Low Amplitude Kink Soliton Excitation in Peyrard-Bishop Double Strand DNA Model

Donny Dwiputra¹, Wahyu Hidayat¹,² and Freddy Permana Zen¹,²
¹Theoretical High Energy Physics, Physics Department, Institut Teknologi Bandung, Indonesia
²Indonesian Center of Theoretical and Mathematical Physics (ICTMP), Indonesia
E-mail: donny.dwiputra@s.itb.ac.id

Abstract. We investigate the feasibility and appearance of a kink-like soliton solution in damped Peyrard-Bishop double-strand DNA model by applying the method Zdravković et al [Chaos Soliton Frac. 45, 1378 (2012)]. We extend the method to a perturbative case, resulting in a low amplitude solution. The importance of the kink excitation is to describe the propagating open state of DNA chain which has a significant role in DNA transcription and replication processes. In this paper, we study the feasibility conditions of a kink-like excitation to appear in DNA chain.

1. Introduction
Modelling a specific biological system that has several crucial interrelated phenomena is highly challenging for most physicists. Lossless transfer of information in DNA involve some intricate mechanism like transcription i.e. how the base-pair as blueprint of information being read effectively and replication process which also includes the transcription process as its initial step.

One most prominent model is given by Peyrard-Bishop (PB) [1]. Their model explains base-pair opening process, first initiated by local openings (the so-called DNA bubbles) and then the bubble grows when the temperature is above critical. Later, some crucial improvements applied to their model, such as in [2] which adds interaction between adjacent base-pairs, and in [zoli2011thermodynamics] which adds a tanh term to explain the solvent effect that stabilizes the double-strand structure. Interaction with protein molecule is also modelled in [4]-[6] by adding a protein and an interaction potential. However, there are no attempt to find a solution of PB model which involves a propagating open state such as in transcription and replication processes.

This paper aims to find a topological kink-like excitation to depict the propagation of base-pair opening in transcription and replication processes. We use the method in [7] to get the kink-like excitation from perturbed PB model up to fourth order in the potential. We will find that the PB model is not fully appropriate to explain the transcription process and at the last section of this paper we suggest some improvements.

2. Perturbative Peyrard-Bishop Model with Damping
The original Peyrard-Bishop (PB) model established a good approximation to the base-pair opening motion of a planar double-stranded DNA chain. However, the model has some major limitation i.e. by the fact that the adjacent base pairs are not independent each other. This factor is corrected by adding the stacking interaction term to the Hamiltonian [2].
For simplicity we only consider the original PB model but with an addition of environmental damping. The source of this damping is due to the fact that the stable DNA structure would not exist in vacuum, in reality the molecule complex is surrounded by viscous solution (in vivo and in vitro) [8]. We introduce the viscosity effect by adapting the Caldiora-Kanai model of damped oscillator [9] to our case, which is done by modifying the Hamiltonian to the time-dependent case. Thus, facilitating mechanical energy change over time. The damped PB Hamiltonian for the base opening (transverse) motion is represented as

$$H = \sum_n \left[ e^{-\gamma t} \frac{p_n^2}{2m} + e^{\gamma t} \left( \frac{K}{2} (y_{n+1}^2 - y_n^2) + V(y_n) \right) \right],$$  

where $y_n$ is the base-pair stretching relative to its equilibrium and $p_n$ is its momentum, while the damping coefficient $\gamma$, nucleotide mass $m$, and inter base-pair stiffness $K$ are taken to be constants. The first term represents the kinetic energy of a nucleotide, the second one is the potential energy of the interaction between adjacent base pairs. The last term is the Morse potential,

$$V(y_n) = \frac{D}{2} (e^{-ay_n} - 1)^2.$$  

where $D$ is the stiffness of the Hydrogen bonds which connect the two strands of a nucleotide and $a$ is the width of the potential well. Morse potential represents the bound-state and unbounded-state of the base-pair. This facilitates closed and open states of a double-strand DNA, respectively.

The model leads to a coupled nonlinear partial differential equation which cannot be solved exactly [10]. To compromise, we keep the first nonlinearities by expanding the Morse potential to fourth order,

$$V(y_n) = \frac{D}{2} \left( a y_n - (a y_n)^3 + \frac{7}{12} (a y_n)^4 + O((a y_n)^5) \right).$$  

This is the minimal setting to keep the boundedness of the potential and thus allows us to get a small, perturbative solution by assuming a weak nonlinearity. To further simplify the problem, we apply a continuum approximation $y_n(t) \rightarrow y(z, t)$ by using the expansion,

$$y_{n\pm1} \rightarrow y \pm y_z l + \frac{1}{2} y_{zz} l^2,$$

where $l = 3.4$ Å is the length between adjacent base pairs. In this paper the subscripts $t$ and $z$ denote time and spatial derivatives, respectively. This approximation valid only for weak coupling $K$. All this brings us to the following equation of motion,

$$m y_{tt} - K l^2 y_{zz} + D a \left( a y - \frac{3}{2} (a y)^2 + \frac{7}{6} (a y)^3 \right) + y y_z = 0.$$  

