Nonlinear dynamics of modified peyrard-bishop DNA model in nosé-hoover thermostat

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Abstract. In this study, we investigate the viscous effect by adding solvent potential into Hamiltonian Peyrard-Bishop DNA model. The dynamics of the modified Peyrard-Bishop DNA model is also considered in time-dependent thermal friction, namely Nose-Hoover Thermostat. Equation of motion formulate by using an analytical method, then solved using a numerical method. We show the pattern of phase space diagrams of the DNA dynamics in each variation of viscous and temperature, the movement of base pairs at a specific temperature, and the thermostat’s energy fluctuation that affects DNA dynamics.

1. Introduction

DNA, as genetic information material [1-3], has been engineered for various purposes. Today, DNA engineering has developed very rapidly in the last decade, especially in communication and technology [4-5]. Genetic information on bacterial DNA can be engineered to be used as a data storage [4-7]. Nevertheless, the transfer principle of the bacterial DNA genetic code is still in the development to be applied optimally. At present, some branches of biomolecular science have discussed DNA in detail [8-9], but their perspective can only interpret DNA statically. Both encryption and decryption processes of DNA genetic code are challenging to observe experimentally [10]. Therefore, multidisciplinary science is needed to discuss structural complexity and dynamics of DNA molecules as a whole. Nonlinear physics exists to describe DNA dynamics when transferring genetic information through the physical modeling of the DNA system.

DNA dynamics has become a topic of interest to physicists [11-18], starting from developing mathematical models [13-15], as well as developing methods used to analyze the amount of physics in DNA systems [16-18]. In the book “What is life” [19], Schrodinger propose a model of aperiodic crystals, which has genetic information, bonding to each other through covalent bonds. Then, Herbert Fröhlich (1983) states that biological activity related to the dynamics of molecular vibrations that occur from coherent excitation of polar modes can be stabilized by the nonlinear effect of the system [20]. Thus, the DNA system will be more representative when reviewed as a nonlinear phenomenon.

The first mathematical model of DNA using nonlinear systems is the Peyrard-Bishop DNA model [21]. The DNA system illustrated in the model only considers local denaturation assuming that the DNA is in a vacuum. This of course is very different from the actual condition of DNA in the cell...
nucleus. The physical condition of the DNA system has been previously reviewed by involving aspects of the interaction of the surrounding environment, such as the effects of thermal friction [18] or solvents [22, 23]. However, the result of these study were not relevant enough to the physical conditions of the DNA system.

In this study, to obtain more relevant results based on the actual DNA physical system, we investigate the modified PB DNA model by including the solvent potential [23] which has thermal contact to a time dependent thermal bath, namely Nose-Hoover thermostat. The equation of motion was obtained by solving the Modified Hamiltonian PB model using analytical methods. Furthermore, those equation will be solved using the numerical method. The dynamic properties of DNA will be examined through numerical results. The base pair’s movement are investigated by analyzing the thermal bath and solvent’s physical factors, e.g., viscosity and temperature through phase space pattern. We also analyze the velocity of base pair stretching related to energy fluctuation from the Nose-Hoover thermostat.

2. Modified Peyrard-Bishop DNA Model

Firstly, we consider the chemical compound of DNA, leading to the DNA model illustration as shown in Figure 1. The phosphate group link to a sugar group in single helix chain. These sugar and phosphate groups are referred to as strands. Furthermore, each sugar chain connects to a base, and then between bases is connected to its base-pair through weak hydrogen bonds.

![Figure 1](image)

**Figure 1.** (a) Chemical compound of DNA for one nucleotide (Sugar, Phosphate, Base), (b) simple and (c) mathematical model double-strand illustration of DNA [24]

The DNA model as illustrated above is proposed by [21] which is defined by the Hamiltonian,

\[
H = \sum_{n=1}^{N} \left[ \frac{m\dot{y}_n^2}{2} + V_{\text{Spring}} + V_{\text{Morse}} \right]
\]

(1)

with \(N\) is the number of homogenous base pairs, \(n\) is index of base pair. Moreover, the potential terms respectively are \(V_{\text{Spring}} = \frac{K}{2}(y_n - y_{n-1})^2\) and \(V_{\text{Morse}} = D(e^{-\alpha y_n} - 1)^2\).

