sugar-phosphate chemical bonds are more rigid than the hydrogen bonds of the two bases [31]. When DNA undergoes vibrations, assuming the n base pair is stretched, the perturbation will be transmitted to the nearest neighbor to $n + 1$ and $n - 1$, so on for the other base pairs. The perturbation in a realistic system is the interaction between DNA and other biomolecules such as protein [29]. To explain this process, we begin by describing the energy states of the DNA system in the Hamiltonian model as follow,

$$H=\sum_{n=1}^{N}\frac{m\dot{y}_n^2}{2}+V_{Spring}\left(y_n,\ y_{n-1}\right)+V_{Morse}\left(y_n\right)+V_{Solvent}\left(y_n\right). \tag{1}$$

The interactions between base pairs [2, 17, 21] describe by the summation of the kinetic and potential energies. The Hamiltonian model shown by Equation 1 has been modified from PB Hamiltonian by adding the potential term, namely the solvent potential. The three potential forms in the Hamiltonian above have different physical representations [13, 21], which are:

$$V_{Spring}\left(y_n,\ y_{n-1}\right) = \frac{K}{2}\left(y_n-y_{n-1}\right)^2, \tag{2-a}$$

$$V_{Morse}\left(y_n\right) = D\left(e^{-\alpha y_n}-1\right)^2, \tag{2-b}$$

$$V_{Solvent}\left(y_n\right) = -D\zeta\left[\tanh\left(\frac{y_n}{L}\right)-1\right]. \tag{2-c}$$

The potential spring arises from the reason when the base in a certain position experiences interaction with the neighboring base. In this case, an overlap occurs, allowing the value y_n to approach the value y_{n-1} at any time, and the potential will be the maximum value when $y_n = y_{n-1}$ [31]. The term of the spring potential is obtained from the approximation of harmonic motion when the DNA vibrates, where K is the coupling constant. In the other hand, Morse potential plays a role in explaining the interactions between base pairs, such as A-T and G-C pairs, where D is the depth of the potential well and α is a spatial scaling factor [21, 31]. For a more realistic case, the DNA system is assumed in a liquid affected by the viscosity effect of the fluid called the dissipation effect; this is represented by the solvent potential [13, 21]. An illustration of the involvement of solvent potential to the base pair stretching is shown in Figure 2.

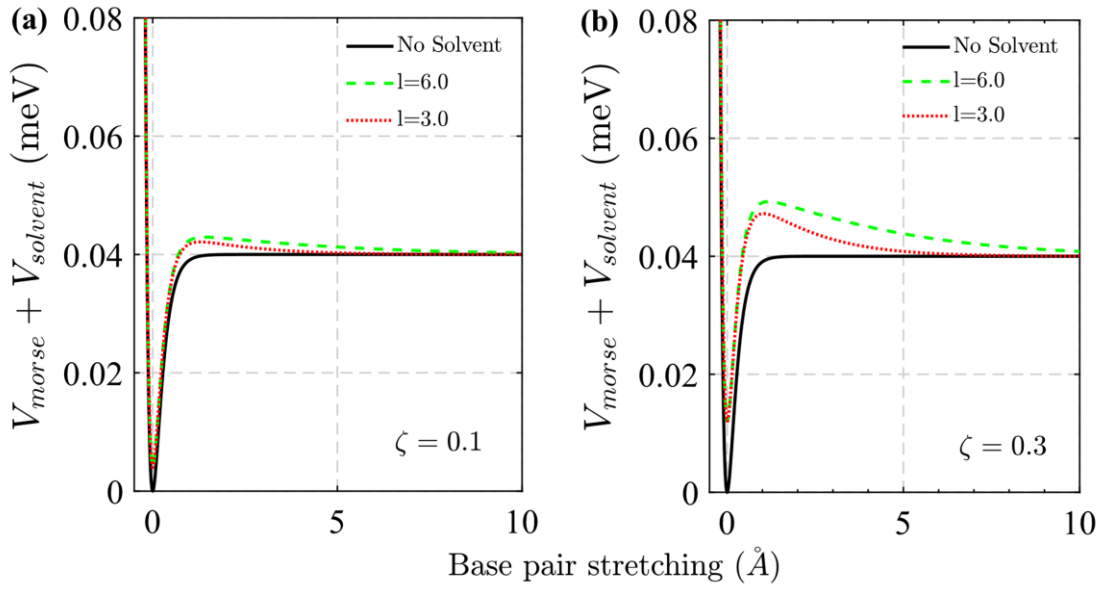

Figure 2. Potential term in DNA system by including the solvent potential with (a) viscosity ζ=0.1 (b) ζ=0.3

The addition of solvent potential in the PB Hamiltonian model allows the motion of DNA to become anharmonic as a precursor to the nonlinear dynamics of DNA [2, 7, and 21]. Completely, the Hamiltonian of DNA model is written as,

$$H=\sum_{n=1}^{N}\frac{m\dot{y}_n^2}{2}+\frac{K}{2}\left(y_n-y_{n-1}\right)^2+D\left(e^{-\alpha y_n}-1\right)^2-D\zeta\left[\tanh\left(\frac{y_n}{L}\right)-1\right]. \tag{3}$$

3- Thermostat as a Bio-Fluid

We investigate the DNA system in an artificial bio-fluid with a specific viscosity, where the dynamic behavior of DNA is influenced by thermal viscosity [2, 13, 21]. The purpose of the idea is to describe the dynamics of DNA more realistically. The system investigation involve a thermal bath in the form of a Nosé-Hoover (NH) thermostat, which was considered through the canonical ensemble approach [2]. In principle, the idea of a thermostat is one of the popular techniques for controlling a specific temperature, including energy fluctuations, by adding and removing energy from the environment around DNA. The NH thermostat is known and used as one of the most powerful methods for describing molecular dynamics at a constant temperature.

