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LONG-RANGE INTERACTIONS AND WAVE PATTERNS IN A DNA MODEL

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Abstract

We propose a spin-like model of DNA nonlinear dynamics with long-range interactions between adjacent base pairs. We show that the model equation is a modified sine-Gordon equation. We perform the linear stability analysis of a plane wave, which predicts high amplitude and extended oscillating waves for high values of the long-range parameter. This is confirmed numerically and biological implications of the obtained patterns are suggested.

1 Introduction

The complexity and role of DNA make it the most important molecule in nature. Describing its dynamics therefore remains a fascinating task for modern physicists and biophysicists alike, because it is nowadays accepted that DNA undergoes dynamical features that are not yet fully unmasked. There have been many attempts to describe that complicated dynamics using appropriate models. The first nonlinear model was suggested by Englander et al. [1]. Later, Yomosa proposed a further theory based on a dynamic plane base-rotor model [2]. Along the same line, Takeno and Homma [3] developed that idea and proposed a general spin-like model, and showed its efficiency in describing open-states in DNA. Further modifications of the same model have recently been introduced by Daniel and Vasumathi [4] and Tabi et al. [5] who showed the importance of helicity in DNA spin-like models. In this letter, we further modify the same model and point out the importance of long-range dispersive interactions of the Kac-Backer type [6, 7] in describing hydrogen bonds oscillations. The importance of long-range interactions is due to the presence of phosphate groups along the strands [8]. Those phosphate groups are shielded by the counter-ions supplied by the medium. The long-range interaction therefore allows to take into account the screening of the interactions or an indirect coupling between base pairs (e.g. via water filaments). This has been justified in the paper of Shafranovskaya et al. [9] who studied experimentally the diffusion of charge in DNA and demonstrated the importance of long-range excitation migration in DNA. Also, experimentally, the evidence for long-range attractive hydration forces was studied by Rau and Parsegian [10]. Besides, there are the results of some recent measurements indicating that moderate long-range repulsive interaction are suitable to describe long-range communication in DNA[11]. This qualitative discrepancy is also shared by theoretical findings so that the real long-range force to be adopted for DNA dynamics remains unclear. Along the same line, Rau and Parsegian [10] also emphasized that many other forces could be responsible for long-range interactions in DNA, a conclusion which motivated the present work. In the rest of this letter we perform the linear stability analysis of a planar wave, solution of a modified sine-Gordon (sG) equation, and predict the appearance of highly localized soliton-like structures in presence of long-range interactions. Numerical simulations further confirm our analytical predictions and bring out the presence of extended breather-like structures.

2 Model

In this work, we consider the so-called B-form of the DNA molecule as presented in Fig.1(a) (S and S' represent the two strands of the molecule). Since in this model we intend to introduce the DNA spin-like model with long-range interaction, we can assimilate that model to the Heisenberg

one by writing the Hamiltonian of the anisotropic model as

$$H_0 = \sum_n \left(-\sum_{j\neq n} J g_{nj} (S_n \cdot S_j) + A (S_n^z)^2 \right), \tag{1}$$

where the summation is over the N base pairs of the DNA lattice. In the above equation, $S_n = (S_n^x, S_n^y, S_n^z)$ represents the spin vector at the n^{th} base pair, and the terms proportional to Jg_{nj} and A stand for the ferromagnetic spin-spin exchange long-rage interaction and uniaxial magnetocristalline anisotropy with the easy axis along the z axis. The long-range interaction constant g_{nj} is given by [6, 7]

$$g_{nj} = \frac{f(1-\nu)}{\nu} \nu^{|n-j|}, \quad \text{with} \ \sum_{j\neq n} g_{nj} = 2f, \tag{2}$$