In this section, we consider the Peyrard-Bishop (PB) DNA model [21] with the viscous effect in the term of solvent potential [23]

\[
V_{\text{Solvent}}(y_n) = -D\zeta \left[ \tanh \left( \frac{y_n}{L} \right) - 1 \right]
\]

(2)

to accommodate the physical representation of energy activation [24]. Whereas solvent potential modulated by a barrier factor \(\zeta\) and by a length \(L\) setting the range of the potential. In this study \(L\) is the length of the DNA chain. The distance between two neighboring pairs of nitrogenous bases is
So that the whole chain length can be used the relation $L = Nl$. This assumption leads the Hamiltonian PB model into

$$H = \sum_{n=1}^{N} \left[ \frac{m \dot{y}_n^2}{2} + V_{\text{total}} \right],$$

so that the total potential of the DNA model system becomes

$$V_{\text{total}} = V_{\text{Spring}} + V_{\text{Morse}} + V_{\text{Solvent}}.$$  \hspace{1cm} (4)

The potential used previously in original PB model is Morse potential, which describes the interaction between two base pairs. $D$ is the dissociation energy of the base pair, $D = 0.04$ eV and $a = 4.45 \text{ Å}^{-1}$. While $V_{\text{spring}}$ is an expression of a harmonic spring potential as an interaction between the $n$-th base pair and the neighboring base pairs. The parameter $K$ is a constant elasticity with value $K = 0.06$ eVÅ$^{-2}$. However, in this PB model, Morse potential still has physical shortcomings. The shape of the well in Figure 2. (blue line) allows the initial deviation of any value. If it is related to the physical system, it is not possible. A nitrogen base pair requires activation energy to bond. Therefore, in this study, the effect of the solvent potential term is added. The solvent potential along with the Morse potential is illustrated in Figure 2.

![Figure 2](image)

**Figure 2.** Potential term in DNA system with of the solvent potential term with barrier factor (a) $\zeta = 0.1$ and (b) $\zeta = 0.3$ [23] with $D = 0.04$ eV and $a = 4.45 \text{ Å}^{-1}$ [21].

### 3. Nosé-Hoover Thermostat

The behaviour of DNA dynamics influenced by thermal viscosuity [10]. In order to simulate realistic way of DNA dynamics, we investigate this system by considering in Nose-Hoover (NH) thermostat, which approximate the canonical ensemble. Thermostat idea is one of popular techniques to control a certain temperature including the energy fluctuations by adding and removing energy from the surrounding environment of the DNA. Therefore, the Nosé–Hoover thermostat has been commonly used as one of the most accurate and efficient methods for constant-temperature molecular dynamics simulations.

In the approach of Nose, the Hamiltonian with an additional degree of freedom for thermal bath, namely $s$, is known as Hamiltonian – Nosé represent in the form

$$H_{\text{Nose}} = \sum_{n=1}^{N} \frac{p_n^2}{2m_n s^2} + V(y) + \frac{p_s^2}{2Q} + f(kT \ln s),$$  \hspace{1cm} (5)
where $Q$ is an effective mass associated to $s$. With $V(y)$ is the potential of modified PB model in (4). Hamiltonian in (5) has additional coordinates in the form of the parameter $s$ and its conjugate $p_s$. From this equation, we can obtain the four equations of motion from the $2N + 2$ coordinate systems,

$$
\dot{y}_n = \frac{\partial H_N}{\partial p_n} = \frac{\bar{p}_n}{ms},
$$

(6)

$$
\dot{s} = \frac{\partial H_N}{\partial p_s} = \frac{P_s}{Q},
$$

(7)

$$
\dot{\bar{p}}_n = -\frac{\partial H_N}{\partial y_n} = \bar{F}_n,
$$

(8)

$$
\dot{\bar{p}}_s = -\frac{\partial H_N}{\partial s} = \frac{1}{s} \left( \sum_{n=1}^{N+1} \bar{p}_n^2 s - f k T \right).
$$

(9)

Furthermore, with the Hoover transformation [26], (i) $\bar{p}_n = \bar{p}_n / s$; (ii) $dt' = dt / s$; (iii) $ds / dt' = d\eta / dt'$; and (iv) $p_s = p_s$, the $2N + 2$ equations of motion are reduced to only $2N + 1$ equations of motion. But what has physical meaning are only the following these equations,

$$
m\ddot{y}_n = K (y_{n+1} + y_{n-1} + 2y_n) + 2a D e^{-\alpha s} \left( e^{-\alpha s} - 1 \right) + \frac{D}{L} \sum_{n=1}^{N+1} \bar{p}^2_n e^{s} \left( \frac{y_n}{L} \right) - \xi m\ddot{y}_n,
$$

(10)

then with the definition $\xi = p_s / Q$ the form of equation of motion from additional degree of freedom is obtained

$$
\dot{\xi} = \frac{1}{Q} \left( \sum_{n=1}^{N+1} m\ddot{y}_n - f k T \right),
$$

(11)

which are coupled to each other. These equations in (10) and (11) solved using numerical approach.

