Time-dependent damping effect for the dynamics of DNA transcription

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Abstract. DNA is an interesting macromolecule to study because it plays a role in the body of living beings. This paper modified the Peyrard-Bishop (PB) DNA model by involving time-dependent damping. Damping on this model is considered a time-dependent perturbation. The dynamics of DNA transcription with time dependent damping effect is described by the damped nonlinear Schrodinger (DNLS) equation. Solution of the equation is obtained by applying variational method. So obtained the required parameters and done analysis using matlab. The simulation for the solution is done for nucleotide mass $5.1 \times 10^{-25}$ kg, distance between base neighbor $3.4 \times 10^{-10}$ m, elastic coefficient 8 N/m, depth of morse potential 0.1 eV, and width of morse potential $2 \times 10^{10}$ m$^{-1}$. This research showed a wave of soliton type of breather and spatial soliton. This paper also showed time-dependent damping causes changes in the amplitude and width of the DNA soliton wave.

Keyword : Dynamics of DNA, soliton wave, DNLS, the variational method

1. Introduction
Deoxyribonucleic acid (DNA) is one of the most interesting and mysterious biological molecules. A living being with other living things has different DNA characteristics. The relationship of human kinship was determined by DNA. DNA is the molecule that shapes life and character in living things. DNA is a polymer consisting of monomers called nucleotides. Each nucleotide consists of three components: sugar (furanose-derivative deoxyribose), heterocyclic base, and phosphate. One of the most important processes in DNA dynamics is the process of transcription. Transcription is the process by which genetic information is copied into mRNA [1, 2, 3].

The Peyrard-Bishop model describes the DNA transcription dynamics as two harmonic oscillator chains coupled by hydrogen bonds on each base. Where interaction between bases is described by potential morse [4]. Since then many researchers have examined this model such as, research on the static nature of DNA opening that forms bubbles at biological temperatures [5], the effect of stacking on bubble dynamics [6,7], and etc.

In the experiment, this process in addition to the thermal dependence also depends on the type of fluid, ion concentration, and PH of the fluid present around the DNA sample [8, 9,10]. The environmental effects of liquid are generally expected to provide damping or dissipation effects on the model. There are several studies on the effects of damping on DNA by means of giving damping on the
equation of system motion [11] and giving of damping through Hamiltonian theory of Cardirola Kanai [12, 13]. However, previous studies indicate that the damping coefficient given is constant. In real, the damping effect is not constant. So in this research, the author tries to model the transcription process with time-dependent damping coefficient.

2. Modification of Peyrard-Bishop DNA model with time-dependent damping

Following the Peyrard-Bishop model, the motion of DNA molecules is represented by two degree of freedom, \(u_n\) and \(v_n\), which correspond to the displacement of the base pair from its equilibrium position. By applying the normal transformation, two new degrees of freedom are obtained, \(x_n = \frac{(u_n + v_n)}{\sqrt{2}}\) and \(y_n = \frac{(u_n - v_n)}{\sqrt{2}}\). However only the variable \(y_n\) is relevant for DNA transcription process. So, the Hamiltonian equation is used

\[
H = \sum_n \left( \frac{\dot{y}_n^2}{2m} + \frac{1}{2}K(y_n - y_{n-1})^2 + D \exp(-\alpha y) - 1 \right)^2, \tag{1}
\]

the Hamiltonian equation is transformed into a Lagrangian function as follows

\[
L = \sum_n \left( m \frac{\dot{y}_n^2}{2} - \frac{K}{2} (y_{n+1} - y_n)^2 - D \exp(-\frac{\alpha}{2} y_n) - 1 \right)^2. \tag{2}
\]

Denaturation is influenced by environmental factors so that denaturation can occur at body temperature. In this case denaturation occurs due to significant PH changes resulting from the interaction of RNA polymerase enzymes with fluid around the DNA. This causes the fluid viscosity conditions around the DNA to be different over time. The viscosity around the DNA affects the damping effect on RNA polymerase enzymes. In this study the damping coefficient is a Gaussian function. So the Lagrangian equation can be obtained from

\[
\frac{d}{dt} \frac{\partial L}{\partial \dot{y}_n} - \frac{\partial L}{\partial y_n} = F_d, \tag{3}
\]

where \(F_d = -\gamma \frac{\dot{y}_n}{dt}\) and \(\gamma = \gamma_0 \cdot \exp(-\beta t^2)\). \(F_d\) is the damping force, \(\gamma\) is the damping coefficient, \(\gamma_0\) is the initial damping coefficient, \(\beta\) is a parameter, and \(t\) is time. Equation (2) becomes the equation of system motion as follows

\[
m \ddot{y}_n + \gamma \dot{y}_n = K (y_{n+1} + y_{n-1} - 2y_n) + \alpha D \left[ \exp(-\frac{\alpha}{2} y_n) - 1 \right] \exp(-\frac{\alpha}{2} y_n). \tag{4}
\]

