Chaotic Behaviour of Modified Hamiltonian Peyrard-Bishop-Dauxois Model on DNA System

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Abstract. DNA research has involved a variety of disciplines across fields, which work complementary and supportive by using the theory, model, and experiment. Physics provides a theoretical basis that can be used for experimentation, as well as developing new physical models. This physical model can explain the nonlinear dynamics of DNA. In this study, we modified Hamiltonian Peyrard-Bishop-Dauxois (PBD) model by adding the influence of the surrounding environment namely thermal bath, in the form of time-dependent thermal friction and stochastic white noise. Both are represented through the Nosé-Hoover-Langevin (NHL) thermostat. Formulations of equation motion are obtained using analytical methods, to be solved using numerical methods. We present the numerical calculations results in phase space images to show chaotic behaviour. Furthermore, we gain an increase in chaotic patterns along with the increase in temperature. In addition, we also obtain the relationship between the distance of the base pair with temperature, especially in the denaturation process.

1. Introduction

In the last half-century, the molecule of DNA is structurally known and now as an icon of modern biosciences. The story of DNA began in 1869 when Frederich Miescher, isolated nucleic acids in the cell nucleus [1]. Then, from the study, Miescher proposed the name of DNA for the first time [2]. Furthermore, Avery’s research [3] and the Hershey-Chase experiment [4], confirmed that DNA is genetic information-carrying material. At present, genetic information well known can be manipulated through genetic engineering technology. However, scientific disciplines that discuss DNA cannot explain so well how the process of transferring the genetic code. Biomolecular science has discussed DNA in detail [5,6], but multidisciplinary science is needed to discuss the overall complexity of the molecular structure and dynamics of DNA. Therefore, physics is present to describe the dynamics of DNA through the physical modelling of DNA systems. Some physicists have tried these complex problems to find the answers. Schrödinger has been a pioneer since 1944 by modelling aperiodic crystals which have genetic information, bonding together through covalent bonds [7]. Until in 1982, Herbert Fröhlich concluded that the nonlinear effects of the system can stabilize biological activity related to the dynamics of molecular vibrations that occur due to coherent excitation of polar modes [8].
DNA dynamics is considered as a nonlinear phenomenon because when reviewed as linear dynamics it becomes unrepresentative [9]. Physical system of the DNA model using a nonlinear system was first developed by Peyrard and Bishop [10]. Furthermore, Dauxois et al. [11] added anharmonic spring potential to [10], which have physical meaning as stacking interactions to become DNA has a helix form. In another study Dauxois et al. [12] also modelled DNA dynamics by involving an artificial thermostat represented by the Nosé-Hoover thermostat. Discussion of DNA dynamics with the helix model in [13-16] has been able to explain several DNA physical phenomena. In other studies, surrounding environmental aspects also reviewed [17,18]. In further developments, Hamiltonian DNA model was modified by adding potential liquid effects [19] or accompanied by external potential effects [20] to obtain denaturation temperatures. The denaturation process does not only involve temperature variables but also involves environmental effects, such as the liquid around DNA. Therefore, to minimize the degree of freedom of the liquid particle collision with DNA, stochastic is present as a representation of the random force in Brownian motion. In this study, random force review in the form of white noise ($\chi$), known as the Nosé-Hoover-Langevin (NHL) thermostat [21]. Moreover, the model initiated needs to be developed using physical parameters to obtain relevant results. We obtain some pattern of phase space diagram on chaotic behaviour phenomena.

2. Hamiltonian of the DNA Model
The molecular structure of DNA is identified through X-ray diffraction experimental data, that DNA is double helix [22]. The standard DNA model that has succeeded in explaining the local denaturation process is the PB DNA model [10]. Peyrard and Bishop assume a set of phosphate groups and sugar groups from DNA are considered as an elastic bar. The two rods (double strand DNA) are interconnected with base pairs, as illustrated in figure 1. (a). By reviewing the direction of motion only in the out-phase $y_n = (u_n - w_n) / \sqrt{2}$, the Hamiltonian DNA system of the PB model is represented in the form

$$H_{\text{hom}}^{(PB)} = \sum_{n=1}^{N} \left[ \frac{m}{2} \dot{y}_n^2 + \frac{K}{2} (y_n - y_{n-1})^2 + D \left( e^{-\alpha y_n} - 1 \right)^2 \right]$$

