SOLITARY WAVE EXCITATION IN DNA UNDER THE INfIUENCE OF MORSE POTENTIAL AND THE EFFECT OF STRETCHING

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Abstract: We investigate the nonlinear dynamics of a DNA molecule system using Peyrard-Bishop model. This model is being considered as a mechanism of internal motion occurring during the assembly of DNA chain. The DNA nucleotide base pair is assumed to have two degree of freedom and the equation of motion is reduced to the discrete nonlinear Schrodinger (NLS) equation by using semi-discrete approximation method. We detect the instability region by using Modulational Instability analysis. We present a detailed analysis of the effect of potential strength of neighboring nucleotides in the process of energy localization in the form of soliton solution and also we present the detailed analysis of Molecular Dynamics Simulations and Stability analysis for short and long time period. We discuss about the effect of varying Morse potential and stretching in DNA nucleotide chain and this effect is playing an important role in the DNA transcription and Translation process.

Keywords: DNA, Nonlinearity, Modulational Instability Analysis Discrete Breathers.

Introduction: The discovery of Deoxyribonucleic Acid (DNA) double helix structure is undoubtedly one of the most important findings in the history of science. DNA is a biological polymer which exists in different form (A, B, Z, E...) but only the B form can be found in living organisms. DNA is basically a complex structure consisting of two strands of long linear polymer of nucleotides [1]. Where each strand is made up of sugars, Purine [adenine (A) and guanine (G)] and Pyrimidine[Thymine(T) and Cytosine(C)] bases and Phosphates. According to Watson and Crick scheme (1953) the bases on opposite strands are connected by relatively weak hydrogen bonds. It is the sequence of these four bases along the backbone that encodes information the mechanical properties of DNA are closely related to its molecular structure and sequence, particularly the weakness of H-bonds and electronic interactions that hold the strands of DNA together compared to the strength of bond with each strand.

The Hamiltonian approaches to denaturation based on the Peyrard-Bishop (PB) model have been proposed (Peyrard and Bishop, 1989). These models treat the base pair displacements as continuous variables thus allowing a description of those intermediate states, essential to the DNA dynamics.

The PB model considers simplified geometry for the DNA chain. n is described by the scalar variable u_n which represents the transverse stretching of the hydrogen bonds connecting between two bases. PB model has the advantage that it can help to describe the DNA sequence and it allows to study the dynamics and also PB model is a strong simplification of actual DNA molecule in solution, the quantitative and qualitative agreement with numerous experimental results given to same as theoretical results. The stacking energy between two neighboring bases is described by an harmonic potentials. This model reduces the myriad degrees of freedom of DNA to a one-Dimensional chain of effective atom describing the relative base -pair separations from the ground-state possions [2, 3]. An important essence of the PB model is the nonlinear stacking interaction which reproduces the experimentally measured sharp phase transition of long homopolymers [4]. Moreover the model, parameterized for heterogeneous DNA chains, has given accurate results for denaturation curves of short heterogeneous DNA sequences [5].

In this work we strongly rely on the impact of Morse potential and stretching in DNA dynamics. We bring out the formation of localized structures through Modulational Instability (MI) in the Peyrard Bishop (PB) model. We present theoretical and numerical results concerning the properties of nonlinear waves on the PB model of DNA dynamics.

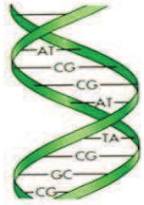

Fig. 1: Structure of DNA

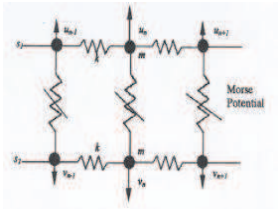

Fig. 2: Morse Potential in DNA

The Modulational Instability (MI) of the linear wave in terms of the energy localization in nonlinear lattice was introduced by Dauxios and Peyrard [6]. The same phenomenon also done in various contexts: in fluid dynamics as called Benjamin-Feir instability, in nonlinear optics and plasma physics. In this paper, we perform the linear stability analysis and analyze the instability domain and point out the crucial role of the nonlinearities and also we checked this analysis by using numerical simulations.

The Model Hamiltonian and Dynamical Equation: We adapt the Morse potential to describe the hydrogen bonds, (1) a harmonic coupling due to the Stacking is assumed between neighboring bases. We use **m** for the mass and **S** for the harmonic constant of longitudinal spring along each strand. We ignore the difference masses and harmonic constants in DNA. The stacking energy between two neighboring bases is described by anhormonic potential:

$$U(u_n, u_{n+1}) = D(e^{-au_n} - 1)^2 + \frac{1}{2}S(1 + \eta e^{-b(u_{n+1}+u_n)}) \quad (1)$$

$(u_{n+1} + u_n)^2$.