Using the Nosé approach, the Hamiltonian of DNA model (Equation 3) is modified by adding one degree of freedom for the thermal bath, i.e., *s*. The Hamiltonian used in this study has the full form,

$$H_{Nose} = \sum_{n=1}^{N} \frac{P_n^2}{2m_n s^2} + V(y_n) + \frac{P_s^2}{2Q} + fk_B T \ln s, \tag{4}$$

known as the Hamiltonian - Nosé. Here, Q is the effective mass of heat bath, having a value related to s. Whereas $V(y_n)$ is the total potential of the modified PB DNA model, i.e., the spring, Morse, and solvent potential. Parameter s is known to have conjugates P_s. From the Equation 4, we derive four equations of motion for the DNA system:

$$\dot{y}_n = \frac{\partial H_n}{\partial \vec{P}_n} = \frac{\vec{P}_n}{ms^2}, \tag{5-a}$$

$$\dot{s} = \frac{\partial H_n}{\partial P_s} = \frac{P_s}{Q}, \tag{5-b}$$

$$\dot{\vec{P}}_n = -\frac{\partial H_n}{\partial y_n} = \vec{F}_n, \tag{5-c}$$

$$\dot{P}_s = -\frac{\partial H_n}{\partial s} = \frac{1}{s}\left(\sum_{n=1}^{N} \frac{\vec{P}_n^2}{ms^2} - fk_B T\right). \tag{5-d}$$

Precisely for the coordinate system $2N + 2$. Furthermore, by applying the Hoover transformation: (i) $\vec{P}_n' = \vec{P}_n / s$, (ii) $dt' = dt/s$, (iii) $ds/sdt' = d\eta/dt'$, and (iv) $P_s = P_\eta$, the equations of motion of the system $2N + 2$, Equations 5-a to 5-d, are reduced to $2N + 1$ equations of motion [34]. However, what is known to have a physical meaning is only the equation,

$$m\ddot{y}_n = K(y_{n+1} + y_{n-1} + 2y_n) + 2\alpha D e^{-\alpha y_n}\left(e^{-\alpha y_n} - 1\right) + \frac{D\zeta}{L}\operatorname{sech}^2\left(\frac{y_n}{L} - 1\right) - \xi m\dot{y}_n \tag{6}$$

by definition $\xi = P_s/Q$. The equation of motion of the additional degrees of freedom is also obtained, namely thermal friction equation, which represent thermal viscosity,

$$\dot{\xi} = \frac{1}{Q}\left(\sum_{n=1}^{N} m\dot{y}_n^2 - fk_B T\right) \tag{7}$$

known have to couple to Equation 6. Furthermore, in Equations 6 and 7, y_n represents stretching between base pairs as DNA in the open state. Whereas m is the mass of the nitrogenous base, K is the coupling constant, α is the spatial scaling factor, D is the energy of dissociation, ζ is viscosity, L is the length of the DNA chain, f is degrees of freedom, k_B is Boltzmann's constant, and T is the absolute temperature.

4- Nonlinear Dynamics Formulations

In this section, we construct a theoretical formulation for obtaining the nonlinear dynamic (soliton) equation of DNA in a bio-fluid (NH thermostat), by taking consideration into Equations 6 and 7. Based on the literature, solitons arise when there is an appropriate balance between linearity, i.e., in the form of perturbations, such as dissipation, and the nonlinearity of a medium (bio-fluid) [35]. The linearity of the system has a consequence that the envelope propagation of a wave in the medium is wide. This process is signed by the intensity of the envelope profile that tends to decrease. Meanwhile, the nonlinearity of the system gives a consequence of propagating the wave envelope, which tends to be narrow and is indicated by the increasing intensity of the envelope profile. Moreover, when the two properties of the medium balance each other, the wave envelope will undergo self-focusing and form a stable wave. This wave maintaining consistency of shape during propagation is refer as a soliton. We investigated the same in the DNA system, where the probability of the emergence of solitons originated from the activity of the field wave modulation instability. Then, this activity is self-focused by a small perturbation given to the DNA system [12].