(1)

for reviewing each $n$-th base pairs are homogeneous. The first term is the kinetic term of the base pair, the second term is the harmonic spring potential as representation of the interaction between neighboring base pairs, $K$ is a spring constant, $K = 0.06$ eV Å$^{-2}$[17]. Whereas the third term is the Morse potential, parameter $D$ and $\alpha$ are respectively the energy of dissociation of the pair and width of the potential well. Figure 1. (b) represents the interaction between base pairs. In this study we investigate the environment around DNA, so anharmonic spring necessary added to accommodate stacking interaction that cause by the surrounding environment [11]. The difference in here, base pairs are review heterogeneously with Hamiltonian in form

![Figure 1](image-url)

**Figure 1.** Illustration of (a) the DNA system of Peyrard-Bishop model and (b) Morse potential as a representation of interactions between base pairs [23].
In the PB model, consideration is only on the DNA strand because of the system assumed to be in a vacuum [10]. But in this research model, the DNA system involved interactions with NHL thermostats, so that the energy possessed by DNA will fluctuate. However, the energy circulation between DNA and NHL thermostat remains conserved. Therefore, the PBD model is more accurate with the actual DNA physical system because of including the environmental aspects [12], as in this study through the Nosé-Hoover-Langevin thermostat.

3. Nosé-Hoover-Langevin Thermostat

In the PB model, consideration is only on the DNA strand because of the system assumed to be in a vacuum [10]. But in this research model, the DNA system involved interactions with NHL thermostats, so that the energy possessed by DNA will fluctuate. However, the energy circulation between DNA and NHL thermostats remains conserved. Before we discuss about NHL thermostat, firstly we consider the DNA system with Hamiltonian in extended phase space, by including s entropy and its momentum conjugate $p_s$. Solving Nosé-Hamiltonian with f degree of freedom [27]

$$H^{(N)} = H^{(PBD)}_{het} + \frac{P^2}{2Q} + f k_B T \ln s. \tag{3}$$

become equations of motion, and using Hoover transformation [27], we get Nosé-Hoover equations

$$m \ddot{y}_n = -\nabla U(y_n) - \xi \dot{y}_n \tag{4}$$

$$\dot{\xi} = \frac{1}{Q} \left( \sum_{n=1}^{N} m \dot{y}_n^2 - f k_B T \right) \tag{5}$$

with, $\dot{y}_n = v_n$, $\xi$ is extra degree of freedom represent thermodynamics friction, and $T$ is temperature. Term $-\nabla U(y_n)$ in equation (4) is a force derived from combination of anharmonic spring potential and a heterogeneous Morse potential. The Boltzmann constant $k_B$ is adjusted to other parameters, equal to $8.61733 \times 10^{-5}$ eV/K. Parameter $Q$ assumed like mass of thermal bath, set proportional to $f k_B T$.

The previous PBD model only reviews the homogenous base pair coupled on the Nosé-Hoover thermostat [12]. Rather than using Nosé-Hoover thermostat and review random force as Langevin dynamics, we use idea to include the stochastic variable as the term of extended phase space [21]. This idea accommodating stochastic terms $\chi(t)$ in additional degrees of freedom greatly to be easier calculations, represent as new thermodynamics friction $\zeta$. We introduce the time evolution of $\zeta$

$$\dot{\zeta} = g(v_n) - \gamma \zeta + \chi(t), \tag{6}$$

in NHL thermostat. The parameter $\gamma$ is the damping coefficient and $g(v_n)$ in form
After adding stochastic terms by using NHL thermostats idea, the equation of motion (4) become

\[ m\dot{v}_n = -\nabla U_{(ab)}(y_n) - \zeta m v_n \]

(8)
couple to external thermal bath in equation (6). Whereas \( \chi(t) \) is a Gaussian white noise with mean, \( \langle \chi(t) \rangle = 0 \), and variance, \( \langle \chi(t) \chi(t') \rangle = 2D_{\text{eff}} \delta(t-t') \). The parameter \( D_{\text{eff}} \) is a diffusion coefficient that satisfies the relation \( D_{\text{eff}} = \gamma k_B T Q^{-1} \). Moreover, \( \delta_{ij} \) is delta Kronecker and \( \delta(t-t') \) is delta Dirac function. If the stochastic term remains to be reviewed as combination of the Langevin dynamics and the Nosé-Hoover thermostat idea, it causes variance relations become time dependent, meaning that changes at any time. Expectation values that always change at any time cause the system to be difficult to observe. Next step, calculating the parts of stochastic differential equations by assuming Brownian motion is a Wiener process, \( \chi(t) \) \( dt = \sigma \, dW \), and define \( \gamma = Q \sigma^2 (2k_B T)^{-1} \). Equation (6) has the following forms of thermal evolution [28]

\[ d\zeta = \frac{1}{Q} \left( \sum_n m v_n^2 - f k_B T \right) dt - \gamma \zeta dt +\sigma dW \]

