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# Dynamics of DNA breathing in the Peyrard–Bishop model with damping and external force

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## ABSTRACT

The impact of the damping effect and external forces on DNA breathing is investigated within the Peyrard–Bishop model. In the continuum limit, the dynamics of the breathing of DNA is described by the forced-damped nonlinear Schrödinger equation and studied by means of the variational method. The analytical solutions are obtained for special cases. It is shown that the breather propagation is decelerated in the presence of a damping factor without the external force, while the envelope velocity and the amplitude increase significantly with the presence of external force. It is particularly found that the higher harmonic terms are enhanced when the periodic force is applied. It is finally argued that the external force accelerates the DNA breathing.

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## 1. Introduction

At room temperature the DNA double helix spontaneously denatures locally, opens up or fluctuates. The so called DNA breathing in particular occurs when it is locally excited with large amplitude [1–3]. It also depends on the dynamics of surrounding fluid molecules [4,5]. Therefore, it is important to take into account the effects of such viscous medium. The effects have actually been investigated by, for instance, Zdravkovic et al. where the solution is described by the damped nonlinear Schrödinger (NLS) equation [6].

Recent experiments show that the DNA breathing might be influenced by external forces like the Terahertz field [7]. They have found that the linear instabilities lead to a dynamics dimerization, while the true local strand separation requires a threshold amplitude mechanism. Within the Peyrard–Bishop–Dauxois (PBD) model, Maniadis et al. have shown that the period-doubled discrete breather appears from the anti-continuum limit of the

driven PBD model [8]. They adopted the discretized PBD model with additional damping (dissipative) term and periodic (cosine) external force as well.

This paper discusses the viscous dissipation effect as well as an external force acting on DNA in the Peyrard–Bishop (PB) model. Then, the dynamics of DNA breathing with such additional terms are investigated using a continuum approach. This means the paper considers a larger scale of DNAs with a typical size of, namely 2  $\mu\text{m}$ , which can be observed using atomic force microscopy (AFM). Using AFM it has been observed that such DNAs generate interesting fractal patterns [9].

The paper is organized as follows. In Section 2 the Hamiltonian of the model under consideration is explained, and its subsequent equation of motion (EOM) containing the damping and external force is derived. The continuum approximation for the DNA breathing is described in Section 3. Thereafter, its solitonic solution using the variational method is given in Section 4, and followed by a discussion of breathing dynamics in terms of solitary waves in Section 5. Finally, the paper is ended with a summary.

## 2. PB Model with damping and external force

Following the PB model, the motion of DNA molecules is represented by two degrees of freedom,  $u_n$  and  $v_n$ , which correspond

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to the displacement of the base pair from its equilibrium position along the direction of the hydrogen bonds connecting the two bases in the pair in the two different strands [10–12]. Further, it can be rewritten by performing a transformation to the center of mass coordinate representing the in-phase and out-of phase transverse motions,  $X_n = (u_n + v_n)/\sqrt{2}$  and  $Y_n = (u_n - v_n)/\sqrt{2}$  respectively. Since, however only the variable  $Y_n$  is relevant for DNA breathing, the PB model is given by Peyrard and Bishop [10],

$$H = \sum_n \frac{1}{2M} (P_n)^2 + \frac{\kappa}{2} (Y_{n+1} - Y_n)^2 + \frac{D}{2} (e^{-\frac{\alpha}{2} Y_n} - 1)^2, \quad (1)$$

where  $D$  and  $\alpha$  are the depth and inverse width of the potential respectively.  $P_n = M\dot{Y}_n$  is the momentum, while  $\kappa$  is the spring constant.

As mentioned above, the studies of PB models with viscosity have already been done by adding a term  $-\epsilon\gamma\dot{Y}_n$  in the EOM [6,13,14]. In Ref. [6], the NLS equation with viscous effect has been solved to study the dynamics of DNA breathing. The interaction between the system and the surrounding environment leads to energy dissipation. This means that the system is no longer conservative and reversible. Unfortunately, there is no standard procedure to include the dissipation effect in a Hamiltonian. It is still an open problem so far. On the other hand, including the dissipation effects is motivated by some measurements in quantum cryptography [15,16]. There are some methods to incorporate dissipation effects, i.e. Caldirola–Kanai [17], and Caldeira–Leggett where the dissipation effects are treated as a collection of oscillator harmonics [18,19]. The first method is rather straightforward. The second method makes use of a Lindblad formulation with a density matrix equation [16,20,21].

In this paper, for the sake of simplicity let us adopt the formulation of Caldirola–Kanai to derive the classical EOM. The corresponding Hamiltonian for a dissipative system in the formulation is called the Caldirola–Kanai Hamiltonian. In general, it is written in the form of a time-dependent Hamiltonian, that is  $H(p, q) = \exp(-\gamma t) p^2/2M + \exp(\gamma t) V(q)$  [17]. Here,  $\gamma = \eta/M$  and  $\eta$  is the damping coefficient. The model describes a dissipative system where its kinetic energy is damped along the time, while its potential is getting larger. This means the energy conservation is broken explicitly within the model, since it describes a kind of open system due to dissipation rather than a conventional closed system. The model has widely been applied to deal with quantum dissipations such as the quantization of an electromagnetic field inside a resonator filled by dielectric medium [22], the susceptibility of identical atoms subjected to an external force [23], the coherent states for a damped harmonic oscillator [23], the dissipative tunneling of an inverted Caldirola–Kanai oscillator [24] and the functional integral for non-Lagrangian systems [25]. In principle one can extend such approaches to describe the denaturation processes in a dissipative system.

The present paper proposes the modified PB model with the damping effect and an external driving force  $F(t)$ ,

$$H = \sum_n \frac{e^{-\gamma t}}{2M} (P_n)^2 + \frac{e^{\gamma t} \kappa}{2} (Y_{n+1} - Y_n)^2 + \frac{e^{\gamma t} D}{2} (e^{-\frac{\alpha}{2} Y_n} - 1)^2 - e^{\gamma t} F_n(t) Y_n. \quad (2)$$

Here,  $F_n(t)$  is a conservative force. Although in principle one can directly start from a certain EOM as derived later, in this paper let us consider this Hamiltonian, because there are certain advantages of this approach, for instance being able to calculate the thermodynamic behaviors of the system under consideration for future studies. Secondly, rather than put the additional forces in the EOMs by hand, one can generate them in a systematical

way. It should be noted however that this paper is focused only on investigating the dynamics governed by the derived EOM.