Descriptively, we have shown instability in the DNA dynamics system through the calculation of the numerical solutions of Equations 6 and 7 [33]. In this study, the formulation is built by firstly examining the perturbation in the DNA system as a cause of self-focusing. This equation is formulated by taking the definition $y_n = \varepsilon\phi_n$ in Equations 6 and 7, which $\varepsilon \ll 1$ are small perturbation. By that definition, Equations 6 and 7 are written as,

$$m\frac{\partial^2 \varepsilon\phi_n}{\partial t^2} = K\left(\varepsilon\phi_{n+1} + \varepsilon\phi_{n-1} + 2\varepsilon\phi_n\right) + 2\alpha D\left[-\left(\alpha\varepsilon\phi_n\right) + \frac{3}{2}\left(\alpha\varepsilon\phi_n\right)^2 - \frac{7}{6}\left(\alpha\varepsilon\phi_n\right)^3 + \frac{5}{8}\left(\alpha\varepsilon\phi_n\right)^4 - O\left(\left(\alpha y_n\right)^5\right)\right] + \frac{D\zeta}{L}\left[1 - \left(\frac{\varepsilon\phi_n}{L}\right)^2 + \frac{2}{3}\left(\frac{\varepsilon\phi_n}{L}\right)^4 + O\left(\left(\frac{y_n}{L}\right)^5\right)\right] - \xi m\frac{\partial\varepsilon\phi_n}{\partial t} \tag{8}$$

and;

$$\dot{\xi} = \frac{1}{Q}\left(\sum_{n=1}^{N} m\frac{\partial\varepsilon\phi_n}{\partial t} - fk_BT\right) \tag{9}$$

obtained by involving a 4th-order Taylor series expansion for the potential term. Here ϕ_n is a new expression of y_n as a representation of base-pair stretching. We prefer to call this condition a local open state of the DNA system.

Equations 8 and 9 are seen as mathematical models of a discrete system, so it would be better to evaluate them through a discrete approximation. In principle, DNA is part of a discrete system because it has several numbers of *n* base pairs [7]. However, to investigate the dynamics of whole DNA sequences with better perspective, including the interaction with thermal bath, we evaluate this using a continuous approximation, i.e., by taking a definition,

$$\phi_n(t) \approx \phi(nl, t) \rightarrow \phi(z,t) \tag{10}$$

$$\phi_{n\pm1}(t) \approx \phi(n\pm l,t) \rightarrow \phi \pm \phi_z l + \frac{1}{2}\phi \pm \phi_{zz} l^2 + \cdots \tag{11}$$

for an expression of each *n* DNA base pair as a continuous unit without losing its identity, i.e., discrete properties. In Equations 10 and 11 above, l = 3.4 Å is the distance between the base pairs. Meanwhile, *z* and *t* are representation of base pairs and time, respectively. Through continuous approximation, Equation 8 for only the 4th order takes the form,

$$m\phi_{tt} + \xi m\phi_t - 4K\phi - Kl^2\phi_{zz} - 2\alpha D\left[-(\alpha\phi) + \frac{3}{2}\varepsilon(\alpha\phi)^2 - \frac{7}{6}\varepsilon^2(\alpha\phi)^3 + \frac{5}{8}\varepsilon^3(\alpha\phi)^4\right] - \frac{D\zeta}{L}\left[\frac{1}{\varepsilon} - \varepsilon\left(\frac{\phi}{L}\right)^2 + \frac{2}{3}\varepsilon^3\left(\frac{\phi}{L}\right)^4\right] = 0 \tag{12}$$

Furthermore, by ignoring the even and higher than the 3rd order terms of ϕ in the expansion, obtained

$$m\phi_{tt} + \xi\phi_t - \alpha\phi_{zz} - \beta\phi + \gamma\varepsilon^2\phi^3 - \frac{\rho}{\varepsilon} = 0 \tag{13}$$

and similarly, for Equation 9 written as follow,

$$\dot{\xi} = \frac{1}{Q}\left(\int m\varepsilon\phi_t\, \partial z - fk_BT\right) \tag{14}$$

to purpose the condition that DNA system as a centrosymmetric system. This condition is important and generally leads to the formation and nonlinear arrangement of the system [35]. Equations 13 and 14 are written by taking the definition,

$$\alpha = \frac{Kl^2}{m}; \qquad \beta = \frac{4K - 2D\alpha^2}{m}; \qquad \gamma = \frac{7D\alpha^4}{3m}; \qquad \rho = \frac{D\zeta}{mL}. \tag{15}$$

In Equation 13, if $\varepsilon \rightarrow 0$, the parameter ρ/ε will take a tremendous value. This condition allows calculation in Equation 13 to become invalid; therefore, it can be negligible. Through the perturbation theory approach, a mathematical model of system dynamics, as shown by Equation 13, will have a solution $\phi = Ae^{i(qz-\omega t)}$, with $A = A(z, t)$ is a wave envelope [14]. From this, we derive the fundamental part of the substitution process of function ϕ into Equation 13,

$$\frac{\partial^2 A}{\partial t^2} + \xi\frac{\partial A}{\partial t} - \alpha\frac{\partial^2 A}{\partial z^2} - \left(\omega^2 - q^2\alpha + \beta\right)A + \gamma\varepsilon^2|A|^2 A = 0 \tag{16}$$

The Equation 16 is the dynamic envelope evolution equation. Here, the dispersion relationship is $\omega^2 \approx q^2$ to cancel each other out. Furthermore, if envelopes are assumed to vary slowly, the term $\partial^2 A/\partial t^2 \ll \partial A/\partial t$ can be ignored. This assumption implies that the envelope moves very fast, but its acceleration is always smaller than its velocity. As a result, a nonlinear partial differential equation is obtained as follow;

$$\xi\frac{\partial A}{\partial t} - \alpha\frac{\partial^2 A}{\partial z^2} - \beta A + \gamma\varepsilon^2|A|^2 A = 0 \tag{17}$$

with,

$$\dot{\xi} \approx \frac{1}{Q}\left(\int m\varepsilon A_t \, \partial z - fk_B T\right) \tag{18}$$

i.e., starting now referred to as the Nonlinear Schrödinger equation (NLS). Both Equations 17 and 18, are coupled. Here, we solve both equations by the split-step Fourier numerical method. How to solve those equations is shown in Figure 3.