which is known as the Kac-Baker potential, where $|n-j|$ measures the absolute distance between the two sites n and j and the parameters f and ν are, respectively, the range of the interactions, with $0 \leq \nu < 1$, and the elastic constant of strands. For a given ν, g_{nj} decreases when j increases. Experimentally, one can relate the parameter ν to the number of neighboring interactions. Note that the limit $\nu \to 0$ reduces to the nearest neighbor problem and the limit $\nu \to 1$ (possible only for $N \to \infty$) defines the infinite-range problem [6, 7]. The above Hamiltonian is considered for one strand, therefore similar considerations can be made for the second strand S' by replacing S_n by $S_n^{'}$. The whole Hamiltonian for the DNA molecule can then be written, after reformulating $S_n = (S_n^x, S_n^y, S_n^z) = (\sin\theta_n \cos\phi_n, \sin\theta_n \sin\phi_n, \cos\theta_n)$ and $S_n^{'} = (S_n^{'x}, S_n^{'y}, S_n^{'z}) = (\sin\theta_n^{'} \cos\phi_n^{'}, \sin\theta_n^{'} \sin\phi_n^{'}, \cos\theta_n^{'})$, as

$$\begin{aligned} H_0 = \sum_n \Bigg[-\sum_{j\neq n} J g_{nj} \Big(& \sin\theta_n \sin\theta_j \cos(\phi_n - \phi_j) + \sin\theta_n^{'} \sin\theta_j^{'} \cos(\phi_n^{'} - \phi_j^{'}) \\ & + \cos\theta_n \cos\theta_j + \cos\theta_n^{'} \cos\theta_j^{'} \Big) + A\cos^2\theta_n + A\cos^2\theta_n^{'} \Bigg]. \end{aligned} \tag{3}$$

In Figs.1(b) and 1(c), we show the horizontal projection of the nth base pair in the xy and xz planes, respectively. In these figures, Q_n and Q_n' denote the tips of the nth bases belonging to the strands S and S'. P_n and P_n' represent the points where the bases in the nth base pair are attached to the strands S and S', respectively.

It has been shown that interstrand base-base interactions or hydrogen bonding energy deeply depend on the distance between the two complementary bases [3]. Thus from Figs.1(b) 1(c), the square of the distance between the edges of the arrows $(Q_nQ_n')^2$ is written as [3, 5]

$$\begin{aligned} (Q_nQ_n')^2 = {} & 2 + 4r^2 + (z_n - z_n')^2 + 2(z_n - z_n')(\cos\theta_n - \cos\theta_n') \\ & - 4r[\sin\theta_n \cos\phi_n + \sin\theta_n' \cos\phi_n'] + 2[\sin\theta_n \sin\theta_n' \\ & \times (\cos\phi_n \cos\phi_n' + \sin\phi_n \sin\phi_n') - \cos\theta_n \cos\theta_n'] \end{aligned} \tag{4}$$

where r is the radius of the circle depicted in Fig.1(b). The corresponding base-base distance can be obtained in terms of S_n and $S_n^{'}$ as follows

$$(Q_nQ_n')^2 = 2 + 4r^2 + 2\left(S_n^x S_n^{'x} + S_n^y S_n^{'y} - S_n^z S_n^{'z} \right) - 4r\left(S_n^x + S_n^{'x} \right), \tag{5}$$

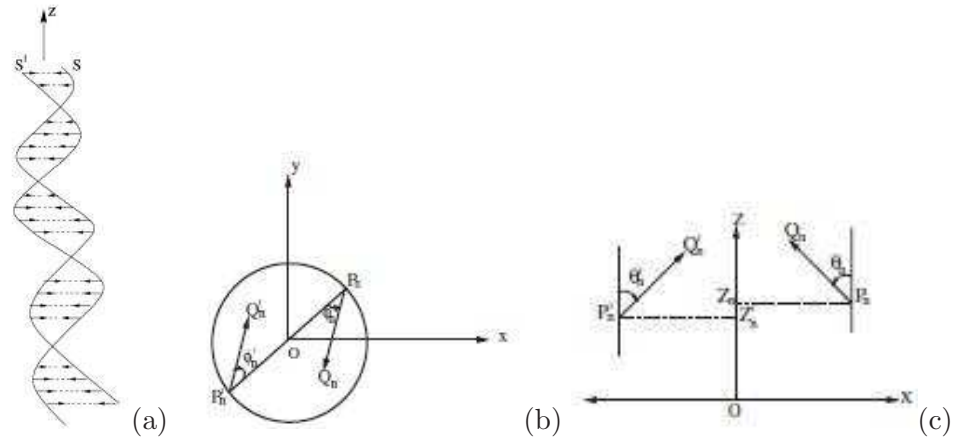

Figure 1: (a) A schematic structure of the B-form of DNA; (b) A horizontal projection of the nth base pair in the xy-plane; (c) A projection of the nth base pair in the xz-plane.