From the Hamiltonian in Eq. (2), one can obtain the canonical coordinates,

$$\dot{Y}_n = \frac{\partial H}{\partial P_n} = e^{-\gamma t} \frac{P_n}{M}, \quad (3)$$

$$\dot{P}_n = -\frac{\partial H}{\partial Y_n} = -e^{\gamma t} \kappa (Y_{n+1} - 2Y_n + Y_{n-1}) - e^{\gamma t} \frac{\alpha D}{2} (e^{-\frac{\alpha}{2} Y_n} - 1) - e^{-\frac{\alpha}{2} Y_n} + e^{\gamma t} F_n(t). \quad (4)$$

Substituting Eq. (3) into Eq. (4) yields a differential equation,

$$M\ddot{Y}_n + M\gamma\dot{Y}_n + \kappa(Y_{n+1} - 2Y_n + Y_{n-1}) + \frac{\alpha D}{2} (e^{-\frac{\alpha}{2} Y_n} - 1) e^{-\frac{\alpha}{2} Y_n} = F_n(t). \quad (5)$$

The damping term  $\gamma M\dot{Y}_n$  is similar to the external force in [6], i.e.  $F_n = -\gamma M\dot{Y}_n$  in their EOM which has been put by hand. Therefore, within the model one can conclude that the term is nothing else than the contribution of a damped kinetic term in an open system governed by the Caldirola–Kanai Hamiltonian.

### 3. Continuum limit approximation

The dynamical behavior of DNA breathing can be studied using the continuum approximation in Eq. (5). Let us assume that the amplitude of oscillation is small, and the nucleotide oscillates around the bottom of the Morse potential. This assumption is plausible to keep the DNA breathing. Then, under the assumption the out-of phase transverse motions can be rewritten as,

$$Y_n \equiv \epsilon \Psi_n \quad (6)$$

with  $\epsilon \ll 1$  [3,6,13].

Substituting Eq. (6) into Eq. (5), up to the third order of the Morse potential one obtains,

$$\ddot{\Psi}_n + \gamma \dot{\Psi}_n = \omega_0^2 (\Psi_{n+1} - 2\Psi_n + \Psi_{n-1}) + C_m^2 (\Psi_n + \epsilon a_1 \Psi_n^2 + \epsilon^2 a_2 \Psi_n^3) + \tilde{F}_n, \quad (7)$$

where  $\omega_0^2 = \kappa/M$ ,  $C_m^2 = (\alpha^2 \bar{D})/(2M)$ ,  $a_1 = -3/4\alpha$ ,  $a_2 = \sqrt{7/24}\alpha$ ,  $\bar{D} = 1/N \sum_n^N D_n$  is the average value of  $D$ , and  $\tilde{F}_n = F_n(\epsilon \Psi_n, t)$ . This result is well known as a semi-discrete equation for investigating the DNA breathing in a viscous medium [6,13]. For a relatively long DNA chain, this equation can be simplified by taking its full continuum limit. Defining the length scale  $l \equiv x/n$  and  $C_0^2 = \omega_0^2 l^2$ , one can rewrite  $\Psi_n(t) \rightarrow \Psi(x, t)$ . The approximation is valid as long as the solution under consideration changes rather slowly and smoothly along the DNA [5]. This then yields,

$$\frac{\partial^2 \Psi}{\partial t^2} + \gamma \frac{\partial \Psi}{\partial t} = C_0^2 \frac{\partial^2 \Psi}{\partial x^2} + C_m^2 (\Psi + \epsilon a_1 \Psi^2 + \epsilon^2 a_2 \Psi^3) + \tilde{F}(x, t). \quad (8)$$

Both terms of  $\epsilon \tilde{F}(x, t)$  and  $\epsilon \gamma \partial \Psi / \partial t$  can be treated perturbatively by assuming that it contributes little enough to the whole DNA motion that is dominated by the first and second terms. Since the first and second terms yield a solution of  $\Psi \sim e^{i(kx - \omega t)}$ , using the multiple scale expansion method, namely by expanding the associated equation into different scale and time spaces [26], one gets,

$$\Psi = \Psi^{(0)} + \epsilon \Psi^{(1)} + \dots, \quad (9)$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_0} + \epsilon \frac{\partial}{\partial t_1} + \dots, \quad (10)$$

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial x_0} + \epsilon \frac{\partial}{\partial x_1} + \dots. \quad (11)$$

Substituting further these expansions into Eq. (8),

$$0 = \epsilon^0 \left[ \frac{\partial^2 \psi^{(0)}}{\partial t_0^2} - C_0^2 \frac{\partial^2 \psi^{(0)}}{\partial x_0^2} - C_m^2 \psi^{(0)} \right] + \epsilon^1 \left[ \frac{\partial^2 \psi^{(1)}}{\partial t_0^2} + 2 \frac{\partial^2 \psi^{(0)}}{\partial t_0 \partial t_1} - C_0^2 \frac{\partial^2 \psi^{(1)}}{\partial x_0^2} + \gamma \frac{\partial \psi^{(1)}}{\partial t_0} - 2C_0^2 \frac{\partial^2 \psi^{(0)}}{\partial x_0 \partial x_1} + C_m^2 \psi^{(1)} - \frac{3}{2} C_m^2 (\psi^{(0)})^2 + \tilde{F} \right] + \epsilon^2 \left[ \frac{\partial^2 \psi^{(2)}}{\partial t_1^2} + 2 \frac{\partial^2 \psi^{(1)}}{\partial t_0 \partial t_1} - C_0^2 \frac{\partial^2 \psi^{(2)}}{\partial x_1^2} - 2C_0^2 \frac{\partial^2 \psi^{(1)}}{\partial x_0 \partial x_1} + \frac{7}{6} C_m^2 (\psi^{(0)})^3 + 2C_m^2 \psi^{(0)} \psi^{(1)} \right] + \dots \quad (12)$$