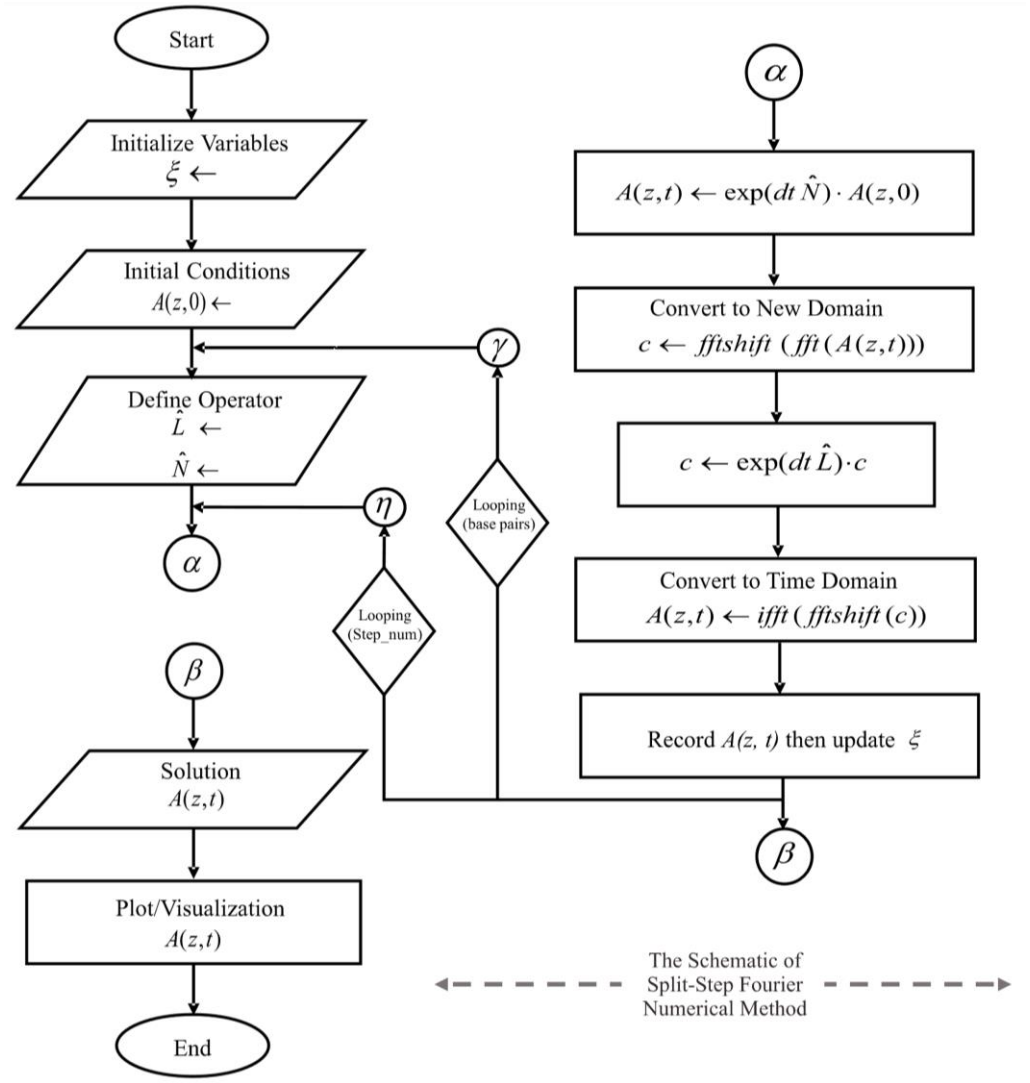

Figure 3. Flowchart of the numerical method to obtain a soliton-like solution from NLS-like equation

5- Numerical Result and Discussion

The main purpose of this study is to investigate how the behavior of DNA, especially when interacting with the bio-fluid. As the result of this study, we find the phenomenon of solitons in a DNA dynamics system. This is a highly expected result because until now, the existence of solitons in DNA dynamics systems is still challenging to find [36-44]. Moreover, we also include the interaction between DNA and bio-fluid. In fact, the existence of solitons gives an exquisite physical meaning for DNA dynamics when transferring genetic information; DNA is open stably [7]. The stability of soliton-like plays an important role in keeping genetic data in the process of transferring information from being lost [7, 12]. In this study, we successfully modeled the DNA system interacting with the artificial thermostat as a bio-fluid. The dynamics of this DNA model is represented by the dynamic equation of a soliton, an NLS-like equation (Equation 17) coupled to a thermostat (Equation 18). In this section, we describe how the soliton from both equations are obtained by using a numerical approach. So far, this DNA model has not been studied, moreover with the Fourier split-step numerical method. This approach is based on the concept of splitting linearity and nonlinearity term of the DNA system—several discussions regarding the application of the split-step Fourier method. Recently, Ripai et al. have successfully demonstrated and applied the method to an NLS equation to investigate soliton dynamics and evolution in a nonlinear medium [36, 37]. We also apply similar principles to the case of DNA by substituting the coupling constant $K = 0.06\ eV/A^2$, dissociation energy $D = 0.04\ eV$, spatial scaling factor $\alpha = 0.04\ A^{-1}$, nitrogenous base mass $m = 300\ amu$, the distance between base pairs $l = 4.3\ \text{Å}$, and Boltzmann's constant $k_B = 8.61733 \times 10^{-5}\ eV/K$