3. Continuum limit approximation

The \(y_n\) approximation is a small amplitude. So \(y_n = \epsilon \psi_n\) with \(\epsilon \ll 1\) and can be expansion using taylor series and equation (4) to be as follows

\[
\psi_n + \frac{\gamma}{m} \dot{\psi}_n = \omega_0^2 (\psi_{n+1} + \psi_{n-1} - 2\psi_n) - C_m^2 (\psi_n + \epsilon a_1 \psi_n^2 + \epsilon^2 a_2^2 \psi_n^3), \tag{5}
\]

where \(\omega_0^2 = \frac{K}{m}\), \(C_m^2 = \frac{\alpha a^2}{2m}\), \(a_1 = -\frac{3\alpha}{4}\), \(a_2 = -\frac{\gamma}{2a}\), with \(m\) is a nucleotide mass. The DNA strand is so long that the system can be viewed as a continuum medium (like a string). Perform a continuum limit approximation as follows

\[
\psi_{xx} = \lim_{t \to 0} \frac{(\psi_{n+1} - 2\psi_n + \psi_{n-1})}{t^2}, \tag{6}
\]

then equation (5) becomes

\[
\psi + \frac{\gamma}{m} \psi = C_m^2 \psi_{xx} - C_m^2 (\psi + \epsilon a_1 \psi^2 + \epsilon^2 a_2^2 \psi^3), \tag{7}
\]
where \( \psi = \frac{\partial^2 \psi}{\partial t^2} \), \( \psi_x = \frac{\partial \psi}{\partial x} \), \( \psi_{xx} = \frac{\partial^2 \psi}{\partial x^2} \), \( C_o^2 = \omega_0^2 l^2 \), and \( \gamma = e \gamma \). Equation (7) can be expanded in different time and space scales. Therefore, multiple scale expansion method is applied as follows

\[
t_0 = e^0 t, t_1 = e^1 t, x_0 = e^0 x, x_1 = e^1 x,
\]

so equation (7) becomes

\[
0 = \frac{\partial^2 \psi}{\partial t_0^2} + \frac{2\epsilon \partial^2 \psi}{\partial t_0 \partial t_1} + \epsilon^2 \frac{\partial^2 \psi}{\partial t_1^2} + \epsilon \frac{\partial \psi}{\partial t_0} + \epsilon^2 \frac{\partial \psi}{\partial t_1} - C_0^2 \left( \frac{\partial^2 \psi}{\partial x_0^2} + \frac{2\epsilon \partial^2 \psi}{\partial x_0 \partial x_1} + \epsilon^2 \frac{\partial^2 \psi}{\partial x_1^2} \right) + C_m^2 (\psi + \epsilon a_1 \psi^2 + \epsilon^2 a_2^2 \psi^3),
\]

(9)

to solve the equation of motion is done approach perturbasi theory as follows

\[
\psi = \psi^0 + e \psi^1,
\]

(10)

with

\[
\psi^0 = \psi_0 (x_1, t_1) e^{i\theta} + \psi_1^* (x_1, t_1) e^{-i\theta},
\]

(11)

\[
\psi^1 = \psi_0 (x_1, t_1) + \psi_2 (x_1, t_1) e^{i2\theta} + \psi_0^* (x_1, t_1) + \psi_2^* (x_1, t_1) e^{-i2\theta},
\]

(12)

where \( \theta = k x_0 - \omega t_0 \). The damping term only gives disturbance to the first harmonic term or in other words the damping term only contribute to \( t_1 \). With \( t_1 \) is the time coordinate on the envelope wave, \( t_0 \) is the time coordinate of the carrier wave, \( x_1 \) is the coordinate of space in the envelope wave, and \( x_0 \) is the coordinate of space in the carrier wave [15].

