EFFECT OF TWISTING AND NONLINEAR DYNAMICS OF THE ANHARMONIC TWIST OPENING MODEL OF DNA

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Abstract: In this paper, we investigate the play role of twisting in the dynamics of DNA by considering anharmonic twist opening model. In this model, we consider the coupling between opening of base pairs and twist of the strand responsible for helicoidal structure of B-DNA. We derive the dynamical equations and recast them as two Coupled Discrete Nonlinear Schrodinger equations (CDNLS) by employing Fourier approximation method. Further, we perform the linear stability analysis and it is observed that the soliton profile is generated when the instability occurs. It is shown that the instability increases with the increase of the degree of twisting and this may cause genetic disorder related diseases in DNA system. The analytical predictions are confirmed with the numerical dynamics of molecular dynamical simulations performed and verified the same.

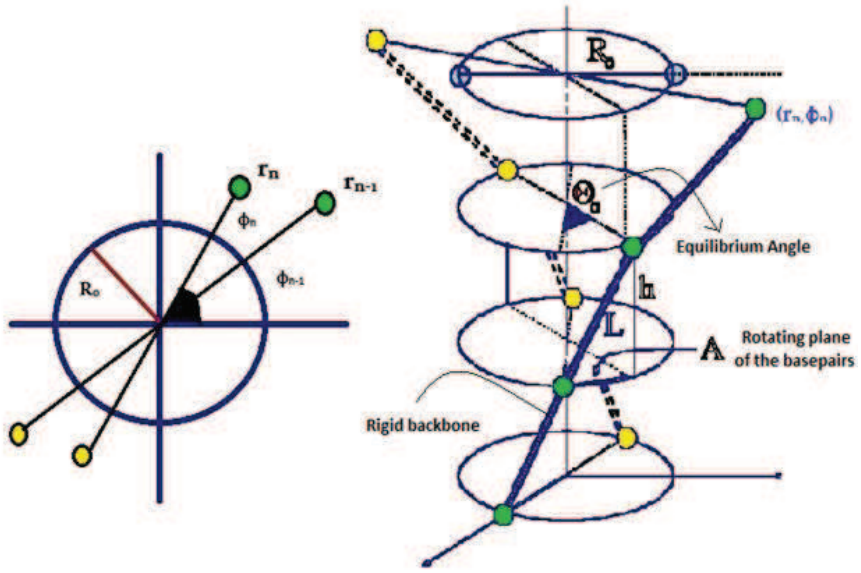
Keyword: DNA Twisting, Fourier Approximation, Modulational Instability Analysis.

1. Introduction: Deoxyribo Nucleic Acid (DNA) is the hereditary material that acts as the fundamental information storage medium to transfer the genetic information for all the living organisms including human beings. In order to fully understand the basic mechanism of biological processes like denaturation, initiation, transcription and translation many simple dynamical models of DNA are studied in the past decades [1],[2]. Englander et al [3], made the first prediction towards the nonlinear modelling of DNA dynamics and suggested the propagation of solitons along the DNA molecule, where an enzyme namely RNA-polymerase binds to a particular site of the double stranded DNA-helix during the process of DNA transcription. We assume the free rotation of base pairs around the molecular axis of DNA leads to twisting of the strands. Yamosa [4] proposed a plane based rotator model and neglected the constraints arising from the sugar phosphate strands of DNA and longitudal motion of the bases. Further, Peyard and Bishop [5] and Christiansen et al [6], investigated the dynamics by considering the transverse and longitudal motion of bases in DNA. The energy associated with the hydrogen bonding between the interstrand base pairs and the stacking energy between the intrastrand adjacent base pairs arising due to the electrostatic, the exchange, the induction, dispersion and deformation in the form of stretching, twisting and bending of the macromolecules. These interstrand and stacking energies are modelled in the form of Morse potential [7] and harmonic potential to ultimately determine the conformation and stability of DNA. Dauxois et al [8] reported that the nonlinear interactions play a leading role in the denaturation of DNA. Barbi et al [9],[10] derived a new

model, in which each base is considered a single, non-deformable point mass by taking into account the topological constraints of the helicoidal structure of DNA molecule.