and the hydrogen bond interaction can be described by the potential

$$H_1 = \sum_n \eta \Big[\sin\theta_n \sin\theta_n^{'} \cos(\phi_n - \phi_n^{'}) - \cos\theta_n \cos\theta_n^{'} \Big], \tag{6}$$

where η represents a measure of the interstrand interactions. In Eq.(5), the longitudinal compression along the direction of the helical axis has been neglected and we have assumed $z_n = z_n^{\prime}$ [3]. The total Hamiltonian is finally given in terms of the variables (θ_n, ϕ_n) and $(\theta_n^{'}, \phi_n^{'})$ by

$$\begin{aligned} H = \sum_n \Bigg[& - \sum_{j \neq n} J g_{nj} \Big(\sin\theta_n \sin\theta_j \cos(\phi_n - \phi_j) + \sin\theta_n^{'} \sin\theta_j^{'} \cos(\phi_n^{'} - \phi_j^{'}) \\ & + \cos\theta_n \cos\theta_j + \cos\theta_n^{'} \cos\theta_j^{'} \Big) + \eta \Big(\sin\theta_n \sin\theta_n^{'} \cos(\phi_n - \phi_n^{'}) - \cos\theta_n \cos\theta_n^{'} \Big) \\ & + A\cos^2\theta_n + A\cos^2\theta_n^{'} \Bigg]. \end{aligned} \tag{7}$$

The equations of motion for the corresponding quasi-spin model in the limit $A \gg J, \eta$ [3] lead to the system $\dot{\phi}_n = 2A\cos\theta_n$ and $\dot{\phi}_n^{'} = 2A\cos\theta_n^{'}$, where the overdot represents the time derivative. With such considerations, we consider the absolute minima of the potential and rewrite the Hamiltonian as [3, 4]

$$H = \sum_n \left[\frac{I}{2} \left(\dot{\phi}_n^2 + \dot{\phi}_n^{'2} \right) - \eta \Big(1 - \cos(\phi_n - \phi_n^{'}) \Big) + \sum_{j \neq n} J g_{nj} \Big(2 - \cos(\phi_n - \phi_j) - \cos(\phi_n^{'} - \phi_j^{'}) \Big) \right], \tag{8}$$

where $I = \frac{1}{2A}$ is the moment of inertia of the bases around the axes at P_n $(P_n^{\prime})$. In this previous step, we have restricted our problem to a plane-base rotor model [3] by assuming $\theta_n = \theta_n^{'} = \pi/2$. The equations of the motions of the base pairs are derived from the Hamiltonian (8). They are

$$I\ddot{\phi}_n = -J \sum_{j \neq n} g_{nj} \sin(\phi_n - \phi_j) + \eta \sin(\phi_n - \phi_n^{'}) \tag{9a}$$

$$I\ddot{\phi}_n^{'} = -J\sum_{j\neq n} g_{nj}\sin(\phi_n^{'} - \phi_j^{'}) + \eta\sin(\phi_n^{'} - \phi_n). \tag{9b}$$

We consider the difference in angular rotation of bases with respect to neighboring pairs along the two strands to be small and therefore assume $\sin(\phi_n - \phi_j) \approx (\phi_n - \phi_j)$ and $\phi_n^{'} = -\phi_n$. After rescaling the time as $t \to \sqrt{J/I}t$ and choosing $\eta = -J/2$ and $\psi = 2\phi$, we finally get the following set of equations

$$\frac{d^2\psi_n}{dt^2} + 2f\psi_n + \sin(\psi_n) = L_n, \tag{10}$$

where the auxiliary quantity L_n, which is defined as $L_n = \frac{f(1-\nu)}{\nu}\sum_{j\neq n}\nu^{|n-j|}\psi_j$, satisfies the recursive relation

$$(\nu + \nu^{-1})L_n = L_{n+1} + L_{n-1} + \frac{f(1-\nu)}{\nu}(\psi_{n+1} + \psi_{n-1} - 2\psi_n). \tag{11}$$