(9)

Equation (9) have a role as an NHL thermostat that can be completed after implicit form of discretization and rewritten in explicit form as,

\[ \zeta_{n+1} = \left( 1 + \Delta t \sigma^2 / 4Q \right)^{-1} \left( \zeta_n + \Delta t \left( \sum_n m v_n^2 - f k_B T \right) + \sigma \sqrt{\Delta t} W \right) \]

(10)

Solution of equations (8) and (10) is carried out using numerical calculations [29,30] presented in the next section. Several numerical parameters need to be initialized, such as time step \( \Delta t \) and variance \( \sigma^2 \). The most important unit in this simulation is the time dimension that has been converted into a time unit that has a relation, 1 t.u. = 1.0214 x 10^{-14} s [17]. This value will affect the friction coefficient \( \gamma = \tau^{-1} \), where \( \tau \) has the dimension of time and its value should be adjusted depending on how and what damping process desires to model. In this model we set \( \tau = 0.5 \) ps [31].

4. Numerical Result and Discussion

4.1. Chaotic Behaviour

Although the definition of chaos has no universally accepted, a commonly used definition formulated by Robert L. Devaney that the dynamical system can be classified as chaotic, following three properties [32]: (1) sensitive to initial conditions, (2) topologically mixing, and (3) have dense periodic orbits. In this case, we consider the first and the last properties by ignoring the second one because of the different discussion. Chaotic behaviour in this DNA model observed based on the results of the phase space system. The initial condition temperature is given in each variation \( \Delta T = 25 \) K with interval 300 K \( \leq T \leq 400 \) K. While the simulation is carried out, the initial distance between the base pair \((n = 1)\) initialized \( y_0 = 0 \) Å and the initial separation velocity is equal to \( v_0 = 0.5 \) Å(t.u.)^{-1}. In addition, for the next base pair \((n \neq 1)\), the initial condition initialized to zero. After calculating using the numerical method, the results of the phase space images are obtained as follows.
The difference of temperature variable in order to the long-range dynamical behaviour associated with chaotic dynamics. Moreover, the behaviour of dynamical systems that are highly sensitive to initial conditions. Increased chaotic patterns tend to chaos with increasing temperature values, represent in figure 2-6. The higher temperature value allowed the higher entropy of system. When thermal energy from the thermostat transferred to mechanical energy for DNA dynamics is too large, the bonding energy in the DNA system is not strong enough to receive the mechanical energy. Furthermore, the DNA system achieved extreme chaotic behaviour. In this case, the bond in the base pair is broken, and DNA can undergo a denaturation process. The energy in the DNA system is transferred back to the thermostat to keep the energy of the system conserved. Besides the increasing pattern of chaos, in higher temperature the trajectory systems also have dense periodic orbits. This result corresponds to the first and third properties of chaos definition by Robert L. Devaney [32].

**Figure 2.** Phase space diagram at temperature 300 K.

**Figure 3.** Phase space diagram at temperature 325 K.

**Figure 4.** Phase space diagram at temperature 350 K.

**Figure 5.** Phase space diagram at temperature 375 K.

**Figure 6.** Phase space diagram at temperature 400 K.
In the study of Behnia et al. [17] PB model using NH thermostats for temperatures of 300 K have results that shown chaotic behaviour. However, in this study, the PBD model with NHL thermostats when the temperature of 300 K had not shown chaotic behaviour. The results of chaotic behaviour only occur when temperatures are greater than 300 K. Thus, the characteristics of NHL thermostats show chaotic behaviour only in high temperature. Physically when the temperature gets higher, the liquid viscosity around the DNA will shrink, this will reduce the external force of the liquid and accommodate the denaturation process. Otherwise, if the temperature gets lower the reverse process occurs which is called the unzipping process.