The substitution of equations (10), (11), and (12) into equation (9). Then do the grouping of the order of the harmonic term. The zero order term contained \( \psi^0 \), the first order term containing \( e^{i\theta} \), and the second order term contained \( e^{i2\theta} \). From the grouping of the zero order term obtained

\[
\psi_0 = -a_1 |\psi_1|^2,
\]

(13)

from the grouping of the second order term and describe \( \omega^2 = C_m^2 + C_0^2 k^2 \) obtained

\[
\psi_2 = \frac{a_1 |\psi_1|^2}{3}.
\]

(14)

then equations (13) and (14) are substituted into the grouping of the first order term. Thus obtained

\[
0 = - \frac{1}{2\omega^2} \frac{\partial^2 \psi_1}{\partial t_1^2} - \frac{c_0^2}{2\omega} \frac{\partial^2 \psi_1}{\partial x_1^2} + \frac{\epsilon \gamma}{2\omega m} \frac{\partial \psi_1}{\partial t_1} - \frac{2c_0^2}{\omega} |\psi_1|^2 \psi_1 - i \left( \frac{\partial \psi_1}{\partial t_1} + V_\theta \frac{\partial \psi_1}{\partial x_1} \right),
\]

(15)

with \( V_\theta = \frac{c_0^2 k}{\omega} \). Equation (15) is written in a better form by transforming it into travelling wave coordinate

\[
\xi = x_1 - V_\theta t_1 \quad \text{dan} \quad \tau = \epsilon t_1.
\]

(16)

Assuming damping only contribute to time and not to space. So, equation (15) forms the damped nonlinear Schrodinger (DNLS) equation as follows

\[
i \frac{\partial \psi_1}{\partial \tau} + \Lambda_1 \frac{\partial^2 \psi_1}{\partial \xi^2} + \Lambda_2 (\tau) \frac{\partial \psi_1}{\partial \tau} + \Lambda_3 |\psi_1|^2 \psi_1 = 0,
\]

(17)
where \( \Lambda_1 = \frac{c_2^2 c_3 h}{2 \omega^3} \), \( \Lambda_2 = \frac{2 c_2 h}{\omega} \), \( \Lambda_2(t) = - \frac{\epsilon r}{2 \omega m} \) with \( r = r_0 \), \( \exp(-\beta r^2) \), \( r_0 = 0.05 \) kg/s, \( \beta = 2 \), and \( t = \frac{z}{v} \). \( r \) is a \( r \) function because the damping is assumed to be small and affects only the envelope wave.

### 4. Variational methods

The motion equation obtained is the damped nonlinear Schrödinger (DNLS) equation with the following solution

\[
\Psi_1(\xi, \tau) = A_0 \text{sech}\left[\frac{1}{L} (\xi - u_e \tau)\right] \exp[-i(k \xi - \omega \tau)],
\]

where \( A_0 = \sqrt{\frac{(u_0^2 - 2u_1 u_1)}{2\Lambda_1 \Lambda_3}}, \quad L = \frac{2\Lambda_2}{\sqrt{(u_0^2 - 2u_1 u_1)}}, \quad k = \frac{u_e}{2\Lambda_1}, \quad \) and \( \omega = \frac{u_e u_2}{2\Lambda_1}. \( A_0 \) is the initial amplitude of the soliton wave, \( L \) is the width of the soliton wave, \( k \) is the wave number, \( \omega \) is the angular frequency, \( u_e \) is the velocity of the envelope wave, \( u_c \) is the velocity of the carrier wave, \( \Lambda_1 \) and \( \Lambda_3 \) is a constant [15, 16]. However, the existence of damping factor that becomes a disruption to the system causes the amplitude, position, velocity, and phase of the soliton wave to be time dependent [17]. So the solution becomes

\[
\Psi_1(\xi, \tau) = \eta(\tau) \text{sech}[\eta(\xi + \zeta(\tau))] \exp[-i(\theta(\tau)\xi + \varphi(\tau))],
\]

there are four time-dependent parameters \( \eta(\tau), \zeta(\tau), \theta(\tau) \) dan \( \varphi(\tau) \). These parameters can be determined using the variational method. With variational methods it can be obtained that is using Lagrangian density function as follows

\[
\mathcal{L} = \frac{i}{2} (\Psi_{1r} \Psi_{1r}^* - \Psi_{1r} \Psi_{1r}^*) - \Lambda_1 |\Psi_{1r}|^2 + \frac{\Lambda_2}{2} |\Psi_{1r}|^4 + \frac{\Lambda_3}{2} (\Psi_{1r}^* \Psi_{1r}^* - \Psi_{1r} \Psi_{1r}) - \frac{1}{2} \frac{\partial \Lambda_2}{\partial \tau} \Psi_{1r}^* \Psi_{1r}.
\]