The continuum approximation of Eq.(10) is written, after rescaling $x \to x/d$, as

$$\psi_{tt} - \frac{\nu}{(1-\nu)^2}\psi_{xxtt} - \left[\frac{f(1+\nu)}{(1-\nu)^2} - \frac{\nu}{(1-\nu)^2}\cos(\psi)\right]\psi_{xx} + \left[1 + \frac{\nu}{(1-\nu)^2}\psi_x^2\right]\sin(\psi) = 0. \tag{12}$$

For $\nu = 0$, the above equation reduces to the standard sG equation.

3 Amplitude equation and oscillations of strands

We proceed with the multiscaling expansion of Eq.(12). For this purpose, due to the presence of the term ψ_{xxtt}, it would be interesting to introduce auxiliary coordinates, $p(x,t)$, $v(x,t)$ and $u(x,t)$ such that [12]

$$\begin{aligned}
&\psi_x = p, \;\; p_t = v, \;\; v_t = u, \\
&\psi_{tt} - \frac{\nu}{(1-\nu)^2}u_x - \left[\frac{f(1+\nu)}{(1-\nu)^2} - \frac{\nu}{(1-\nu)^2}\cos(\psi)\right]\psi_{xx} + \left[1 + \frac{\nu}{(1-\nu)^2}p^2\right]\sin(\psi) = 0.
\end{aligned} \tag{13}$$

It is, therefore, possible to write the analogue of (13) by using its partial finite-difference expression, in order to take discreteness effects into account in our study, as follows

$$\begin{aligned}
&\frac{1}{2}[\psi(n+1,t) - \psi(n-1,t)] = p(n,t), \;\; \frac{\partial p(n,t)}{\partial t} = v(n,t), \;\; \frac{\partial v(n,t)}{\partial t} = u(n,t), \\
&\frac{\partial^2\psi(n,t)}{\partial t^2} - \frac{\nu}{2(1-\nu)^2}[u(n+1,t) - u(n-1,t)] \\
&- \left[\frac{f(1+\nu)}{(1-\nu)^2} - \frac{\nu}{(1-\nu)^2}\cos(\psi(n,t))\right][\psi(n+1,t) + \psi(n-1,t) - 2\psi(n,t)] \\
&+ \left[1 + \frac{\nu}{(1-\nu)^2}(p(n,t))^2\right]\sin(\psi(n,t)) = 0.
\end{aligned} \tag{14}$$

$p(x,t)$, $v(x,t)$ and $u(x,t)$ are taken in the form of the following series [5, 12]

$$\begin{aligned}
\psi(n,t) &= \sum_{p=1}^{\infty}\sum_{l=-p}^{p}\epsilon^p\eta_p^{(l)}(m,\tau)A^{(l)}(n,t) &(15)\\
p(n,t) &= \sum_{p=1}^{\infty}\sum_{l=-p}^{p}\epsilon^p\varphi_p^{(l)}(m,\tau)A^{(l)}(n,t) &(16)\\
v(n,t) &= \sum_{p=1}^{\infty}\sum_{l=-p}^{p}\epsilon^p\chi_p^{(l)}(m,\tau)A^{(l)}(n,t) &(17)\\
u(n,t) &= \sum_{p=1}^{\infty}\sum_{l=-p}^{p}\epsilon^p\Xi_p^{(l)}(m,\tau)A^{(l)}(n,t), &(18)
\end{aligned}$$

with $A^{(l)}(n,t)=\exp(il(\Omega t+qn))$, $\eta_p^{(-l)}=\left(\eta_p^{(l)}\right)^*$, $\varphi_p^{(l)}=\left(\varphi_p^{(l)}\right)^*$, $\chi_p^{(l)}=\left(\chi_p^{(l)}\right)^*$, and $\Xi_p^{(l)}=\left(\Xi_p^{(l)}\right)^*$. We have also considered the change of variables $\tau=\epsilon(t+n/v_g)$ and $\xi=\epsilon^2 n$. After introducing the trial solutions (15)-(18) into Eqs.(14), the leading order $(1,l)$ of Eq. (14) constitutes a linear homogeneous system for $\eta_1^{(l)}$, $\varphi_1^{(l)}$, $\chi_1^{(l)}$ and $\Xi_1^{(l)}$. For $l=0$ and $l=1$ we have