The first and second terms in the leading order (LO) and next-to-leading order (NLO) terms in Eq. (12) provide the harmonic solutions, while the remaining terms lead to the non-harmonic ones. Then it is plausible to consider [6,13],

$$\psi^{(0)}(x_1, t_1) = \psi^{(1)}(x_1, t_1) e^{i(kx_0 - \omega_0 t_0)} + cc, \quad (13)$$

$$\psi^{(1)}(x_1, t_1) = \psi^{(0)}(x_1, t_1) + \psi^{(2)}(x_1, t_1) e^{2i(kx_0 - \omega_0 t_0)} + cc, \quad (14)$$

$$\tilde{F} = \tilde{f}(x_1) e^{i(kx_0 - \omega_0 t_0)} + cc. \quad (15)$$

Having Eqs. (13)–(15) at hand and using the dispersion relation  $\omega_0^2 = \bar{D} + C_0^2 k^2$ , Eq. (12) becomes,

$$\psi^{(0)} = 3 |\psi^{(1)}|^2, \quad (16)$$

$$i \frac{\partial \psi^{(1)}}{\partial \tau} + \Lambda_1 \frac{\partial^2 \psi^{(1)}}{\partial \xi^2} + \Lambda_2 \frac{\partial \psi^1}{\partial \tau} + \Lambda_3 |\psi^{(1)}|^2 \psi^{(1)} = \tilde{f}, \quad (17)$$

$$\psi^{(2)} = \frac{1}{2} |\psi^{(1)}|^2, \quad (18)$$

where  $\Lambda_1 = C_0 \bar{D} / (2C_m^3)$ ,  $\Lambda_2 = \gamma / (2C_m)$ ,  $\Lambda_3 = 2\bar{D} / C_m$ ,  $\tau \equiv t_1 - \epsilon t_0$ ,  $\xi \equiv x_1 - (C_0 k) / C_m t_0$ ,  $x_1 = \epsilon x_0$ . This set of EOMs is nothing else than the forced-damped nonlinear Schrödinger (FDNLS) equation.

#### 4. Variational methods

The solution of the FDNLS equation with cosine force leads to a chaotic behavior [8,27]. However, the present paper investigates the breathing dynamics which is still in the solitonic behavior. This situation is realized by putting the damping terms and external force to remain perturbative. Therefore the basic solution is still the solitonic NLS. This problem can be solved using the variational method [19].

It is also well know that for the case with  $\gamma = 0$  and  $\tilde{f} = 0$ , the NLS equation admits the following traveling wave solution [5,6,13],

$$\psi^{(1)}(\xi, \tau) = A_0 \operatorname{sech} \left[ \frac{1}{L} (\xi - u_e \tau) \right] e^{-i(k\xi - \tilde{\omega}\tau)}, \quad (19)$$

where,

$$A_0 = \sqrt{\frac{u_e^2 - 2u_e u_c}{2\Lambda_1 \Lambda_3}}, \quad (20)$$

$$L = \frac{\sqrt{2\Lambda_1}}{\sqrt{u_e^2 - 2u_e u_c}}, \quad (21)$$

$$\tilde{k} = \frac{u_e}{2\Lambda_1}, \quad (22)$$

$$\tilde{\omega} = \frac{u_e u_c}{2\Lambda_1}. \quad (23)$$

Here,  $u_e$  is the envelope wave velocity and  $u_c$  is the carrier wave velocity satisfying  $u_e^2 - 2u_e u_c > 0$ . Using Eqs. (9), (13) and (14) one obtains the soliton solution,

$$\psi(x, t) = 2\psi^{(1)} \cos(kx - \omega_0 t) + \epsilon |\psi^{(1)}|^2 [3 + \cos(2(kx - \omega_0 t))], \quad (24)$$

where  $\psi^{(1)}$  is given by Eq. (19).

Based on the corresponding variational methods to solve the FDNLS equation, one may use the solution in Eq. (19) as the related basic form. Considering that the amplitude, width, phase velocity and position of the soliton should be time dependent [26,28], let us write the 1-soliton in the following form,

$$\psi^{(1)}(\xi, \tau) = \eta(\tau) \operatorname{sech}[\eta(\xi + \zeta(\tau))] \times \exp(-i[\theta(\tau)\xi + \phi(\tau)]). \quad (25)$$

In order to obtain the dynamics of functions  $\eta$ ,  $\theta$ ,  $\zeta$  and  $\phi$ , one should first derive the Lagrangian for the FDNLS. The appropriate Lagrangian is,

$$\mathcal{L} = \frac{i}{2} (\psi_\tau^{(1)} \psi^{(1)*} - \psi_\tau^{(1)*} \psi^{(1)}) - \Lambda_1 |\psi_\xi^{(1)}|^2 + \Lambda_3 |\psi^{(1)}|^4 + \frac{\Lambda_2}{2} (\psi_\tau^{(1)} \psi^{(1)*} - \psi_\tau^{(1)*} \psi^{(1)}) - (\tilde{f} \psi^{(1)*} + \tilde{f}^* \psi^{(1)}), \quad (26)$$

which satisfies the FDNLS equation through the Euler-Lagrange equation [26],

$$\frac{\partial}{\partial \tau} \left( \frac{\partial \mathcal{L}}{\partial \psi_\tau^{(1)*}} \right) + \frac{\partial}{\partial \xi} \left( \frac{\partial \mathcal{L}}{\partial \psi_\xi^{(1)*}} \right) - \frac{\partial \mathcal{L}}{\partial \psi^{(1)*}} = 0. \quad (27)$$