4.2. Denaturation Process

The denaturation process has a very important role in the process of transferring the genetic code. In this process the information stored on genes is copied to be used in the process of protein synthesis or DNA replication. During the process of transcription and replication, when the polymerase enzyme approaches the DNA strand, there is an extreme change in pH in the fluid around the DNA [5,6,9]. As the previous study [10], this physics models a DNA system can explain the dynamics of the denaturation process. The value of denaturation temperature is strongly influenced by various aspects, not least the concentration and type of liquid. Under normal conditions, the liquid around the DNA has a high concentration with a neutral pH at room temperature. When extreme pH or temperature changes occur, the viscosity of the liquid will decrease significantly. Changes in extreme pH and a significant increase in temperature can destabilize the hydrogen bonds in DNA causing to weaken and denaturation occurs. In this study, to accommodate that condition the friction coefficient is set by choosing the value of $\tau = 5$ ps [31].

The numerical simulation results are shown in figure 7. The DNA system succeeded in identifying a denaturation temperature of 400 K. Another calculation on different temperature have no result for denaturation process, the distance between base pair remains bonding reciprocally. The base pair reviewed is the first 7 pairs, due to the DNA sequences of L60B36 only to 60 pairs in length [25] so the review of 5-10 pairs are representative enough. In the actual denaturation process, there is a base pair that does not participate in separation, only certain pairs are involved in denaturation process [5,6,9]. For example, the first base pair ($n = 1$), there is no separation at any time except only in the denaturation process. This is because the left-hand neighbor of the base pair considered as fixed end. Physically, this condition is like noncoding regions that are not involved in the genetic coding process [5,6,9]. In the case of a base pair which has a separation value ($y$), suddenly the distance becomes decrease after previously the distance increase monotonously over 5 Å, this indicates that there is an influence coming from the surrounding environment just before the denaturation process occurs. Firstly, the base pair will be close to each other and then move away and apart, reach over 10 Å. From the previous study, this

![Figure 7](image_url)
value tends to lead denature [20]. The denaturation process does not occur spontaneously and simultaneously, but rather gradually and coordinated.

DNA denaturation temperature obtained based on experiments around 375 K [33]. The difference in denaturation temperature values obtained in this study can be due to the viscous and heat capacity of the liquid. In addition, temperature 400 K is the value of the simulation results, which need to be calibrated with the results of measurements or experiments. Furthermore, the viscous and heat capacity of the liquid and the percentage of the base pairs number of the type G-C can also affect the temperature of denaturation [24]. Because each base pair G-C has three hydrogen bonds, this causes more stability than the base pair A-T, which has only two hydrogen bonds [5,6]. Moreover, parameter values from Morse potential in PBD model are different for G-C and A-T pairs [13]. The percentage of base pairs of this type of G-C depends on the sequence of DNA that is reviewed or the degree of heterogeneity of artificial DNA modelled.

4.3. Comparison of PBD and PB Models

The fundamental difference between the PBD model and the PB model is the term of the anharmonic spring. The PBD model can be reviewed into a PB model when stacking interaction \((\rho)\) is zero or the other way reviewed the deviation locally. The linearized PBD model has no potential anharmonic term, but only terms harmonic spring and thermal bath represent by NHL thermostat. Both comparisons are only shown at temperature 300 K, due to the system remain has no chaotic behaviour. In PBD model by numerical and by linearization, the distance between base pair \((y)\) fluctuates periodically. The difference between figure 8. (a) and figure 8. (c) because of the dynamics factor in the linearization model without anharmonic terms. The Morse potential term after linearization is not much different from the harmonic oscillator term, because it only has a \(\Delta y\) term. In figure 8. (a) show the plot result of the PBD model system, which represents the physical system that the \(y\) value cannot be negative too large due to the minimum distance limit received by each base pair. In other hand, figure 8. (c) and 8. (d) show the maximum kinetic energy at the same period. Moreover, the modified DNA system has interactions with the NHL thermostat, so that the energy circulation between DNA and NHL thermostats fluctuate periodically. Overall the energy of the system remains conserved.

![Figure 8](image.png)

**Figure 8.** (a) The distance between the first base pair and (b) strand separation velocity of PBD model by numerical calculation. (c) The distance between the first base pair and (d) strand
separation velocity of PBD model by linearization. Both of PBD model review deviation locally with $\tau = 5$ ps.