in the calculation process. The simulation is carried out over a range of temperature values 300 $K \leq T \leq 450$ K, number of base pairs $N = 100$, with the perturbation parameter $\varepsilon \ll 1$ and degrees of freedom $f = N + 1$. Applying an assumption in a mathematical model, namely ansatz, to the calculation process confirms the existence of a soliton-like in the DNA system proposed (Figure 4). Ansatz is chosen in the bright soliton model, namely $A(z, 0) = \text{sech}(z)$, as the initial complex envelope condition for each time it approaches the value $A(z, t) \approx \text{sech}(z) \exp(i\xi t/2)$. The ξ is a representation of the fluid thermal viscosity effect of the DNA system.

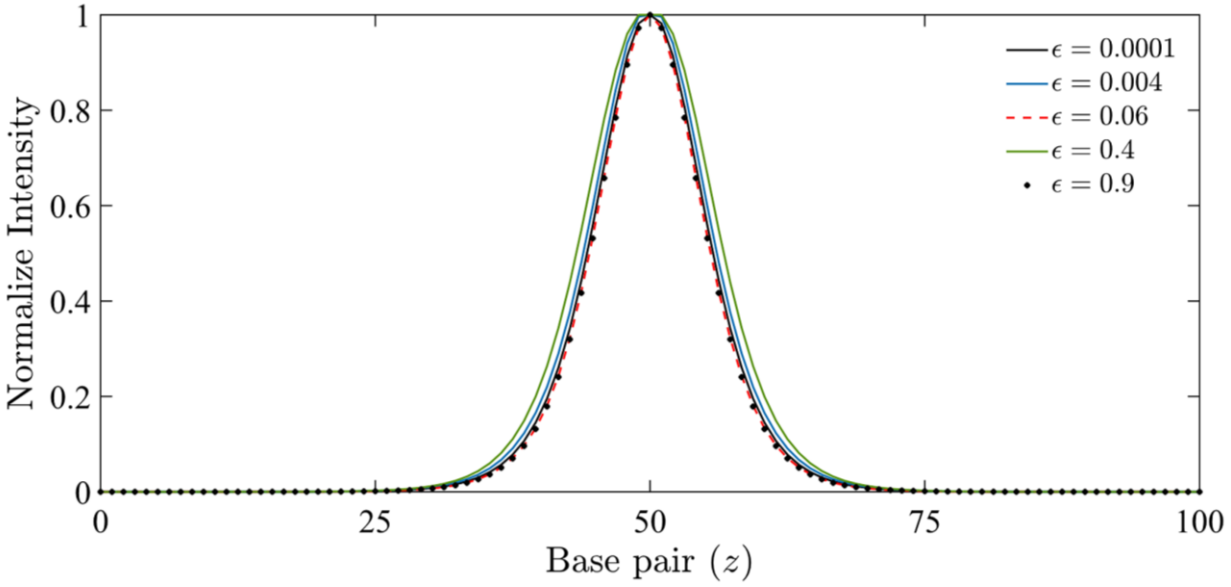

Figure 4. Soliton-like of DNA system in the NH Thermostat for the several values of the perturbation parameter ε = 0.0001, ε = 0.004, ε = 0.06, ε = 0.4, and ε = 0.9

The soliton-like presence in the DNA system appears to represent stretching of base pairs; the open state of the DNA chain. Here, a bright soliton-like model was confirmed to be relevant for representing the local opening of the DNA system, given the intensity of the envelope profile toward zero in the minimum and maximum base pair z sequences (Figure 4). This localization is considered to play an essential role in transferring genetic information. Solitons in the DNA system is seen to be present from the right balance between perturbation and nonlinearities that arise from the surrounding environment, such as interactions between nucleotides, interactions between base pairs, and the effect of fluid thermal viscosity; as expressed by three potential forms in Equations 2-a, 2-b and 2-c. Nonlinearity affects the instability of plane wave modulation (representation of DNA motion), making DNA motion nonlinear. Previous studies have shown the nonlinear motion of DNA based on the instability of this type of modulation in a chaotic form with a regular pattern [2, 33]. When the perturbation is considered, it contributes to the process of plane wave self-focusing. So that the instability that is thought to cause the periodic waveform deviation, indicated by the change in the dispersion relationship, is canceled by the self-focusing process, which finally maintains a stable waveform, called the soliton, as shown in Figure 4.