Substituting Eq. (25) into Eq. (26) yields,

$$L = 2\eta\zeta\dot{\theta} + \eta\dot{\phi} + 2i\Lambda_2\eta\zeta\dot{\theta} + i\Lambda_2\eta\dot{\phi} + 4\Lambda_1\eta\theta^2 + \frac{4}{3}\Lambda_3\eta^3 - \eta\bar{F}, \quad (28)$$

by making use of relations  $L = \int_{-\infty}^{\infty} \mathcal{L} d\xi$ ,  $\int_{-\infty}^{\infty} \operatorname{sech}(a\xi) d\xi = \pi/a$  and  $\int_{-\infty}^{\infty} \operatorname{sech}^2(a\xi) \tanh(a\xi) d\xi = 0$ . Here,

$$\bar{F} = \int_{-\infty}^{\infty} \left( \tilde{f} e^{i[\theta(\tau)\xi + \phi(\tau)]} + \tilde{f}^* e^{-i[\theta(\tau)\xi + \phi(\tau)]} \right) \times \operatorname{sech}[\eta(\xi - \zeta\tau)] d\xi. \quad (29)$$

Eq. (28) is the Lagrange function in terms of  $\theta$ ,  $\eta$ ,  $\phi$  and  $\zeta$ . The EOM can be easily obtained by again using the Euler-Lagrange equation,

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{X}} \right) - \frac{\partial L}{\partial X} = 0, \quad (30)$$

where  $X = (\eta, \theta, \phi, \zeta)$ . Eqs. (28) and (30) lead to the following set of EOMs,

$$2(1 + i\Lambda_2)\eta\dot{\zeta} + 2(1 + i\Lambda_2)\zeta\dot{\eta} = 8\Lambda_1\eta\theta - \eta \frac{\partial \bar{F}}{\partial \theta}, \quad (31)$$

$$2(1 + i\Lambda_2)\zeta\dot{\theta} + (1 + i\Lambda_2)\dot{\phi} = 4(\Lambda_1\theta^2 - \Lambda_3\eta^2) - \eta \frac{\partial \bar{F}}{\partial \eta} - \bar{F}, \quad (32)$$

$$(1 + i\Lambda_2)\dot{\eta} = -\eta \frac{\partial \bar{F}}{\partial \phi}, \quad (33)$$

$$2(1 + i\Lambda_2)\dot{\theta} = -\frac{\partial \bar{F}}{\partial \zeta}. \quad (34)$$

Further substitution of Eqs. (33) and (34) into Eqs. (31) and (32) provides,

$$(1 + i\Lambda_2)\eta\dot{\zeta} - 4\Lambda_1\theta = 2\eta\frac{\partial\bar{F}}{\partial\eta} - \frac{\partial\bar{F}}{\partial\theta}, \quad (35)$$

$$(1 + i\Lambda_2)\dot{\phi} - 4(\Lambda_1\theta^2 - \Lambda_3\eta^2) = \zeta\frac{\partial\bar{F}}{\partial\zeta} - \eta\frac{\partial\bar{F}}{\partial\eta} - \bar{F}. \quad (36)$$

Unfortunately, the analytic and general solutions for Eqs. (31)–(34) do not exist. The solutions are still derivable only for special conditions. From here, let us consider a few special cases of  $\bar{F}$ .

First of all, let us consider a special case when the damping factor and external force vanish, that is  $\Lambda_2 = 0$  and  $\bar{F} = 0$ . As a result,  $\eta = \eta_0$  in Eq. (33) is a constant, while Eq. (34) yields  $\theta = \theta_0$  to be also a constant. Eqs. (31) and (32) lead to a simple solution,

$$\zeta = 4\Lambda_1\theta_0\tau, \quad (37)$$

$$\phi = 4(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2)\tau. \quad (38)$$

Therefore the single soliton has the form of,

$$\Psi^{(1)}(\xi, \tau) = \eta_0 \operatorname{sech}[\eta_0(\xi + 4\Lambda_1\theta_0\tau)] \times \exp\{-i[\theta_0\xi + 4(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2)\tau]\}. \quad (39)$$

This coincides with the single soliton solution of the conventional NLS equation.

In the second case, let us ignore the external force,  $\bar{F} = 0$ . Again,  $\eta = \eta_0$  and  $\theta = \theta_0$  in Eqs. (33) and (34) become constant as well. The time dependent variables are  $\zeta$  which represents the soliton velocity and the phase of soliton  $\phi$ . The EOM then has a simple form,

$$(1 + i\Lambda_2)\frac{d\zeta}{d\tau} - 4\Lambda_1\theta_0 = 0, \quad (40)$$

$$(1 + i\Lambda_2)\frac{d\phi}{d\tau} - 4(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2) = 0. \quad (41)$$

These yield,

$$\zeta(\tau) = 4\frac{\Lambda_1\theta_0}{(1 + \Lambda_2^2)}(1 - i\Lambda_2)\tau, \quad (42)$$

$$\phi(\tau) = 4\frac{(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2)}{(1 + \Lambda_2^2)}(1 - i\Lambda_2)\tau, \quad (43)$$

and the single soliton solution becomes,

$$\Psi^{(1)}(\xi, \tau) = \eta_0 \operatorname{sech}[\eta_0(\xi + \bar{\zeta}\tau) + i\eta_0\bar{\zeta}\Lambda_2\tau] \times e^{-i(\theta_0\xi + \bar{\phi}\tau)}, \quad (44)$$

where  $\bar{\zeta} = 4\Lambda_1\theta_0/(1 + \Lambda_2^2)$  and  $\bar{\phi} = 4(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2)/(1 + \Lambda_2^2)$ .