The Lagrangian function is obtained by substituting equation (20) into the following equation

\[
L = \int_{-\infty}^{\infty} \mathcal{L} d\xi,
\]

so

\[
L = 2\eta \theta \zeta - 2\eta \varphi + \frac{2}{3} \eta^3 (\Lambda_3 - \Lambda_2) - 2\Lambda_2 \eta \theta^2 - 2i \Lambda_2 \eta \theta \zeta + 2i \Lambda_2 \eta \varphi - \Lambda_2 \eta.
\]

The Lagrangian function in equation (22) is used to obtain the sought parameters by substituting to the Lagrange equations. Then obtained

\[
\theta = \theta_0,
\]

\[
\eta(\tau) = \eta_0 ,
\]

\[
\zeta(\tau) = -2\Lambda_2 \theta_0 \tau,
\]

and

\[
\varphi(\tau) = [\eta_0^2 (\Lambda_3 - \Lambda_2) - \Lambda_1 \theta_0^2] \tau + i \ln(1 - i \Lambda_2).
\]

After obtaining the sought parameters then substitute the parameters on solution equation (19). So that

\[
\Psi_1(\xi, \tau) = \frac{\eta_0}{\sqrt{1 + \Lambda_2^2}} \text{sech}[\eta_0 (\xi - 2\Lambda_2 \theta_0 \tau)] \exp[-i(\theta_0 \xi + \eta_0^2 (\Lambda_3 - \Lambda_2) - \Lambda_1 \theta_0^2) \tau + 
\]

\[
tan^{-1}(-\Lambda_2)].
\]

\[\text{ DOI:10.1088/1742-6596/1204/1/012012}\]
The result is
\[ \psi = \psi^0 + \epsilon \psi^1, \]  
(28)
with
\[ \psi^0 = \frac{\eta_0}{\sqrt{1 + \lambda_2^2}} \text{sech}[\eta_0(\xi - 2\Lambda_1 \theta_0 \tau)] \exp\{i[\theta_0 \xi + \eta_0^2(\Lambda_3 - \Lambda_1) - \Lambda_1 \theta_0^2] \tau + \tan^{-1}(\lambda_2)]\} \exp\left\{i(kx_0 - \omega t_0)\right\} + \frac{\eta_0}{\sqrt{1 + \lambda_2^2}} \text{sech}[\eta_0(\xi - 2\Lambda_1 \theta_0 \tau)] \exp\{-i[\theta_0 \xi + \eta_0^2(\Lambda_3 - \Lambda_1) - \Lambda_1 \theta_0^2] \tau + \tan^{-1}(\lambda_2)]\} \exp\{-i(kx_0 - \omega t_0)\}, \]  
(29)
and
\[ \psi^1 = \frac{\eta_0}{\sqrt{1 + \lambda_2^2}} \text{sech}[\eta_0(\xi - 2\Lambda_1 \theta_0 \tau)] \exp\{i[\theta_0 \xi + \eta_0^2(\Lambda_3 - \Lambda_1) - \Lambda_1 \theta_0^2] \tau + \tan^{-1}(\lambda_2)]\} \exp\{-i(kx_0 - \omega t_0)\}. \]  
(30)

5. Nonlinear dynamics of DNA transcription

The simulation for the solution is done for nucleotide mass \( m \) is \( 5.1 \times 10^{-25} \) kg, distance between base neighbor \( l \) is \( 3.4 \times 10^{-10} \) m, elastic coefficient \( K \) is 8 N/m, depth of morse potential \( D \) is 0.1 eV, width of morse potential \( \alpha \) is \( 2 \times 10^{-10} \) m, the velocity of carrier wave \( u_c \) is \( 4 \times 10^9 \) m/s, and the velocity of envelope wave \( u_e \) is \( 1 \times 10^5 \) m/s. The result plot of equation (28) is as follows

Figure 1. The dynamics of DNA transcription.

