

Torsional Travelling Waves in DNA

Tomasz LIPNIACKI

Institute of Fundamental Technological Research

Świętokrzyska St. 21, 00-049 Warsaw Poland

E-mail: tlipnia@ippt.gov.pl

Abstract

The simple model of the non-linear DNA dynamics [4] is pursued in order to study the local untwisting of DNA double helix. It is shown how the advancing RNA polymerase may force the motion of the torsional solitary wave along DNA.

1 Introduction

The basic form of DNA is double helix, consisting of two sugar-phosphate backbones and a base pairs chain inside. A schematic drawing of the duplex DNA in an unwound hypothetical state, which one can call planar ladder state, is shown in Fig. 1. Because the four bases composing DNA are hydrophobic substances, they tend to stay together, rather than let the surrounding water fill gaps between them. If the adjacent base pairs in the sequence are in contact, the distance between their centers is $A \approx 3.3 \text{ \AA}$, smaller than the distance between the adjacent sugars in backbones $B \approx 6 \text{ \AA}$. This is because the sugar-phosphate backbones must wrap around the base pair chains in order to preserve their length.

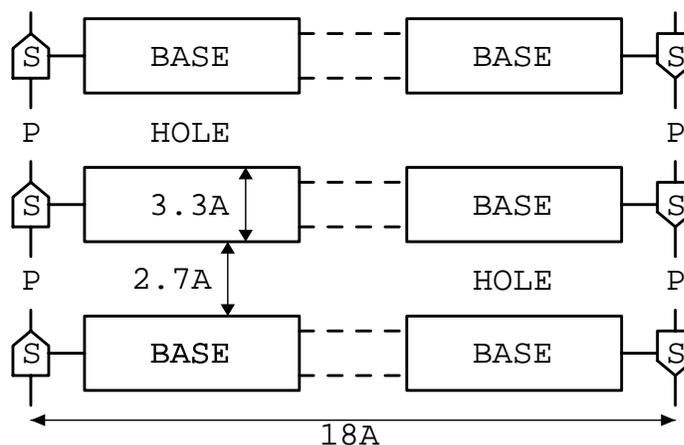


Figure 1. The scheme of DNA, the hypothetical planar DNA ladder with its key dimensions S — sugar, P — phosphate.

The base sequence codes the genetic information, but from the mechanical point of view it is a non periodic chain. The four bases composing DNA have different masses. This

poses a problem for all models. Fortunately, the masses of two base pairs composing DNA, namely the adenine–thymine (A–T) and guanine–cytosine (C–T) are almost equal. Only in an approximation in which one neglects internal degrees of freedom of the base pairs, and treats each base pair as a rigid body, can DNA be regarded as a periodic structure.

The interest in the nonlinear dynamics of DNA started when Englander *et al.* [1] suggested that the existence of solitons propagating along the DNA molecule may be important in a process called “RNA transcription”. In the last decade several models were proposed in order to substantiate this idea in quantitative terms (see Gaeta *et al.* [2] and Yakushevich [3]).

2 Description of the model

The approach to DNA dynamics presented in the current paper is based on the non-linear model of DNA dynamics proposed in Ref. [4]. The constructed model allowed us to describe analytically torsional travelling waves propagating along the DNA molecule. The purselike solutions described the propagation of an untwisted (or oppositely twisted) region along the molecule. Such solution has been connected with the mechanical aspects of transcription of the messenger RNA — one of the most important processes of DNA evolution. During transcription the DNA untwists locally to let one strand serve as a template for synthesis of new RNA strand. The untwisted open region, 15–20 base pairs long, then moves along the DNA.

In the previous paper, the energy dissipation (damping) was not included in the model. However it seems obvious that the motion of DNA leads to some energy dissipation due to nonelasticity of the DNA molecule or to interaction with the solvent. Moreover it is easy to check that when the energy dissipation is present, the purselike solutions cannot exist, unless the energy is somehow added to the system. The present work pursue the already proposed model, connecting the mechanism of energy input with the fact that DNA untwists and opens close to the RNA polymerase. The main idea is the following. In the vicinity of the polymerase the hydrophobic forces between base pairs are different (probably weaker) from those in the rest of the DNA molecule. This is due to the fact that the RNA polymerase is accompanied by flat oily amino acids, which can insert themselves between the base pairs. Thus, close to polymerase it is easier to separate base pairs and so untwist the DNA strands. The motion of the untwisted region is then forced by the motion of the RNA polymerase, which moves along the DNA due to chemical reactions.