The third one is another simple case when  $\bar{F} = \bar{F}_0$  is a constant. Again,  $\eta = \eta_0$  and  $\theta = \theta_0$  are constants. The EOMs in Eqs. (35) and (36) have simple forms as follows,

$$(1 + i\Lambda_2)\frac{d\zeta}{d\tau} - 4\Lambda_1\theta_0 = 0, \quad (45)$$

$$(1 + i\Lambda_2)\frac{d\phi}{d\tau} - 4(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2) = -\bar{F}_0. \quad (46)$$

These lead to,

$$\zeta(\tau) = 4\frac{\Lambda_1\theta_0}{(1 + \Lambda_2^2)}(1 - i\Lambda_2)\tau, \quad (47)$$

$$\phi(\tau) = \left[ \frac{4(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2)}{(1 + \Lambda_2^2)} - \frac{\bar{F}_0}{(1 + \Lambda_2^2)} \right] (1 - i\Lambda_2)\tau. \quad (48)$$

Finally, the single soliton solution for this case is,

$$\Psi^{(1)}(\xi, \tau) = \eta_0 \exp(-\bar{\phi}\Lambda_2\tau) e^{F^*\tau} e^{-i(\theta_0\xi + \bar{\phi}\tau - F^*\tau)} \times \operatorname{sech}[\eta_0(\xi + \bar{\zeta}\tau) + i\eta_0\bar{\zeta}\Lambda_2\tau], \quad (49)$$

where  $F^* = \bar{F}_0/(1 + \Lambda_2^2)$ . The external force contributes through the positive exponential term, and then should increase the amplitude of the soliton.

For the last one, let us assume that the amplitude and phase are both constants, i.e.  $\eta = \eta_0$  and  $\theta = \theta_0$ , while the external force is assumed to have an exponential form,  $\bar{f} = f_0 \exp(-i\theta_0\xi)$  with  $f_0$  a constant. The EOM becomes,

$$(1 + i\Lambda_2)\eta_0\dot{\zeta} - 4\Lambda_1\theta_0 = 0, \quad (50)$$

$$(1 + i\Lambda_2)\dot{\phi} - 4(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2) = \zeta\frac{\partial\bar{F}}{\partial\zeta} - \bar{F}, \quad (51)$$

while Eq. (29) becomes,

$$\bar{F} = \int_{-\infty}^{\infty} (f_0 e^{-i\theta_0\xi} e^{i[\theta_0\xi + \phi(\tau)]} + f_0 e^{i\theta_0\xi} e^{-i[\theta_0\xi + \phi(\tau)]}) \times \operatorname{sech}[\eta(\xi - \zeta\tau)] d\xi = \frac{4f_0}{\pi} \cos(\phi). \quad (52)$$

Finally one can find,

$$\dot{\zeta} = \frac{4\Lambda_1\theta_0}{(1 + i\Lambda_2)\eta_0}, \quad (53)$$

$$\dot{\phi} = -\frac{4f_0}{\pi(1 + i\Lambda_2)} \cos(\phi) + \frac{4(\Lambda_1\theta_0^2 - \Lambda_3\eta_0^2)}{(1 + i\Lambda_2)}. \quad (54)$$

The Eq. (54) can be solved numerically. It should be noted that its solution is a complex function, i.e.  $\phi = \phi_R + i\phi_I$ . Therefore the soliton profile is given by,

$$\Psi^{(1)}(\xi, \tau) = \eta_0 e^{\phi_I\tau} e^{-i(\theta_0\xi + \phi_R\tau)} \times \operatorname{sech}[\eta_0(\xi - \bar{\zeta}\tau) + i\eta_0\bar{\zeta}\Lambda_2\tau]. \quad (55)$$

Now, in the next section let us discuss in more detail the dynamics of DNA breathing in the four cases given above.

### 5. Nonlinear dynamics of DNA breathing

The external effects of DNA usually lead to inhomogeneities in the DNA model. The inhomogeneity in stacking energy has been found to modulate the width and speed of the soliton depending on the nature of inhomogeneities [29]. The author used the dynamic plane-base rotator model by considering the angular rotation of bases in a plane normal to the helical axis, and found that the DNA dynamics is merely governed by the perturbed sine-Gordon equation. In this paper, it has been shown that the inhomogeneities of DNA breathing dynamics is governed by the FDNLS equation. The solutions of the homogeneous case represent a large amplitude with localized oscillatory mode. This seems to be a good explanation for the breathing of DNA that is spontaneously formed [2,3,5].

In the first case mentioned in the preceding section, it is easily shown that by performing certain transformations, that is  $\eta_0 = A_0$  and  $\theta_0 = 1/(2u_e A_1)$ , the solution coincides with Eq. (19). The simulation for the solution is done for  $\kappa = 8 \text{ N m}$ ,  $M = 5.1 \times 10^{-25} \text{ kg}$ ,  $\alpha = 2 \times 10^{10} \text{ m}^{-1}$ ,  $D = 0.1 \text{ eV}$  and the length scale  $l = 3.4 \times 10^{-10} \text{ m}$  [6]. The solution demonstrates a sort of modulated solitonic wave where the hyperbolic and cosine terms correspond to the envelope wave number and the carrier wave respectively.

In the second case with  $\bar{F} = 0$  and damping constant  $\gamma = 0.05 \text{ kg/s}$ , the breathing behavior is depicted in Fig. 1. The figure shows that the breathing propagation along the DNA molecule is

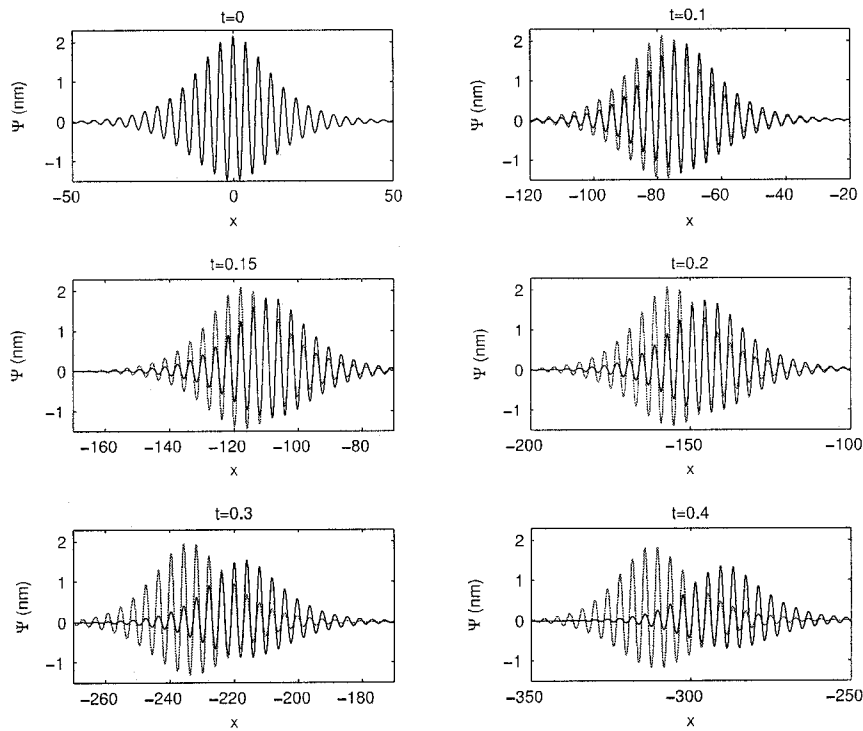


Fig. 1. The DNA breathing in the second case where  $x$  denotes the continuum base pair in the present model (black) and the original PB model (red) with  $g = 0.05$  and  $F = 0$ . (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