Figure 1 showed that it is soliton wave, soliton type of breather, because of the ups and downs of the patterned amplitude and periodically [18, 19]. This type of soliton wave is also said to be a spatial soliton. Because the soliton wave propagates in the \( x \) plane, it showed that the soliton in the DNA propagate along the DNA strands. Over time the amplitude of the soliton in DNA changes. The amplitude of the soliton wave decreases and then increases again. The soliton of amplitude was decreased can identified the occurrence of renaturation in DNA strands. This happens because the PH around the DNA is stabilized so that the viscosity increases again and the damping effect increases. So that damping effect causes the DNA strands to associate of strands into double strands.
The soliton of amplitude was increased can identified the transcription process begins. The RNA polymerase enzyme interacts with a double strand of DNA, the interaction causes the base pair become unstable and the hydrogen bond is weak until the DNA opens its double strands (denaturation). In addition to interacting with base pairs in the DNA strands, the RNA polymerase enzyme interacts with fluid around the DNA. When the RNA polymerase enzyme approaches and interacts with the environment around the DNA, it causes an extreme PH increase. The PH is greater than 7 so that the H$^+$ concentration and the viscosity around the DNA decreases [20]. The reduced viscosity causes the damping effect to decrease and it allows the DNA to open its double strands.

It showed that damping around DNA is not constant but time-dependent. The following comparison of the behavior of the soliton without damping, the soliton with a constant damping, and the soliton with time-dependent damping can be seen from the following graphs:

Figure 2. Graphes of soliton without damping (black curve), soliton with constant damping (red curves), and soliton with time-dependent damping (blue curves)

In general, the amplitude of soliton with time-dependent damping (blue curve), soliton with constant damping (red curve), and soliton without damping (black curve) at $t = 0.1$ seconds decreased. When $t = 0.2$ seconds, the amplitude of soliton with time-dependent damping has increased while the amplitude of soliton with constant damping has slightly increased and the amplitude of soliton without damping still decrease. At $t = 0.3$ seconds, the amplitude of soliton with time-dependent damping decreased again, the amplitude of soliton with constant damping still increase, and the amplitude of soliton without damping still decrease.

It showed that the soliton with constant damping and soliton with time dependent damping are easy to renaturation (decreasing amplitude) because the damping of fluid around the DNA plays a role in the closure of the DNA strands. However, during the denaturation process, the soliton with constant damping is more difficult to open the strands than the soliton with time dependent damping. This is because of the constant damping force inhibits the opening of DNA strands. While on the soliton with time-dependent damping is easy to do the opening strands of DNA. This is due to decreasing damping effect when the process of opening DNA strands. Thus, the decrease in damping effects can help the opening of DNA strands. In the process of opening the DNA strands, there is an enzyme RNA polymerase that can change the PH fluid around the DNA becomes larger, so the H$^+$ concentration in around the DNA decreases, and damping effect becomes reduced.
In addition, the velocity of soliton with time-dependent damping slower than others. This is to compensate for the soliton characteristics that maintain constant carrying energy. The soliton with time-dependent damping undergoes significant damping changes, to maintain a stable condition, the velocity of soliton with time-dependent damping will be slower than others.

6. Summary
The dynamics of DNA transcription with time-dependent damping can be explained by the damped nonlinear Schrodinger (DNLS) equation. The solution of equation showed that soliton type of breather and spatial soliton, because of the ups and downs of the patterned amplitude and the wave propagates along the DNA strands. The analysis showed that damping on DNA not only play a role in the closure of DNA strands but in the process of opening the DNA strands damping also plays a role. It can be seen in the graph of the study that when the process of opening the DNA strands, damping effect helped the process by reducing the damping effect around the DNA as a result of an increase in PH and causes the H+ concentration in around the DNA is reduced. Likewise, in the process of closing the DNA strands, damping plays a role in the process of closing the DNA strands by increasing the damping effect around the DNA as a result of the change in PH to become neutral again so that the H+ concentration in around the DNA increased into stable condition.

Acknowledgements
S.F.R gratefully acknowledge support for LPDP. S.F.R also thanks to all members of Theoretical Physics Laboratory, Institut Teknologi Bandung for the hospitality and valuable support. F.P.Z would like to thanks to Kemenristek DIKTI for the financial support.

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