$$\begin{aligned}
&\eta_1^{(0)}=\varphi_1^{(0)}=\chi_1^{(0)}=\Xi_1^{(0)}=0\\
&\eta_1^{(1)}=\eta(m,\tau),\ \ \chi_1^{(1)}=-\Omega\sin(q)\eta(m,\tau),\ \ \Xi_1^{(1)}=-i\Omega^2\sin(q)\eta(m,\tau),\ \ \varphi_1^{(1)}=i\sin(q)\eta(m,\tau).
\end{aligned} \tag{19}$$

In the particular case of $l=1$, we should stress that the determinant of the system $\eta_1^{(1)}$, $\varphi_1^{(1)}$, $\chi_1^{(1)}$ and $\Xi_1^{(1)}$ is zero if $\Omega(q)$ verifies the dispersion relation

$$\Omega^2=\frac{(1-\nu)^2+4[f(1+\nu)-\nu]\sin^2\left(\frac{q}{2}\right)}{(1-\nu)^2+\nu\sin^2(q)}. \tag{20}$$

At order $(2,l)$, setting $l=0$ gives

$$\eta_2^{(0)}=\varphi_2^{(0)}=\chi_2^{(0)}=\Xi_2^{(0)}=0. \tag{21}$$

For $l=1$, we get an inhomogeneous system for $\eta_2^{(1)}$, $\varphi_2^{(1)}$, $\chi_2^{(1)}$ and $\Xi_2^{(1)}$. The determinant of the corresponding system is zero owing to the dispersion relation (20). The system will further have a solution for the Fredholm solvability condition, which is fulfilled for

$$v_g=\frac{\partial\Omega}{\partial q}=\frac{\Omega\cos(q)}{(1-\nu)^2+\nu\sin^2(q)}\left[\frac{f(1+\nu)-\nu}{\Omega^2}\tan(q)-\nu\sin(q)\right], \tag{22}$$

which gives the group velocity. For non-vanishing values of v_g we write

$$\begin{aligned}
\eta_2^{(1)} &= \zeta(m,\tau)\\
\chi_2^{(1)} &= -\Omega\zeta(m,\tau)\sin(q)+i\left(\frac{\Omega}{v_g}+\sin(q)\right)\frac{\partial\eta(m,\tau)}{\partial\tau}\\
\Xi_2^{(1)} &= -i\Omega^2\zeta(m,\tau)\sin(q)-\left(\frac{\Omega^2}{v_g}+2\Omega\sin(q)\right)\frac{\partial\eta(m,\tau)}{\partial\tau}\\
\varphi_2^{(1)} &= i\zeta(m,\tau)\sin(q)+\frac{1}{v_g}\frac{\partial\eta(m,\tau)}{\partial\tau}\cos(q),
\end{aligned} \tag{23}$$

where $\zeta(m,\tau)$ is an arbitrary function.

At order $(3,l)$, for $l=0$, we have

$$\eta_3^{(0)}=\varphi_3^{(0)}=\chi_3^{(0)}=\Xi_3^{(0)}=0. \tag{24}$$

For $l=1$, we find the nonlinear evolution of $\eta(m,\tau)$. The obtained inhomogeneous linear system for $\eta_3^{(1)}$, $\varphi_3^{(1)}$, $\chi_3^{(1)}$ and $\Xi_3^{(1)}$ is of determinant zero. Once more, we will have a solution of the system if the Fredholm solvability condition holds. The condition gives the nonlinear evolution for $\eta(m,\tau)$ in which the term $\zeta(m,\tau)$ coming from $\eta_2^{(1)}$, $\varphi_2^{(1)}$, $\chi_2^{(1)}$ and $\Xi_2^{(1)}$ cancels out. The equation for $\eta(m,\tau)=\eta_m$ is finally given by