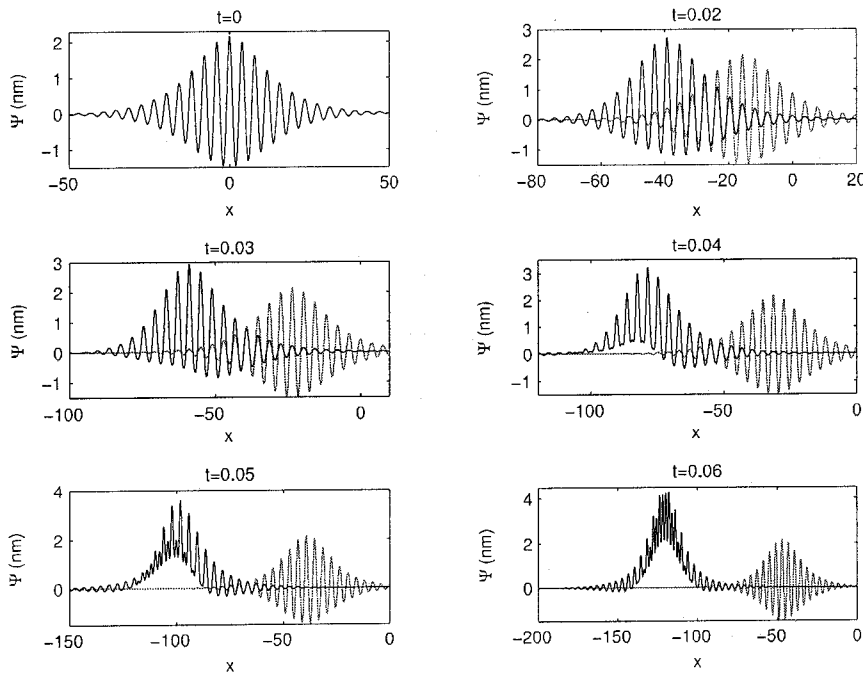


Fig. 2. The solitonic solution of DNA breathing in the model with damping effect and external force  $\bar{F}$  (black) and in the original PB model (red) with  $\gamma = 0.05$  kg/s and  $\bar{F} = 15$  pN. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

affected by the damping. It is obvious from the figure that the damping term decelerates the propagating soliton while retaining its amplitude profile. This indicates that the corresponding damping term does not affect the soliton mass.

Now, the solution with damping effect and  $\bar{F} \neq 0$  is depicted in Fig. 2. The figure is generated with  $F = 15$  pN and a damping factor  $\gamma = 0.05$  kg/s. The external force tends to increase the breathing

amplitude and is damped out by the damping effect. Consequently, the presence of external force increases the envelope velocity significantly, in particular around  $\Delta u_e = \Delta \xi / \Delta \tau \sim O(1)$ .

These results are actually motivated by previous works in [30]. In a cell, DNA strands are separated by the external force [30,31], or in chemical terms by enzymes whose interactions with DNA make strand separation thermodynamically favorable at ambient

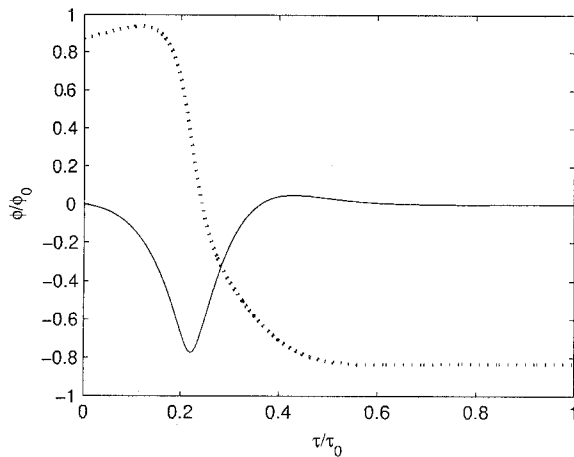


Fig. 3. The solution of Eq. (54) for real (dot line) and imaginary (solid line) parts.

temperature [32]. It has been shown that two strands of double-stranded DNA can be separated (unzipped) by the application of 15 pN force applied at room temperature. Their model predicts that the melting temperature should be a decreasing function of applied force. The paper shows that the external force can increase the amplitude of the breathing and may separate the double helix into single helices.

Finally, let us discuss the fourth case. The behavior of this case is described by the numerical solution of Eq. (54) with a complex function of  $\phi$ . The real and imaginary parts of the solution are associated with the carrier wave and the envelope velocity respectively. The profiles of both parts are shown in Fig. 3. The real part seems to have an anti-sigmoid-like function. In contrast, the imaginary part has negative values. The negative value means the solution propagates to the left.

Now we can discuss the solution of the FDNLS equation using Eq. (54). The result is depicted in Fig. 4. The soliton solution of FDNLS shows an increasing amplitude and velocity with time. The amplitude is relatively high and the shape of the soliton tends to be of step form during its propagation.

The DNA breathing in the fourth case using the solution of  $\psi^{(1)}$  given in Fig. 4 is depicted in Fig. 5. The amplitude of DNA breathing is around 2 nm where the result is similar to that previously reported in [6] for the same parameters. The amplitude is relatively increasing as it propagates to the left. The high amplitude indicates that the DNA is going to be unzipped and finally separated into single helices.