This paper is organised as follows; in section 2, we derive the dynamical equation for the anharmonic twist opening model of DNA and we derive the resultant equation of motion the two Coupled discrete Nonlinear Schrodinger equation for DNA dynamics using Fourier Approximation method. We involve modulational instability analysis in section 3 and generate coherent solitonic profile through instability.

2. Model and Dynamical Equation: The twist opening model of the DNA contains both radial and torsional effect that gives the form of B-DNA. In this model, the bases are considered as the point mass 'm'. The bases are located on the same plane 'A' linked by the hydrogen bond. 'L' is the length of the elastic rod. L/h ratio gives the helicity structure which fixes the strand slant. Helicity is based on the angle of rotation of the base pairs with respect to the equilibrium twist angle θ. The diameter of the DNA is 2Ro. Let's assume bases in each pair moves symmetrically. The Lagrangian of the model is,



$$L=\sum_n\left(m\dot{r}_n^2+mr_n^2\dot{\phi}_n^2\right)+D\left(e^{-a(r_n-R_o)}-1\right)^2+S_l\left(l_n-L\right)^2.R+S_{nl}\left(r_n-r_{n-1}\right)^2e^{-b(r_n+r_{n-1}-2R_o)} \quad , \quad (1.1)$$

where the overdots represents the time derivative. The first term of the Lagrangian represents the kinetic energy. The second term represents the interaction between the hydrogen bonds between the base pairs which are modelled by Morse potential. The term D designates the dissociation energy and 'a' is a parameter which is homogeneous to the inverse of the length. The third term represents the elastic energy of the backbone rods between the base pairs on each strand and S_l is the coupling constant for harmonic elastic interaction of the adjacent bases which characterizes the twisting term R. The last term of the Lagrangian designates the stacking interaction between the neighbouring base pairs. l_n is length of phosphodiester chain which link the base pairs at the n-1 and n+1 sites on the same chain.
The equations of motion for the coupled motion are given by,

$$\ddot{y}_n=\frac{1}{R_o^2}\left(y_n+R_o\right)\ddot{\phi}_n-\frac{K_{y\phi}}{2}\left(\phi_{n+1}-\phi_{n-1}\right)-K_{yy}\left(y_{n+1}+y_{n-1}\right)-w_g^2\left(\alpha y_n+\beta y_n^2+\gamma y_n^3\right)-$$

$$\frac{K_{11}}{b}\left[2\left(y_{n+1}+y_n\right)\left(y_{n+1}-y_n\right)-2\left(y_{n+1}+y_n\right)\left(y_n-y_{n-1}\right)-\left(y_{n+1}-y_n\right)^2-\left(y_n-y_{n-1}\right)^2\right]- \quad . \quad (1.2)$$

$$K_{11}\left[\left(y_{n+1}-y_n\right)^2\left(y_{n+1}+y_n\right)-\left(y_n-y_{n-1}\right)^2\left(y_n+y_{n-1}\right)\right]+S\theta^2$$

$$\ddot{\phi}_n = -\frac{1}{R_o^2} y_n^2 \ddot{\phi}_n - \frac{2}{R_o} y_n \dot{\phi}_n \dot{y}_n - \frac{2}{R_o^2}\left(y_n + R_o\right) \dot{y}_n \dot{\phi}_n - K_{\phi\phi}\left(\phi_{n+1} + \phi_{n-1} - 2\phi_n\right) - \frac{K_{y\phi}}{2}\left(y_{n+1} - y_{n-1}\right) + S\theta^2 \quad . \qquad (1.3)$$