$$-i\beta(\eta_{m+1}-\eta_{m-1})+\alpha\frac{\partial^2\eta_m}{\partial\tau^2}+\gamma|\eta_m|^2\eta_m=0, \tag{25}$$

where

$$\begin{aligned}
\alpha &= \frac{1}{(1-\nu)^2}\left[(1-\nu)^2-\frac{1}{2}\left(\frac{1}{v_g}\right)^2\nu\Omega^2\sin(q)-(f(1+\nu)-\nu)\left(\frac{1}{v_g}\right)^2\cos(q)-\left(\frac{1}{v_g}\right)^2\nu\Omega^2\sin(q)\right.\\
&\quad\left.+\frac{\Omega\nu}{2v_g}\sin(2q)+\nu\left(\frac{\Omega}{v_g}+\sin(q)\right)\sin(q)+\nu\left(\frac{\Omega^2}{v_g}+2\Omega\sin(q)\right)\cos(q)\right]\\
\beta &= \frac{1}{(1-\nu)^2}\left\{\left[\nu\left(1-\frac{\Omega^2}{2}\right)-f(1+\nu)\right]\sin(q)+\frac{\nu\Omega^2}{2}\sin(2q)\right\}\\
\gamma &= \frac{1}{(1-\nu)^2}\left[\frac{1}{4}(1-\nu)^2-\nu\cos^2(q)\right].
\end{aligned} \tag{26}$$

From relation (15), the approximate solution $\psi_n(t)$ of Eq.(9b) can be written as

$$\psi_n(t)=\epsilon\eta_m(\tau)e^{i(qn-\Omega t)}+\vartheta(\epsilon^2)+c.c.. \tag{27}$$

The plane wave solution

$$\eta_m=Be^{i(\lambda m-\mu\tau)} \tag{28}$$

for (25) is characterized by the nonlinear dispersion relation

$$\mu^2=\frac{1}{Q}\left(\frac{2\beta}{\gamma}\sin(\lambda)+|B|^2\right). \tag{29}$$

An instability will develop in the system if the right-hand side of (29) is negative. This implies that both the sign of $Q(q)=\frac{\alpha}{\gamma}$ and $\frac{2\beta}{\gamma}$ will be significative. According to Fig.2(a), where we have plotted the function $Q(q)$, there is a point $q\in[0.35\pi;0.4\pi[$ where Q passes from negative values to positive values. This means that for $Q<0$ the condition for modulational instability (MI) is fulfilled if $\frac{2\beta}{\gamma}\sin(\lambda)+|B|^2>0$. Since λ is bounded and fixed so that $\sin\lambda=1$ (since $\beta<0$ and $\gamma>0$ for all $q\in]0;\pi[$), there will be MI in the DNA lattice if

$$|B|^2>-\frac{2\beta}{\gamma}=B_{cr}^2. \tag{30}$$

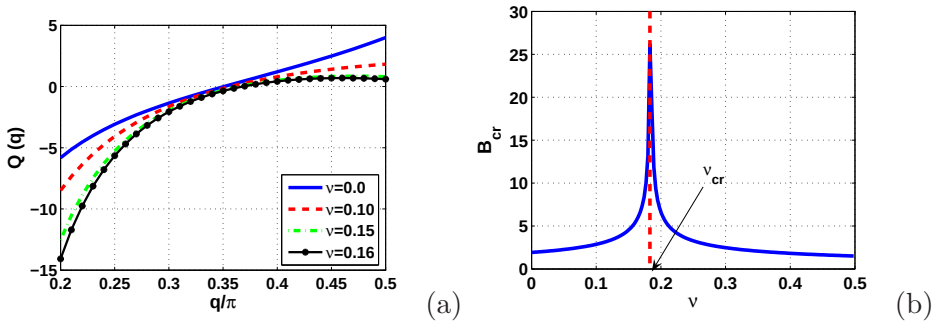

Figure 2: The first panel shows the plot of $Q = \frac{\alpha}{\gamma}$ versus q for different values of the range parameterν and $f = 1.5$. The second panel depicts the threshold amplitude B_{cr} versus the range parameter ν for $q = \pi/10$ and $f = 1.5$.