Finally, it is interesting to note the case of decreasing envelope and carrier velocity respectively up to one order lower. The results are given in Fig. 6. In this case, the solution of FDNLS propagates much more slowly than the previous one. At  $\tau = 0.3$  s the soliton with periodic external force tends to increase the amplitude and velocity. Further at  $\tau = 0.6$  s the amplitude is increased and the corresponding form changes significantly. At  $\tau = 0.7$  s the higher harmonic term is developed and completed at  $\tau = 0.9$ . Together with the time propagation, the amplitude tends to decrease and to disperse into a wider form, and then the higher harmonic term is generated and increasing the amplitude. It is interesting to point out that the harmonic term is coming from the solution of Eq. (54) which is a nonlinear equation.

The DNA breathing corresponding to the previously mentioned  $\psi^{(1)}$  is depicted in Fig. 7. From the figure, the amplitude is about 0.2 nm which is more or less the same as the previous result in [14], where they made use of the Forinash–Cretary–Peyrard model with helicosity. In that work it has been argued that the opening of the DNA double helix is controlled by the resonance mode.

The present results show that the periodic external force and damping effect generate a higher harmonic term in the dynamics of the FDNLS solution. Then it can be concluded that this phenomenon might be responsible for the dynamics of DNA breathing. In particular the early propagation imposes the DNA breathing to decrease its amplitude and disperse into a wider form. The condition changes as the higher harmonic terms of the FDNLS soliton begin to develop which increases the amplitude of DNA breathing significantly.

## 6. Summary

The effects of viscous fluid and external forces on the Peyrard–Bishop DNA breathing have been investigated. In particular, a PB

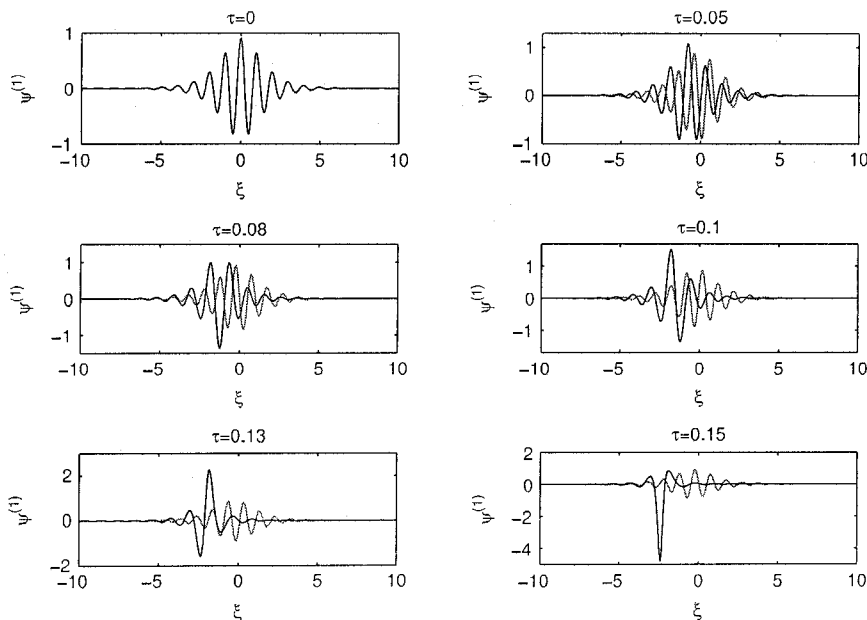


Fig. 4. The solution of the soliton in the FDNLS (black) and the NLS (red) with  $\gamma = 0.05$  kg/s,  $\bar{F} = 15 e^{i\kappa}$  pN,  $v_e = 10^5$  m/s and  $u_e = 4 \times 10^4$  m/s. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

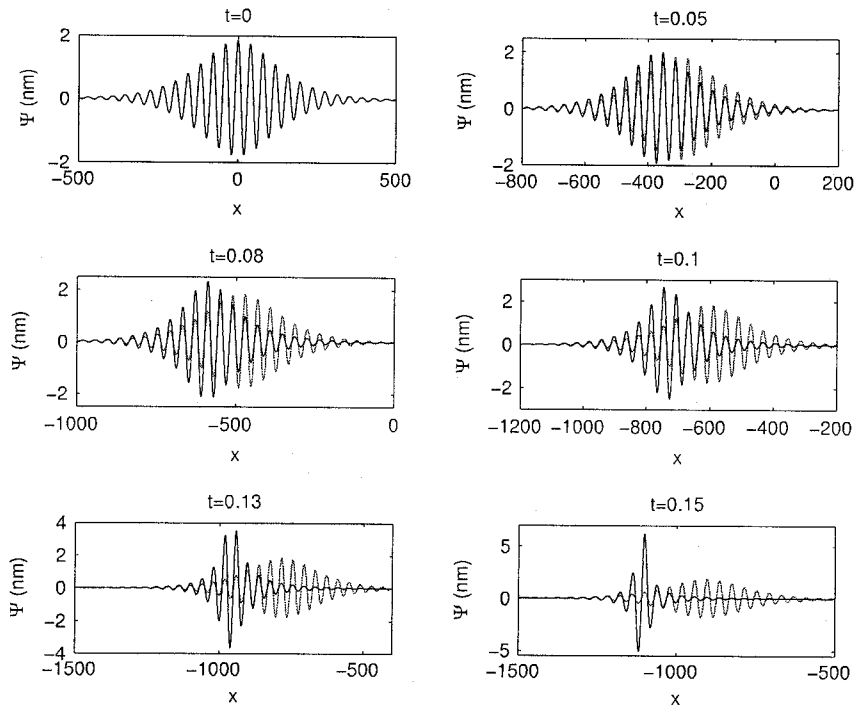


Fig. 5. The DNA breathing propagation for the fourth case in the present model (black) and the original PB model (red) with  $\gamma = 0.05$  kg/s,  $\bar{F} = 15 e^{46}$  pN,  $v_e = 10^5$  m/s and  $u_c = 4 \times 10^4$  m/s. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