Here we can see that the factor $\exp(\pm \gamma t)$ in our Hamiltonian contribute to the last term in right-hand side which is a standard drag force, $f = -y y_z$. As we are interested in traveling kink-like solitons, we define $\xi = k x - \omega t$ as the moving frame. Substitution of this to Eq. (5) by introducing a dimensionless coordinate $\phi$, defined through the relation $y = \epsilon \phi / a$ with $|\epsilon| < 1$, leads to a much more convenient ODE:

$$\alpha \phi'' - \rho \phi' + \frac{3}{2} \epsilon \phi^2 + \frac{7}{6} \epsilon^2 \phi^3 = 0,$$

where $\phi' \equiv \phi \xi$ and the dimensionless parameters are,

$$\alpha = \frac{m a^2 - k^2 l^2 k}{D a^2} \quad \text{and} \quad \rho = \frac{\gamma a}{D a^2}.$$
3. Modified Extended tanh-function Method

In this section we apply the method of Zdravković et al [7] to solve Eq. (6). The desired solution is in the form of tanh-function, which depicts a kink-like excitation of this system. We look for the solution in the form

$$\phi = a_0 \sum_{m=1}^{N} (a_m \Psi^m + c_m \Psi^{-m}),$$

(8)

where $\Psi(\xi)$ is the solution of Riccati equation

$$\Psi' = b + \Psi,$$

(9)

whose derivative form is

$$\Psi'' = 2b\Psi + 2\Psi^3.$$  

(10)

The Possible solution of Eq. (9), if $b \in \mathbb{R}$, depend on the value of $b$ [7]:

(i) $b > 0 \Rightarrow \Psi = \sqrt{b} \tan(\sqrt{b}\xi)$ or $\Psi = -\sqrt{b} \coth(\sqrt{b}\xi)$,

(ii) $b = 0 \Rightarrow \Psi = -\frac{1}{\xi}$

(iii) $b < 0 \Rightarrow \Psi = -\sqrt{-b} \tan(\sqrt{-b}\xi)$ or $\Psi = -\sqrt{-b} \coth(\sqrt{-b}\xi)$,

This does not restrict that $b$ should be a real number to make Eq. (9) solvable, in fact we can still use (i) as a solution if $b \in \mathbb{C}$. If our system gives a negative $b$ (iii), the kink-like solution exists in the tanh term. Otherwise the solution blows up in some region. Thus, as an attempt to get a biophysically plausible solution, we shall look the solution in the case $c_m = 0$. This prevents divergent functions such as tangents and cotangents.

First, we determine $M$: the highest power of $\Psi$ in $\phi$. This is done by simply inserting Eq. (8) to our equation of motion Eq. (6). One can observe that each coefficient $a_m$ has nontrivial value if the highest derivative, $\phi''$, and the highest power, $\phi^3$ contribute the same highest order of $\Psi$ which is $\Psi^{M+2}$ and $\Psi^{3M}$, respectively. Hence, we get $M = 1$. Inserting Eq. (8) to Eq. (6), we get these following relations for each order of $\Psi$:

$$\Psi^0: \quad \frac{7}{6} \epsilon^2 a_0^3 - \frac{3}{2} a_0^2 + a_0 - \rho a_1 b = 0,$$

(11)

$$\Psi^1: \quad b = \frac{1}{2\alpha} \left( 3\epsilon a_0 - \frac{7}{2} \epsilon^2 a_0^2 - 1 \right),$$

(12)

$$\Psi^2: \quad \rho = \frac{\epsilon}{2} (7\epsilon a_0 - 3),$$

(13)

$$\Psi^3: \quad \alpha = -\frac{7}{12} \epsilon^2 a_0^2.$$  

(14)

By a little algebra involving Eqs. (11)-(14) one obtains the cubic equation for $a_0$,

$$a_0^3 + pa_0^2 + qa_0 + r = 0,$$

(15)

where

$$p = -\frac{12}{7\epsilon}, \quad q = \frac{41}{49\epsilon^2}, \quad r = -\frac{9}{49\epsilon^3}.$$  

(16)
We can make substitution \( x \equiv a_g - p/3 \) to remove the second and zeroth order of \( a_g \), the above equation reads
\[
x^3 + \mathcal{P}x + \mathcal{Q} = 0,
\] (17)
with the coefficients [11]
\[
\mathcal{P} = \frac{3q - p^2}{3} \quad \text{and} \quad \mathcal{Q} = \frac{1}{27} (2p^3 + 27r - 9pq).
\] (18)
The cubic equation has discriminant \( D = \mathcal{Q}^2/2 + \mathcal{P}^3/27 > 0 \) and thus it has one real root that can be written as follows [7],
\[
x = -\frac{2}{\sin(2\varphi)} \sqrt{-\frac{\mathcal{P}}{3}}, \tan\varphi = \left[ \frac{\tan \frac{w}{3} \right]^3, w = \arcsin \left[ \frac{2}{q} \left( -\frac{\mathcal{P}}{3} \right)^{3/2} \right].
\] (19)

Figure 1. The amplitude \( y(z, t) \) for \( t = 0 \) and (a) \( x = 1.109/\epsilon \) and (b) \( x = (0.302 + 0.272i)/\epsilon \), with \( Re[y(z, t)] \) (solid line) and \( Im[y(z, t)] \) (dashed line). These solutions travel to the right.