In the proposed model (Fig. 2) base pairs are represented by rigid plates situated along the z axis. The sides of slabs are connected by rods representing the sugar-phosphate chains. It is assumed that these rods can bend but cannot stretch. The mass and inertial momentum of each plate is equal to the mass and momentum per base pair. Every slab can move along and turn around the z axis, and its position is described by a displacement w and a torsional angle Θ .

Elementary geometric considerations lead to the constraint connecting these two degrees of freedom

$$\Delta\Theta = 2 \arcsin \left(\frac{(B^2 - \Delta w^2)^{1/2}}{2R} \right), \quad (1)$$

where r_o is the distance between backbone springs and the duplex axis going through the centers of the slabs and B is the length of the side rods segments.

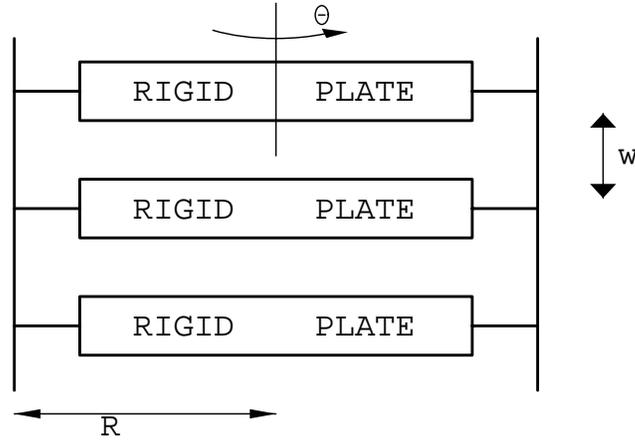


Figure 2. The schematic picture of the mechanical model. Each slab can move along and rotate around z axis; displacement is denoted by w , and torsional angle by Θ .

Now we construct the Lagrangian $L = T - \Phi$. The potential energy

$$\Phi_{i,i+1} = h_o(\Delta w - A, z, t), \quad (2)$$

follows from hydrophobic interaction between subsequent slabs. We assume that $h_o(\Delta w - A, \cdot, \cdot)$ has a single minimum at $\Delta w = A \approx 3.3 \text{ \AA}$. Let us note that because of the fact that $A < B$, the system has two natural minimum energy states: left and right twisted ladder; the relative angle $\Delta\Theta$ between two subsequent base pairs is given by Eq. (1) with $\Delta w = A$. With $A = 3.3 \text{ \AA}$, $B = 6 \text{ \AA}$ and $R = 9 \text{ \AA}$ one gets $\Delta\Theta = \pm 32^\circ$ what closely agrees with experiment.

The Φ dependence on position z and time t is due to the fact that hydrophobic forces may be influenced by RNA polymerase.

In the continuum limit,

$$\Delta w = w' A, \quad \Delta\Theta = \Theta' A, \quad (3)$$

with the primes denoting differentiation with respect to z .

Then the potential energy of the whole chain is

$$\Phi = A \int \left[h(w' - 1, z, t) + \frac{e_o \Theta'^2}{2} \right] dz, \quad (4)$$

where $h(w' - 1, z, t) = h_o(\Delta w - A, z, t)/A$. The term

$$A \int \frac{e_o \Theta'^2}{2} dz \quad (5)$$

has been added to Eq. (4) in order to describe the energy associated with the additional curvature of the side rods when Θ'' differs from zero.

The kinetic energy T is

$$T = \frac{1}{A} \int \left[\frac{m \dot{w}^2}{2} + \frac{J \dot{\Theta}^2}{2} \right] dz, \quad (6)$$

where m and J are the mass and moment of inertia per base pair, and the dot denotes time derivative.