On the other hand, if $Q > 0$, a plane wave solution will be unstable if

$$|B|^2 > |B_{cr}|^2. \tag{31}$$

A patient reader could remark that we have chosen values of ν as 0.0, 0.1, 0.15 and 0.16 to plot Q. He could therefore wonder why such small values for ν have been chosen. In fact, while performing the linear stability analysis, we have remarked that the threshold amplitude is very sensitive to the value of ν. We have also remarked that B_{cr} has a singular point for ν, where the amplitude of wave starts decreasing. This is depicted in Fig. 2 (b). In other words, when $\nu < \nu_{cr}$ the wave amplitude increases and decreases for $\nu > \nu_{cr}$. Considering the case $\nu < \nu_{cr}$, we have plotted the threshold amplitude for different values of ν and the following features have been observed

- for $\nu = 0$, we recover the features of the simple spin-like model of DNA [5, 13]. This implies that plane waves are unstable for all q [see Fig. 3 (a)].
- For $\nu = 0.15$ and $\nu = 0.16$, the threshold of instability exists at any carrier wave number $[q_{cr}; \pi[$ [see Fig. 3 (b) and 3 (c)]. Furthermore, the threshold amplitude in these two cases is an increasing function of the range parameter. This means that for values of ν approaching ν_{cr} highly localized structures are expected. This also implies that the role of long-range interactions in the present model could be to enhance and trap waves that undergo large oscillations in order for chemical reactions between enzymes and bases to be possible.

To verify our analytical predictions we have performed the numerical study of wave modulation in this DNA model, because the linear stability analysis is based on the linearization around the unperturbed carrier wave, which is valid only when the amplitude of the perturbation is small in comparison with that of the carrier wave. Furthermore, the linear stability analysis cannot tell us the long time evolution of a modulated nonlinear plane wave. In that respect, we have integrated the discrete Eq.(10) through the fourth-order Runge-Kutta computational

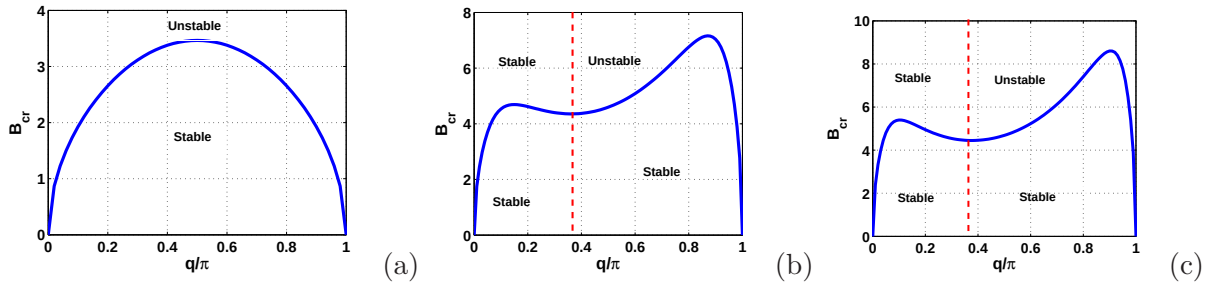

Figure 3: The panels show the threshold amplitude B_{cr} versus the wave number q for different values of ν with $f = 1.5$ and (a) $\nu = 0$; (b) $\nu = 0.15$; (c) $\nu = 0.16$.