We employ the Fourier approximation method, the amplitude solution for y_n and ϕ_n can be written in the form of $y_n(t) = \sum_{p=-\infty}^{+\infty} a_n^{(p)} e^{ipw_b t}$ and $\phi_n(t) = \sum_{p=-\infty}^{+\infty} b_n^{(p)} e^{ipw_b t}$ respectively, where ω_b is the linear oscillation frequency and the Fourier coefficients $a_n^{(p)}$ and $b_n^{(p)}$ are explicitly depending on time. We obtain the final equations as, (1.4)

$$i\dot{v}_n + P_1\left(v_{n+1} + v_{n-1}\right) + \sigma_1 |v_n|^2 v_n + \sigma_2 |\varphi_n|^2 v_n + \sigma_3\left[|v_{n+1} - v_n|^2 \left(v_{n+1} - v_n\right) + |v_n - v_{n-1}|^2 \left(v_n - v_{n-1}\right)\right] + s\theta^2 = 0$$
$$i\dot{\varphi}_n + P_2\left(\varphi_{n+1} + \varphi_{n-1}\right) + \sigma_4 |v_n|^2 \varphi_n + s\theta^2 = 0 \quad , (1.5)$$

3. Modulational Instability Analysis: We involve the modulational instability analysis by assuming the monochromic wave solutions in the form of, $v_n = v_0 e^{i(k_1 n - w_1 t)}$ and $\varphi_n = \varphi_0 e^{i(k_2 n - w_2 t)}$ respectively, and by substituting the wave solutions in (1.4) and (1.5) we get the dispersion relations as,

$$w_1 = -2P_1 \cos k_1 - \sigma_1 v_o^2 - \sigma_2 \varphi_o^2 + \sigma_3 v_o^2 4i \sin k_1 \left(\cos k_1 - 1\right) + s\theta^2$$
$$w_2 = 2P_2 \cos k_2 - \sigma_4 v_o^2 + s\theta^2 \quad , \qquad (2.1)$$

We would like to examine the stability of the initial plane waves, and substitute $v_n = (v_0 + \delta v_n) e^{i(kn - wt)}$ and $\varphi_n = (\varphi_0 + \delta\varphi_n) e^{i(kn - wt)}$, to get the solution with real and imaginary part as follows,

$$\sigma_4\left[v_0\varphi_0 v_1 + v_0\varphi_0 v_2\right] + \left(\Omega + w + 2P_2 \cos\left(Q + k\right) + \sigma_4 v_o^2\right)\varphi_1 + s\theta^2 +$$
$$i(\sigma_4\left[v_0\varphi_0 v_1^* + v_0\varphi_0 v_2^*\right] + \left(-\Omega^* + w + 2P_2 \cos\left(Q - k\right) + \sigma_4 v_o^2\right)\varphi_1^* + s\theta^2 = 0) \quad . \qquad (2.2)$$

This set of homogeneous equations can be written in the form of a matrix as,

$$M \times \begin{pmatrix} v_1 & v_2 & \varphi_1 & \varphi_2 \end{pmatrix} = 0$$
$$M = \begin{bmatrix} a_{11} + \Omega & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} - \Omega & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} + \Omega & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} - \Omega \end{bmatrix} . \qquad (2.3)$$

The Ω is determined from the dispersion relation with k and Q. The instability gain is the imaginary part of complex frequency which means that *G= Im* (Ω). The main concern of this work is to observe the influence of twisting parameter θ, on the dynamics of DNA with anharmonic twist opening model.

4. Molecular Dynamical Simulation: The modulational stability discussed in the previous section is deduced from the linear stability analysis. This linear stability analysis is only based on the linearization around the unperturbed carrier wave. If the wave vector falls inside the instability domain, the wave mixing processes become more significant which generates the combination of waves. Unfortunately, these waves are neglected at the large time scale. In order to analyse the long time behaviour of the nonlinear waves, we perform the molecular dynamics simulation in this section. The molecular dynamical simulation is performed by considering the DNA chain of 256 atoms with periodic boundary conditions and in the lattice the wave vector k is defined by modulo 2π in the form of k =$\frac{2\pi l}{N}$ and Q =$\frac{2\pi l}{N}$, where *l* and L are the integers which is lower than $\frac{N}{2}$. The time evolution of large amplitude zone centre mode is perturbed by the random noise in the Fourier and real space.

5. Result and Discussion: We investigated the influence of twisting in the DNA dynamics with anharmonic twist opening model. We observe from the Figures (a),(b),(c) and (d) that when the degree of twisting increses the instability regime grows exponentially, which may lead the generation of highly robust and coherent solitonic profile which supports the bio-energy transport along the DNA. This may be helpful in prediction to genetic disorder and the associated diseases nin near future.

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