To write the Lagrangian L in a simpler form, we employ units in which $A = 1$. Let

$$\phi := R\Theta, \quad e = e_o/R^2, \quad I = J/R^2. \quad (7)$$

The potential and kinetic energies of the system are now

$$\Phi = \int \left[h(w' - 1, z, t) + \frac{e\phi'^2}{2} \right] dz, \quad (8)$$

$$T = \int \left[\frac{m\dot{w}^2}{2} + \frac{I\dot{\phi}^2}{2} \right] dz. \quad (9)$$

In addition, from (1), replacing sinus by argument, we have the constraint

$$w'^2 + \phi'^2 - B^2 = 0. \quad (10)$$

3 Equations of motion

The evolution equations for w and ϕ , given by Euler–Lagrange equations with Lagrangian

$$L = T - \Phi + \lambda (w'^2 + \phi'^2 - B^2), \quad (11)$$

where λ is the Lagrange multiplier, are

$$I\ddot{\phi} + (e\phi''' + 2\lambda\phi')' - p\dot{\phi}'' = 0, \quad (12)$$

$$m\ddot{w} - \left(\frac{\partial h}{\partial w'} - 2\lambda w' \right)' = 0, \quad (13)$$

$$w'^2 + \phi'^2 - B^2 = 0. \quad (14)$$

The inelastic damping term $p\dot{\phi}''$ (where $p = \text{const} > 0$) was included in Eq. (12). This term is proportional to the speed with which the curvature of the sugar-phosphate chains changes. The role of the dissipation term will become more evident when we come to the final ordinary equation for ϕ' .

Assuming

$$w(z, t) = w(z - vt) = w(\tau), \quad \phi(z, t) = \phi(z - vt) = \phi(\tau), \quad (15)$$

$$h(w' - 1, z, t) = h(w' - 1, z - vt) = h(w' - 1, \tau), \quad (16)$$

we transform the system (12), (13), (14) into ODE's. After integration we obtain the system of equations

$$Iv^2\dot{\phi} = -e\ddot{\phi} - 2\lambda\dot{\phi} - vp\ddot{\phi} + C_2, \quad (17)$$

$$mv^2\dot{w} = \frac{\partial h}{\partial \dot{w}} - 2\lambda\dot{w} + C_1, \quad (18)$$

$$\dot{w}^2 + \dot{\phi}^2 - B^2 = 0. \quad (19)$$

where now the dot denotes differentiation with respect to τ . C_1 and $C_2' = C_2 - 2qc$ are the integration constants, where C_1 and $-C_2$ represent, respectively, the torsional moment and the stretching force applied to the chain at its ends. After some algebra we obtain the following equation for $X = \dot{\phi}$

$$e\ddot{X} = X(m-I)v^2 + \left(\frac{\partial h}{\partial \dot{w}} + C_1 \right) \frac{\partial \dot{w}}{\partial X} - vp\dot{X} + C_2, \quad (20)$$

with

$$\dot{w} = \sqrt{B^2 - X^2}. \quad (21)$$

Finally

$$\ddot{X} = -\frac{\partial W(X, \tau)}{\partial X} - \delta\dot{X}, \quad (22)$$

where

$$W(X, \tau) = -\frac{1}{e} \left(\frac{(m-I)v^2 X^2}{2} + C_2 X + (h(\dot{w}(X), \tau) + C_1 \dot{w}) \right) \quad (23)$$

and $\delta = vp/e$.

If $h(\dot{w}, \tau)$ is a single minimum function with respect to \dot{w} for any τ then $h(X, \tau)$ is a symmetric double well function since \dot{w} is symmetric with respect to X . The potential function $W(X, \tau)$ has precisely two maxima with respect to X (for any τ), provided that C_2 and C_1 are not too large; when $C_2 = 0$, $W(X, \tau)$ is symmetric. When $C_2 \neq 0$, $W(X, \tau)$ is not symmetric, and one maximum is higher than the other.

The homoclinic (heteroclinic) solutions of Eq. (22) correspond to traveling wave pulse-like (kink like) solutions of the initial system (12), (13), (14).