In Figure 4, the bright-soliton-like model varies for each different value of the perturbation parameter. As shown in the figure, this parameter suggests a bright-soliton-like evolution in the proposed DNA system, indicated by the envelope profile's widening and narrowing. Qualitatively, the envelope profile narrows for values closer to zero $\varepsilon = 0.0001$. Next, it becomes more comprehensive for the value after $\varepsilon = 0.004$. However, a return narrowing occurs, in the value of $\varepsilon = 0.06$ and $\varepsilon = 0.9$. Instead of finding a profile that progressively narrows values closer to one $\varepsilon \rightarrow 1$, it becomes the widest for $\varepsilon = 0.4$. The process of widening the envelope profile occurs when the nonlinearity in the DNA system is weakened. On the other hand, narrowing occurs when the influence of nonlinearity increases or dominates. We add perturbation parameters to the DNA dynamics formulation to regulate nonlinearity, as shown in Equation 17. Finally, the bright-soliton-like formation confirmed the disruption in the DNA system's nonlinearity.

The involvement of perturbation in the proposed DNA system occurs quadratically (Equation 17) so that is possible to generate nonlinear quadratic effects on the system. Based on the principles of nonlinearity, this type of effect is an essential part of supporting the existence and evolution of solitons, for this case, as shown in Figure 4. Nevertheless, the perturbation parameter increment does not necessarily indicate an evolution with a narrower envelope profile, meaning that the DNA system's nonlinearity increases. Physically, we consider this evolution to occur not only by nonlinearity but also by the system's linearity due to the dynamics of DNA. Increasing in nonlinearity from the increase in the parameter value that allows the evolution of the envelope to become narrower still can be canceled by the linearity effect. In the formulation, the linearity is expressed by the second and third terms Equation 17 and exerts a widening effect on the soliton envelope. Here, we confirm that the solitons, which in principle exist from the balancing between

linearity and nonlinearity in the DNA system in the NH Thermostat, have not occurred without applying the perturbation theory as a nonlinearity controller. As argued earlier, we prefer to say that solitons in this DNA system come from the perfect fit and balance between perturbation and nonlinearity.

After obtaining a soliton-like solution for the proposed DNA system, we tried to observe the temporal behavior of the solution over a range of temperatures 300 $K \leq T \leq 450$ K. The simulation result is presented in Figures 5-a to 5-g, which verifies the temporal state of the soliton-like solution in a DNA system on a thermal bath, i.e., the NH Thermostat. The modified PB DNA model in the NH Thermostat as a bio-fluid has been reduced to an NLS-like equation by applying a perturbation theory and continuous approach. Numerical calculations are performed to predict the analytical results by involving ansatz in the bright soliton model. Soliton-like evolution has also been obtained and studied based on the principles of systems nonlinearity. Here, we observe the temporal behavior of a soliton-like solution based on variations in temperature T (Figure 5). Soliton-like stability fluctuates as temperature T increases. In principle, this condition is known as fluctuational openings of DNA, which is a state of fluctuation in the process of opening DNA due to thermal activity in solvents [38]. Thus, the theoretical framework built in this study is said to confirm the previous research arguments.