4. Numerical Results and Discussion

We have obtained numerical results for the modified DNA system by adding the effects of thermal solvent potential in thermal bath. According to [13, 11], the dynamics of DNA not only depend on a very large temperature, but there is also depend on the influence from the solution concentration around the DNA. In this study, that condition represent by the solvent potential in (2). As the development from the previous study [13], the viscous effect also reviewed in time evolution through $\xi$ in (11). The nonlinear dynamics of DNA is presented in phase space diagram illustrated by Figure 3 for various viscous and temperatur.

Nevertheless, for temperature 400K the streching of base pair decrease. In [11], the thermostate has a role to increase streching of base pair lead to denaturation process. Furthermore, the solvent potential play important role for bubble or unzipping process in DNA dynamics [13]. This model has realistic way that the process of denaturation DNA not only depend on temperature [10, 18]. Apart from the effect of the temperature, the effect of the viscous constant does not indicate how much different the base pairs can occur.
Figure 3. Phase space diagram of modified PB DNA model based on the addition of the solvent potential with barrier factor (a) $\zeta = 0.1$ and (b) $\zeta = 0.3$ in various temperature.
Figure 4. Velocity of stretching for the 10th base pairs with $\zeta = 0.1$ at temperature (a) 300K and (b) 400K; and $\zeta = 0.3$ at temperature (c) 300K and (d) 400K (1 t.u. = 1.0214 $\times 10^{-14}$ s)

In this study, we assume the initial condition of the thermal bath in a state of thermal equilibrium at a specific temperature value. Beside that, the base pair is given a stretching initial value which is analogous to realistic condition from the interaction between DNA and protein or surrounding environment [25]. Moreover, the DNA movement (Figure 4) causes the energy of thermal bath fluctuate, vice versa, so that energy circulation occurs between the DNA system and the thermal bath.
The energy changes that occur in the thermal bath shown in the following figure 5. Here, we only interest at the highest given temperature values, for each variation of viscous constant.

![Figure 5](image)

**Figure 5.** Energy fluctuation of thermal bath at temperature 400K for (a) $\zeta = 0.1$ and (b) $\zeta = 0.3$.

Energy fluctuation of thermostat affects the distance and velocity stretching of base pair. However, thermal bath would fluctuate differently when the DNA systems are different, i.e., the length of the DNA chain, the heterogeneity of the base pairs, and the initial temperature [11]. When the DNA dynamics achieve a condition where the temperature can cause the double strand DNA separate into a single strand, the denaturation process occurs [25]. Nevertheless, this research is limited to the nonlinear dynamics of DNA in a thermal bath that evolves with time. In this model, increasing the temperature does not necessarily mean that the DNA has a greater distance. The viscous potential also causes the base pair to close again or namely the unzipping process. In order to obtain the relevant DNA denaturation temperature, more physical quantities and modeling idea that involves various
aspects are required, such as DNA twisting coefficient [23]. In addition, hopefully the properties obtained in this study will be useful for application in DNA engineering.

DNA structure stability is mostly determined by the interactions between atoms in DNA. The stacking of base pairs can be considered with each other, namely stacking interactions, through the London force and hydrophobic force. Both of these forces play an essential role in the stability of the double helix shape. As previously explained, the base pairs are bonded to each other by hydrogen bonds. This bond gives a weak van der Waals force, by which an external force can easily break the bond between partners, i.e. thermal denaturation of DNA. The denaturation process is an essential part of the DNA replication process. The process does not occur spontaneously and simultaneously, but rather gradually and coordinated. Several base pairs separate firstly, which is known as the denaturation bubble. More specifically, a denaturation bubble is defined as opening the double helix strand of DNA through a coordinated separation of base pairs [27]. In this study we gain only the early of denaturation process, denaturation bubble, the dynamics of base pair stretch into certain distance and then close again, i.e. unzipping process. Furthermore, the denaturation process can occur due to significant changes in pH or temperature [18].

DNA applications have been widely applied to information systems like data storage, but this idea have not been well optimized due to the process of transferring the genetic code of DNA is complicated to model. Therefore, the nonlinear dynamics of DNA need to discuss in order to find the right process for transferring the genetic code. Scientific disciplines are required to cover this process in a comprehensive manner for developing the DNA model that resembles the realistic condition.

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