4 Existence of the homoclinic orbit

We confine our considerations to the case when

$$W(X, \tau) = W_o(X) + \epsilon V(X, \tau) \quad (24)$$

and there exists a pair $\tau_1 < \tau_2$ such that support of $V(X, \cdot) \subset [\tau_1, \tau_2]$ for any X . Let

$$G(X, \tau) := \frac{\partial V(X, \tau)}{\partial X}. \quad (25)$$

We also assume that $W_o(X)$ has precisely two maxima at X_1 and X_2 and $W(X_1) > W(X_2)$ (i.e. torsional moment $C_2 \neq 0$). Equation (22) can then be written

$$\ddot{X} = \frac{\partial W_o(X)}{\partial X} + \epsilon G(X, \tau) - \delta\dot{X}. \quad (26)$$

The last two terms of Eq. (26) will be treated as a perturbation, and the equation

$$\ddot{X} = \frac{\partial W_o(X)}{\partial X} \quad (27)$$

we will call the unperturbed equation. Let $X_o(\tau)$ be a homoclinic solution of unperturbed equation such that $X_o(\tau) = X_o(-\tau)$, satisfying $\lim_{\tau \rightarrow \pm\infty} X(\tau) = X_2$. Obviously $X_o(\tau + \tau_o)$ is also the homoclinic solution for any τ_o .

Now we may formulate the following:

Theorem. *Assume*

(i) *there exists τ_o such that*

$$\int_{\tau_1}^{\tau_2} G(X_o(\tau + \tau_o), \tau) \dot{X}_o(\tau + \tau_o) d\tau \neq 0, \quad (28)$$

(ii) *$G(\cdot, \cdot) \in C(R^2)$ and $W_o(\cdot, \cdot) \in C^1(R^2)$.*

Then there exists $\epsilon_o > 0$, such that for all $\epsilon \in (0, \epsilon_o)$ there exists $\delta_o > 0$, such that for all $\delta \in [0, \delta_o]$ there exists a homoclinic solution of Eq. (26) such that $X(-\infty) = X(\infty) = X_2$. Simply put, if the variable part of the potential function $\epsilon V(X, \tau)$ is not too large, then for sufficiently small friction term $\delta \dot{X}$ there exists a homoclinic solution to Eq. (26).

The proof can be found in Ref. [5].

5 Conclusion

The existence of torsional traveling waves, within the limits of the proposed model, is due to two main facts.

(i) The potential energy of the DNA chain Φ is a double well function of the twist density Θ' . In the relaxed state the chain has a uniform twist densities $\Theta' = \Theta'_o = (B^2 - A^2)^{1/2} / (AR)$ (from Eq. 1) or $\Theta' = -\Theta'_o$. Let us focus on the first case. Now, applying the torsional moment at the ends of the chain, one can add some positive twist to the system. This additional twist will spread uniformly over the chain, making the twist density $\Theta > \Theta_o$. On the other hand, applying the opposite torsional moment, one can remove twist from the chain, making the average twist density $\Theta < \Theta_o$. When the average twist density is getting smaller the energy of the chain grows up to some critical point when the system can jump to a state in which a part of the chain has a twist opposite to the rest. If the parameter e_o at Θ'' is small, then it is “energetically worth” to create an oppositely twisted segment of the chain even if the average twist density is close to Θ'_o . The untwisted (or oppositely twisted) segment thus created can then move along the chain.

(ii) The energy dissipated due to local twisting and untwisting of the DNA molecule is balanced by the energy pumped by the varying hydrophobic potential of the base pair interaction. Without that additional energy, any nonzero dissipation makes that purselike solutions cannot exist.

The purselike solutions obtained in the model correspond to local untwisting of the DNA molecule during RNA transcription. The transcription process (and so the untwisting of the DNA molecule) takes place in the vicinity of RNA polymerase. In the vicinity of the polymerase the hydrophobic forces between the base pairs get weaker. This is due to the fact that the RNA polymerase is accompanied by flat oily amino acids such as phenylalanine, tyrosine, and tryptophan, which can insert themselves between the base pairs. Within the frames of our model this effect is interpreted as variation of the hydrophobic potential. The advancing RNA polymerase forces, by chemical processes, a large scale “mechanical” motion (the untwisting) of DNA molecule.

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