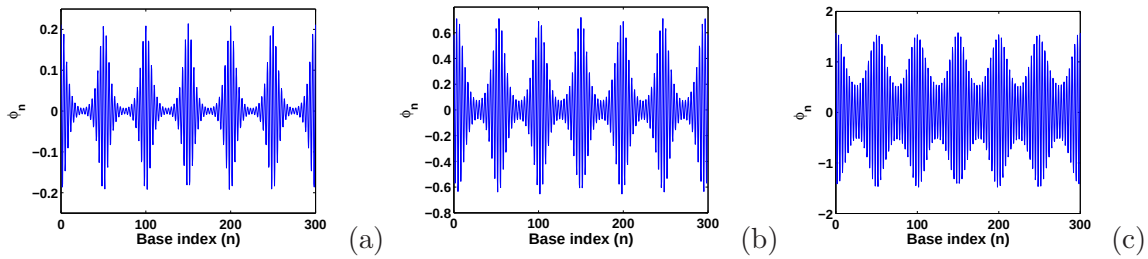

Figure 4: The panels show how the initial plane solution wave breaks into wave train which has the shape of soliton-like object in the present DNA model, as predicted by the analytical predictions, for $\epsilon = 0.01$, $f = 1.5$, $\lambda = 0.45\pi$, $q = 0.98\pi$, $t = 750$, and: (a) $\nu = 0.1$; (b) ν=0.13; (c) $\nu = 0.16$.

scheme. Periodic boundary conditions have been used and the initial condition has been chosen so as to satisfy the combined solutions (27) and (28) (the resulting expression is a modulated wave). As a first remark, the introduced plane-wave breaks into trains of waves, which have the appearance of multisoliton shapes with breathing motion, as expected from the linear stability analysis when appropriate values of wavenumbers q and λ are chosen. Such oscillations have been shown to be at the initiation of the so-called transcription of DNA. In order to understand the effect of long-range interaction on MI, we have plotted in Fig.4 oscillations of strands for different values of the range parameter ν. From Fig. 4 (a) to 4 (c) we observe that increasing the long-range parameter brings about extended or broadened localized soliton-like structures. In other words, long-range interaction in our DNA model makes a large number of base pairs to oscillate [compare Fig.4 (a), Fig.4 (b) and Fig.4 (c)] and to participate in the process of DNA opening. In fact, large oscillations of strands facilitate chemical interactions between the hydrogen bonds and the enzymes involved in the dynamical processes that take place in DNA. In a recent paper, Tabi et al. [14] showed that there exist two types of waves that flow in DNA models. Waves that describe the open-states of DNA lattices are highly localized on specific sites, while waves that describe the breathing mode are broadened with small amplitude. The amplitude of such oscillations increases under the action of RNA-polymerase in order for the hydrogen bonds to be broken. We can therefore say, according to that conclusion, that increasing the range parameter better contributes to DNA breathing. Within such a process,

certain local DNA openings termed origins with specific nucleotide sequences (replicators) work as repressors for an origin recognition complex. The origin recognition complex is considered to be the best candidate for an initiator protein. But only origin recognition complex liganded with ATP (adenosine triphosphate) can recognize and bind to DNA origins in the double helix. The ensemble should be hydrolyzed according to some coordinated signaling pathway. Small oscillations of the dsDNA can therefore be amplified and undergo large fluctuations, which finally transform into bubbles and solitons leading indubitably to the unzipping of the molecule.

4 Conclusion

The main concern of this letter was to propose a spin-like model of DNA which takes long-range dispersive interactions into consideration and to show that long-range interactions can bring about highly localized oscillations in DNA. Through the linear stability of a plane wave, we predicted the appearance of highly localized soliton-like objects. The fundamental question for the existence of nonlinear excitations with soliton-like shape in our DNA model, as predicted by analytical predictions, appears to have been answered by numerical experiments. The presence of these localized excitations confirms the fact that in DNA models, with long-range interactions, interplay between dispersive and nonlinear effects are associated with oscillations of strands that become important and extended as the long-range parameter increases. Such large oscillations of strands contribute to expose bases, that contain the genetic code, to chemical reactions with enzymes leading to the unzipping and breaking of hydrogen bonds of the dsDNA.

The DNA molecule is highly heterogeneous and study on DNA models would be more realistic if the effect of base sequence is taken into account. Up to now, different models have been proposed to study such a complex dynamics on the basis of homopolymers of DNA. This study intends first to introduce the model we propose and works that consider the randomness of base sequence are being carried out. In forthcoming papers we intend to investigate realistic values of parameters in order for the characteristics of AT and GC pairs to be determined. That is why the model, as it is introduced here, uses dimensionless parameters and is applied to an homopolymer model of DNA.

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