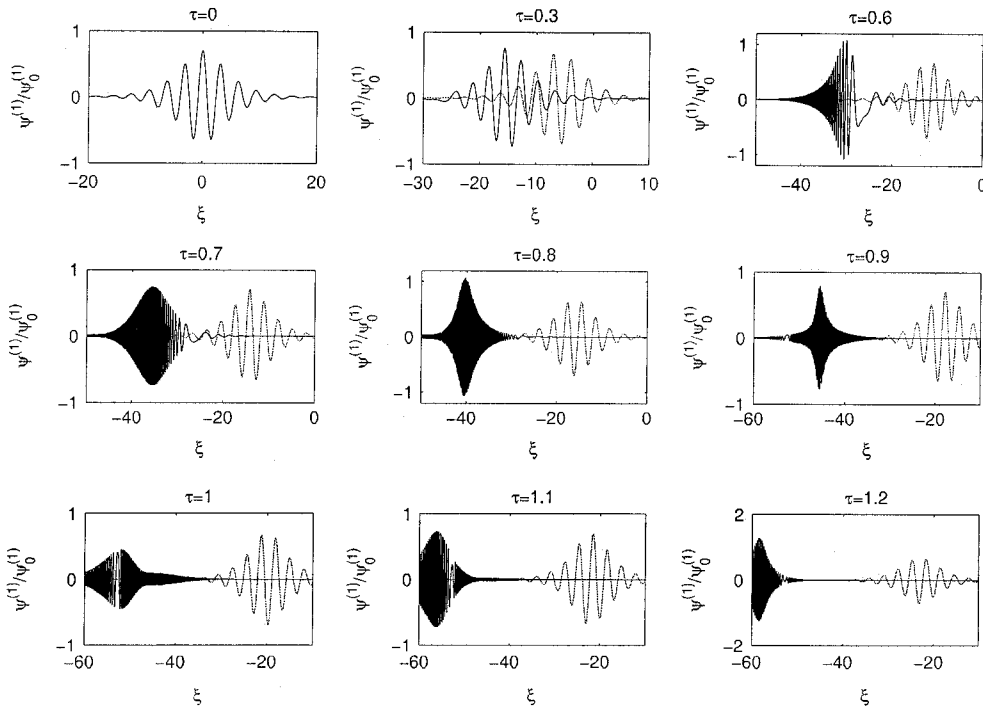


Fig. 6. The solution of FDNLS (black) and NLS (red) with  $\gamma = 0.05$  kg/s,  $\bar{F} = 15 e^{46}$  pN,  $K = 4$  N m,  $v_e = 10^4$  m/s and  $u_c = 4 \times 10^3$  m/s. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

model with the damping effect and the external driving force have been proposed to describe a time-dependent Caldirola–Kanai Hamiltonian. Taking into account the full continuum approximation and using the multiple scale expansion method, it has been shown that the EOM reproduces the FDNLS equation. Assuming that the damping and external forces are perturbative, the FDNLS

equation has been solved using variational methods through Lagrangian formalism.

The analytical solutions have also been obtained for special cases. In the case with constant damping factor and without external force, the breathing propagation is decelerated by the damping effect. In the presence of external force, the velocity and

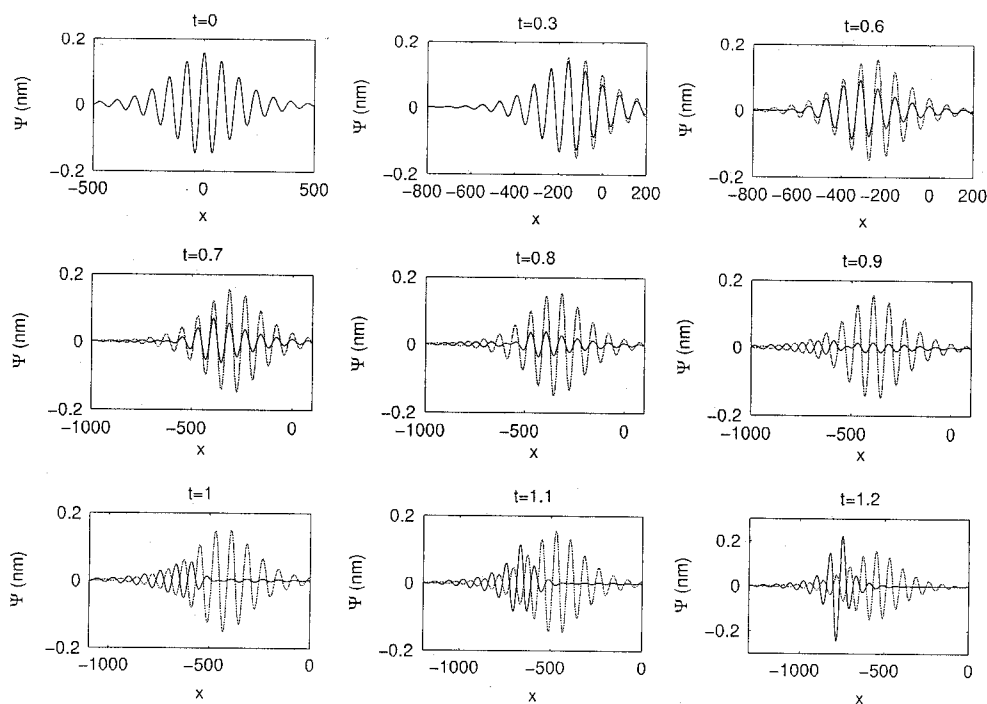


Fig. 7. The DNA breathing in the model (black) and the original PB model (red) with  $\gamma = 0.05$  kg/s,  $\bar{F} = 15 e^{\kappa}$  pN,  $K = 4$  N m,  $v_e = 10^4$  m/s and  $u_c = 4 \times 10^3$  m/s. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

the amplitude increase significantly. It has also been found that the higher harmonic terms are enhanced when the periodic force is applied. These results show that the external force contributes constructively to accelerate the separation of the double helix into single helices.

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