The other two roots are a complex conjugate pair. The roots are approximately
\[
x_1 \approx \frac{1.109}{\epsilon} \quad \text{and} \quad x_{2,3} \approx \frac{1}{\epsilon} [0.302 \pm 0.272i].
\] (20)

4. Discussions and Conclusions
The real root, \( x_1 \), gives the value \( a_0 \approx 0.537/\epsilon \) and from Eq. (12) we get \( b \approx -\frac{0.399}{2\alpha} \). But from Eq. (14) we get \( \alpha < 0 \) for the real nonzero \( a_0 \) (and thus \( a_1 \) is also). This implies \( b > 0 \) and hence the tanh solution representing the low amplitude kink-like excitation does not exist!

In figure 1a, we can see that the solution of type (i) diverges periodically. Strictly speaking, this behaviour is uneven because we have treated this system perturbatively. However, from a biophysical perspective this may be interpreted as the case when DNA is denatured (becomes fully open) at many specific sites because of the highly fluctuated nature of a DNA double-helix structure in noisy environment such as in calcium ion solvent. But apparently, we do not have a sound explanation and lack of experimental evidence for this. Moreover, we can calculate the velocity of this wave defined by \( v = \frac{\omega}{k} \). Some algebra involving Eqs. (7) and (11)—(14) result in the velocity as follows,
\[ v^2 = \frac{KL^2}{m + \frac{4\gamma^2}{3\epsilon(7a_0 - 3)^2Da^2}}. \]  

(21)

We take the DNA parameters from [12] and the viscosity \( \gamma \) from [13]:

\[
\alpha = 1.2\sqrt{2}\text{ A}^{-1}, \quad D = 0.14\text{ eV}, \quad K = 12\text{ N/m}, \\
\kappa = 0.18\text{ A}^{-1}, \quad \gamma = 0.05m\text{ kg/s}.
\]

and we take \( \epsilon = 0.2 \). The wavenumber \( \kappa \) corresponds to about 10 base pairs, each base pair has effective mass of \( m = 5.1 \times 10^{-25}\text{ kg} \). In this case we get \( v \approx 10^{-7}\text{ A}^*/\text{ps} \) which means that our wave is effectively at rest instead of travelling which as in the DNA transcription process. So, at the end, our solution appears to be non-physical and perturbatively incorrect.

But how if we take another root of \( x \), the pair of complex conjugate instead? Surprisingly the complex solution has finite amplitude in its real and imaginary part! The value \( x = (0.302 + 0.272i)/\epsilon \) will result in \( b = 0.111 - 0.173i \) and \( \nu = (5.530 + 6.955i) \times 10^{-8}\text{ A}^*/\text{ps} \). We can see this solution, figure 1b, has a resemblance with the anti-kink solution, but perturbed in the transition region. This solution at a glance pays off our effort in finding kink-like excitation. In other word, we do not yet know the biophysical interpretation of the imaginary part of \( y \) in this case. Unfortunately, however, the kink solution in figure 1b is somewhat unphysical because its velocity is a complex number. Hence further effort is needed if one wants to further contemplate about this kind of non-standard solution.

The inexistence of a kink-like excitation in this perturbed and damped PB model can be explained with the absence of a local maximum of the perturbed potential, Eq. (3). We conjecture that for a discrete, one-dimensional Hamiltonian lattice system to have a kink-like excitation, its potential should have at least a local maximum adjacent to a local minimum so that the canonical position can jump or fall between the peak and valley of the potential and transfers energy to its neighbour in the lattice, corresponding to a topological anti-kink or kink soliton.

Thus, according to our conjecture, the original PB model is unable to excite a kink-like soliton because it lacks a local maximum. This shows that the PB model cannot be used to explain phenomena like transcription and replication properly because it cannot predict a propagating open-state which is the basis of these processes. There are modifications to PB model that poses a local maximum in the potential, such as the one used by Zoli [3] to model the solvent effect to DNA double-strand. The model adds a tanh term which make the tip of the Morse plateau increase locally, here an already-open state cannot evolve to a closed-state (inside the potential well) with no energy cost. This setting is more realistic because a molecule that has undergone a disassociation reaction cannot instantaneously bonds again unless given an activation energy.

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