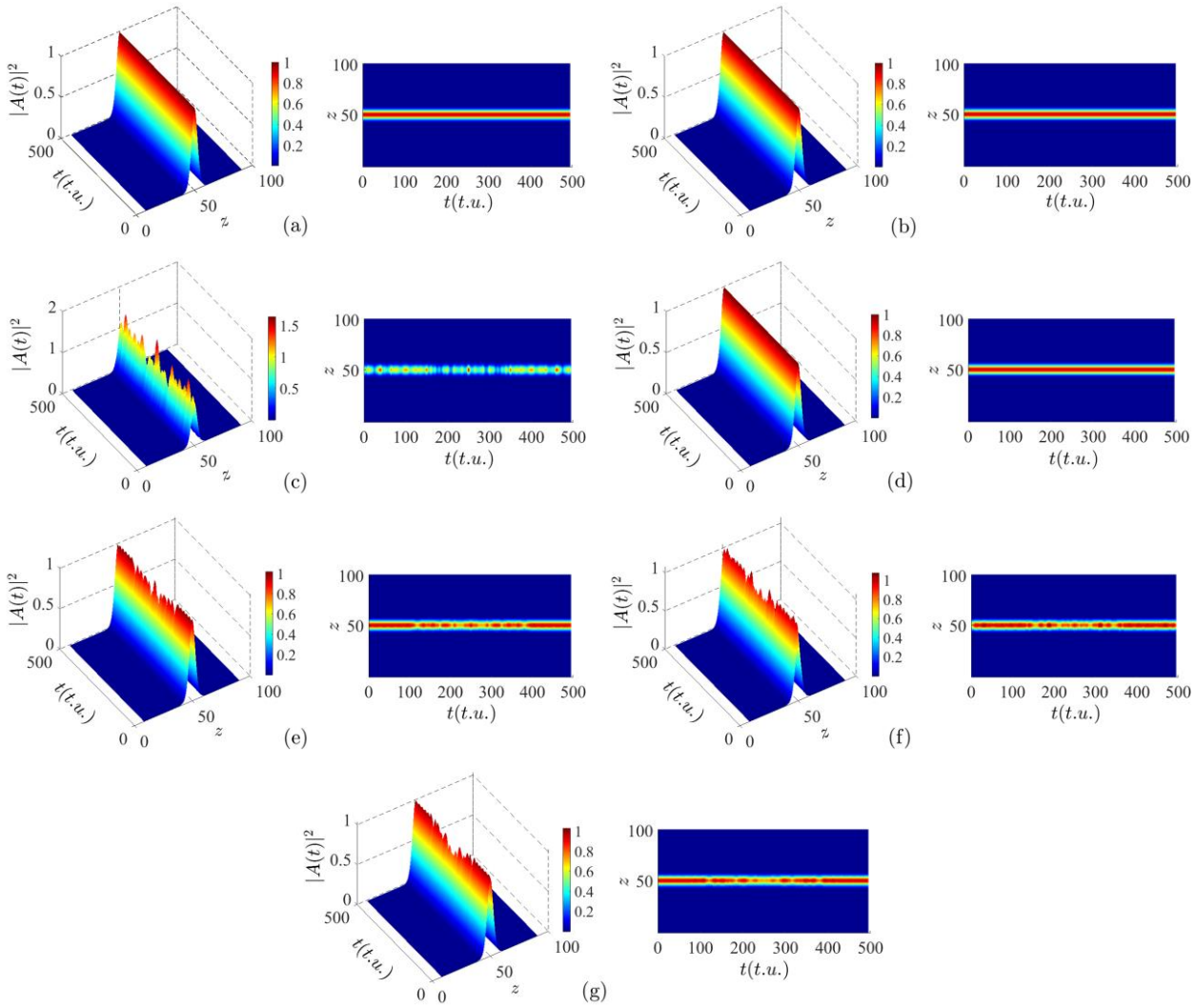

Figure 5. The temporal behavior of the soliton-like on DNA system in the NH Thermostat for temperature values: (a) T = 300 K, (b) T = 325 K, (c) T = 350 K, (d) T = 385 K, (e) T = 400 K, (f) T = 425 K, and (g) T = 450 K [left is surface; right is contour].

In Figure 5, we intend to show fluctuations in soliton-like intensity as fluctuational openings of DNA. For $T = 300$ K (Figure 5-a) and $T = 325$ K (Figure 5-b), a soliton-like solution with a very well-established level of stability was found. Meanwhile, it has fluctuated for $T = 350$ K (Figure 5-c), the state with the most significant fluctuation. Furthermore, for $T = 385$ K (Figure 5d), it is seen that soliton-like stability is maintained. Finally, for $T = 400$ K (Figure 5-e), $T = 425$ K (Figure 5f), and $T = 450$ K (Figure 5-g), the stability undergoes small fluctuations. We are trying to study and find a state of increasingly large fluctuations that contribute to the local denaturation process. This denaturation process is

presented in Figure 6 by simulating the temperature 300 $K \leq T \leq 450\ K$. In principle, Toko et al. have shown that large fluctuations allow the denaturation process to occur. In addition, several other researchers also suspect local denaturation at temperatures approaching $T = 400\ K$ [38]. Whereas DNA denaturation temperature based on experiments is around 375 K [45]. Our observations found large fluctuations from $T = 350\ K$ with a similar denaturation process occurring at 370 $K \leq T \leq 380\ K$, as shown in Figure 6.