However, more specific than that, the nonlinear differential equations can represent overall system behaviour. Whereas linear differential equations can only represent system behaviour at short intervals and locally. By completing the set of linear differential equations, in general it has helped to solve a set of nonlinear differential equations. In addition, for systems that are quite complex and cover wide range, the linear and local approximation cause ignoring much of the information that the variable has in the nonlinear equation, in this case the anharmonic potential. Therefore, approximation of linearity only applies to certain cases such as in steady state conditions or for very small deviation values.

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References
[1] Dahm R 2008 Human Genetics 122(6) pp 565–81
[2] Dahm R 2005 Developmental Biology 278 pp 274–88
[3] Avery O T, Macleod C M and McCarty M 1944 The Journal of Exp. Medicine 79(2) 137–58
[4] Hershey A D and Chase M 1952 The Journal of General Physiology 36(1) pp 39–56
[5] Nelson D L and Cox M M 2012 Principles of Biochemistry (New York: W. H. Freeman and Company) pp 273–300
[6] Voet D, Voet J G and Pratt C W 2008 Fundamental of Biochemistry vol 3 (New York: John Wiley and Son) pp 223–467
[7] Schrödinger E 1944 What is Life? The Physical Aspect of the Living Cell (Cambridge: Cambridge University Press)
[8] Frölich H 1983 International Journal of Quantum Chemistry 23(4) pp 1589–95
[9] Yakushevich L 2004 Nonlinear Physics of DNA (Weinheim: Wiley-VCH Verlag GmbH & Co. KgaA)
[10] Peyrard M and Bishop A R 1989 Phys. Rev. Lett. 62 2755
[11] Dauxois T, Peyrard M and Bishop A R 1993 Phys. Rev. E 47(1) R44(R)
[12] Dauxois T, Peyrard M and Bishop A R 1993 Phys. Rev. E 47(1) 684
[13] Campa A and Giantsanti A 1998 Phys. Rev. E 58(3) pp 3585–88
[14] Choi C H, Kalosakas G, Rasmussen K Ø, Hiromura M, Bishop A R and Usheva A 2004 Nucleic Acids Research 32(4) pp 1584–90
[15] Ares S, Voulgarakis N K, Rasmussen K Ø and Bishop A R 2005 Phys. Rev. Lett. 94(3) 035504
[16] Voulgarakis N K, Redondo A, Bishop A R and Rasmussen K Ø 2006 Phys. Rev. Lett. 96(24) 248101
[17] Behnia S, Akhshani A, Panahi A, Mobarakia A and Ghaderian M 2012 Phys. Lett. A 376 pp 2538–47
[18] Dwiputra D, Hidayat W and Zen F P 2017 J. Phys.: Conf. Ser. 856 012005
[19] Zdravkovic S, Tuszyński J A and Sataric M V 2005 Journal of Comp. and Theoretical Nanoscience 21 pp 1–9
[20] Hidayat W, Sulaiman A, Viridi S and Zen F P 2015 Journal of Phys. Chem. and Biophysics. 5(5) 186
[21] Samoletov A A, Dettmann C P and Chaplain M A J 2007 Journal of Stat. Phys. 128(6) pp 1321–36
[22] Watson J D and Crick F N C 1953 Nature 171 pp 737–8
[23] Peyrard M 2004 Institute of Physics Publishing 17 R1–R40
[24] Behnia S, Akhshani A, Panahi A, Mobarakia A and Ghaderian M 2011 Phys. Rev. E 84 031918
[25] Zeng Y, Montrichok A and Zocchi A 2004 Journal of Mol. Biology 339(1) pp 67–75
[26] Mandelkern M, Elias J G, Eden D and Crothers D M 1981 Journal of Mol. Biology 152(1) pp 153–61
[27] Tuckerman M 2009 Statistical Mechanics: Theory and Molecular Simulation (New York: Oxford University Press)
[28] Leimkuhler B, Noorizadeh E and Theil F 2009 Journal of Stat. Phys. 135(2) pp 261–77
[29] Chapra S and Canale R 2015 Numerical Methods for Engineers vol 7 (New York: McGraw-Hill Education) pp 735–37
[30] Nakamura S 1993 Applied Numerical Methods in C vol 1 (London: Prentice-Hall Internat) pp 313–76
[31] Manghi M and Destainville N 2016 Physics Reports 631(9) pp 1–41
[32] Boris H and Katok A 2003 A First Course in Dynamics: With a Panorama of Recent Developments (Cambridge: Cambridge University Press)
[33] Zoli M 2010 Phys. Rev. E 81(5) 051910