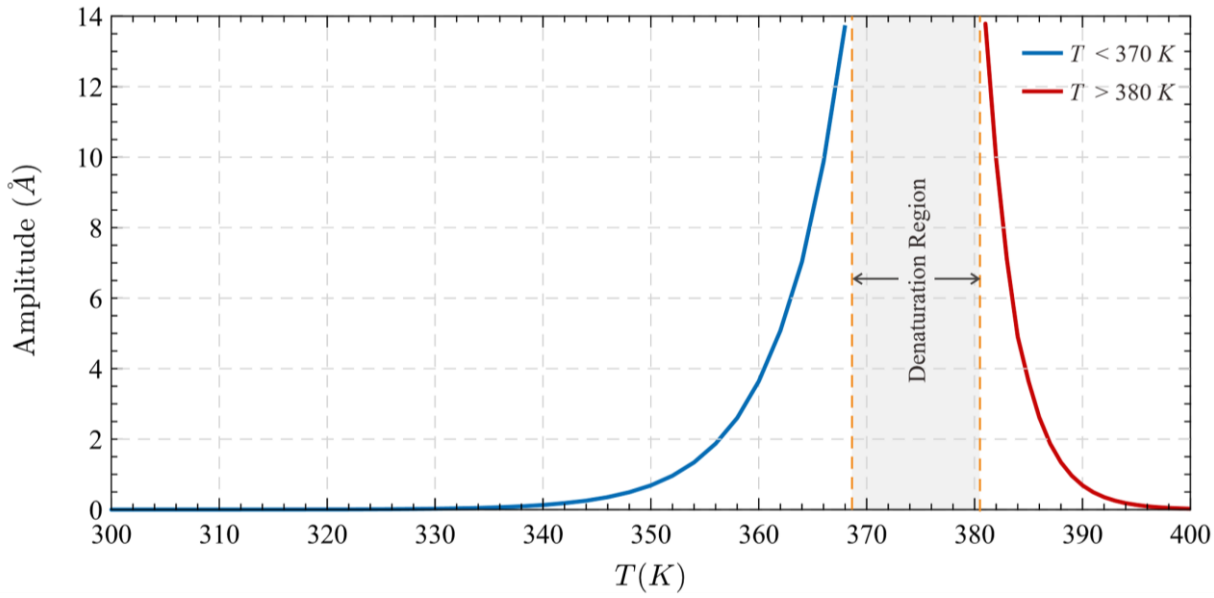

Figure 6. Local denaturation model of the DNA system in the NH Thermostat

The fluctuation in the intensity of the soliton-like solution occurs due to energy fluctuations in the DNA system, caused by thermal activity in the solvent. In this case, the solvent is a liquid with a specific viscosity, which we previously described in terms of the solvent potential and the thermal friction equation (Equations 2-c and 7). More viscous the solvent, the greater the power to impede DNA motion, allowing instability of motion known as the dissipation effect [13]. The dissipation effect allows a decrease in the power of the DNA dynamic process (Figure 2). When thermal activity is involved, the increase in temperature of a thermal bath allows motion in the interactions between molecules of nucleotides to be accelerated. Thus, the dynamic energy fluctuation of DNA is possible to occur. For this case, we found fluctuations in the intensity of the soliton-like solution in the review of the solution's temporal behavior (Figure 5). For stability and small fluctuations, soliton-like solutions are predicted to have a higher energy level than the dissociation energy of the hydrogen bond so that their contribution to denaturation becomes smaller than before. Furthermore, the heat capacity and viscosity of the liquid and the percentage of heterogeneity of the base pairs can also affect the temperature of denaturation [46, 47]. The G-C base pair has three hydrogen bonds; this causes more stability than the base pair A-T, which has only two hydrogen bonds [32]. Moreover, parameter values from Morse potential are also different for G-C and A-T pairs [48]. Lastly, the denaturation process does not occur simultaneously and spontaneously but gradually and coordinated.

6- Summary and Conclusion

We find that the dynamics of the modified PB DNA model while interacting with the bio-fluid is represented by the NLS-like equation. We obtain this equation by implementing a perturbation review and a continuous approximation to the DNA system. The solution of the NLS-like equation is a soliton-like wave, which is attained by applying the Fourier split-step numerical method. Soliton-like solutions are initiated using a mathematical assumption, namely ansatz in the formulation and numerical simulation. Based on observations, soliton-like solutions are relevant to describing DNA's nonlinear dynamics, primarily the phenomenon of local DNA opening, which is essential to explaining the process of transferring genetic information. Soliton-like solutions emerge from a precise balance between perturbation and nonlinearity of the DNA system. Meanwhile, the evolution of the soliton-like arises from the differences in perturbation parameters. This prediction occurs due to the increase and decrease in the nonlinearity property of the DNA system. In this case, the involvement of perturbation works as a control of nonlinearity for the existence of soliton. However, the nonlinear differential equations can represent the overall system behavior more precisely. In contrast, linear differential equations can only represent system behavior locally. Furthermore, for systems that are quite complex and cover a wide range, the linear and local approximations lead to ignoring much of the information in the nonlinear equation.

Furthermore, we also observed the temporal behavior of a soliton-like solution; the fluctuation of the temporal soliton intensity represents the fluctuational openings of DNA. The fluctuations in the DNA system are divided into two levels:

large fluctuations that contribute to the local denaturation process, i.e., DNA strains splitting, and small fluctuations that contribute to the minimum denaturation process, i.e., denaturation bubble. Soliton-like intensity fluctuations emerge as a consequence of energy fluctuations in the DNA system due to the thermal activity of the solvent of a bio-fluid. Subsequently, we find the denaturation process at a temperature of $370\ K \leq T \leq 380\ K$. Finally, the theoretical principles established in this paper confirm the findings of previous researchers. Overall, the proposed model is able to explain the dynamics of DNA interacting with the bio-fluid in the form of a soliton-like. In addition, this model can also explain the phenomenon of denaturation for specific thermal viscosity. Nevertheless, the result is still an approximation, where DNA is reviewed using continuous approximation. Therefore, the DNA system needs to be investigated in a discrete manner to discover other essential things in future studies.

7- Declarations

7-1- Author Contributions

Conceptualization, T.E.P.S. and F.P.Z.; methodology, W.H.; software, Z.A. and A.R.; validation, F.P.Z., W.H., and T.E.P.S.; formal analysis, T.E.P.S.; investigation, A.R.; resources, Z.A. and A.R.; data curation, T.E.P.S.; writing—original draft preparation, A.R.; writing—review and editing, T.E.P.S.; visualization, A.R.; supervision, T.E.P.S.; project administration, T.E.P.S.; funding acquisition, T.E.P.S. All authors have read and agreed to the published version of the manuscript.

7-2- Data Availability Statement

The data presented in this article are available on request from the corresponding author.

7-3- Funding

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7-4- Conflicts of Interest

The author declares that there is no conflict of interest regarding the publication of this manuscript. In addition, the authors have completely observed the ethical issues, including plagiarism, informed consent, misconduct, data fabrication and/or falsification, double publication and/or submission, and redundancies.

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