Hence, the Hamiltonian of the system is written as folows:

$$\mathbf{H} = \sum_{n=1}^{N}[\frac{1}{2}\mathbf{m}(\dot{\mathbf{u}}_n^{\ 2} + \mathbf{U}(\mathbf{u}_n, \mathbf{u}_{n+1}))]. \quad (2)$$

The bases are related by the hydrogen bonds; in this system Morse potential also describes the chemical reactions within the base pairs. While twisting or stretching the hydrogen bonds connecting between the bases are broken then the molecule structure also changes to the stacking interaction between complementary or adjacent bases. The stacking is denoted by the quadratic term $(u_{n+1} - u_n)^2$, which governed by the factor $\frac{1}{2}S(1 + \eta e^{-b(u_{n+1}+u_n)})(u_{n+1} + u_n)^2$. This factor decreases from $\frac{1}{2}S(1+\eta)$ to $\frac{1}{2}S$ when either one or both base pair are stretched. The parameters used in this work are those derived from the thermo dynamical denaturation of DNA. They are m = 300amu, S = 0.04eV. The period of the harmonic oscillations at the bottom of the Morse potential is then $T_o = 2\pi/\omega_g$ = 86.4t.u From Hamiltonian (2), the equation governing the stretching of the base pairs is written as:

$$m\ddot{u}_n = S(u_{n+1} + u_{n-1} - 2u_n) + \frac{1}{2}S[2 + b\eta(u_{n+1} - u_n)]$$

$$(u_{n+1} - u_n)e^{-b(u_{n+1}+u_n)} - \frac{1}{2}S[2 - b\eta(u_n - u_{n-1})]$$

$$(u_n - u_{n-1})e^{-b(u_n+u_{n-1})} - 2aD(e^{-au} - e^{-2au}).$$

Expanding the terms in exponential $e^{-b(u_{n+1}+u_n)}$, $e^{-b(u_n+u_{n-1})}$ and e^{-au} respectively, until the second and third orders, we obtain the following equation of motion:

$$\ddot{u}_n = K_1(u_{n+1} + u_{n-1} - 2u_n) + \alpha' b[(u_n - u_{n-1})^2 -$$
$$(u_{n+1} + u_n)^2] + \alpha' b^2[(u_{n+1} - u_n)^2(u_{n+1} + u_n) -$$
$$(u_n - u_{n-1})^2(u_n - u_{n-1})] + 2\alpha' b[(u_{n+1} - u_n) \quad (3)$$
$$(u_{n+1} + u_n) - (u_n - u_{n-1})(u_n + u_{n-1})] -$$
$$\omega_g^2(u_n + \alpha u_n^2 + \beta u_n^3),$$

Where $K_1 = \frac{S}{m} - 2\alpha', \omega_g^2 = \frac{2a^2D}{m}, \alpha = -\frac{3a}{2}$ and $\beta = \frac{7a^2}{6}, \alpha' = \frac{S\eta}{2m}$.

Very often, the equation in question can take the form of the nonlinear Schrodinger equation (NLS) or the complex Ginzburg-landau (CGL) equation. Two interesting aspects of the latter are (a) that it exhibits the interesting phenomenon of modulational instability, the possibility of the plane wave's bursting into a series of localized pulses and (b) that it accepts solitary wave solutions. The nonlinearity in the dynamics of the lattice might be imposed either by the anhormonicity of the interaction between the atoms or by the existence of an on-site potential. In the first case, it has been shown in a general manner that a constant term (a non oscillating nonlinear wave) appears in the same order as the small amplitude phonon considered (first order perturbation) and hints have been made that its existence might influence the stability of the modulated envelope soliton [6]. The way of deriving the NLS equation consists in studying the nonlinear (amplitude dependent) dispersion relation obtained by considering a phonon in first order of perturbation, in the discrete (or continuum) equation of motion. The next method consists in considering the continuum limit only for the amplitude ,but treating the phase exactly. To do so, however, one must suppose a specific form for the solution [7, 8]. Kivshar and Peyrard [9, 10] have developed an interesting approach to derive the NLS equation in a chain of Klein-Gordon. Recently], Johansson [11, 12] has derived the Klein-Gordon /Fermi-Pasta/Ulam-NLS equation from the Klein-Gordon /Fermi-Pasta/Ulam chain using the Fourier series. Hence, we use this approach to study the existence of soliton-like solutions in the PBD model of the DNA molecule. The small amplitude solutions u_n of the above expanded equation can be written in the form of a Fourier series as:

$$u_n(t) = \sum_{p=-\infty}^{+\infty} a_n^{(p)} e^{ip\omega_b t}, \tag{4}$$

Where ω_b is close to some linear oscillation frequency and the Fourier coefficients are slowly depending on time, $a_n^{(p)}(\varepsilon^2 t)$. Due to exponential decay of the Fourier coefficient in p, they must satisfy $a_n^{(p)} - (\varepsilon^p)$ for p≥o. Moreover $a_n^{(p)} = a_n^{(-p*)}$ since u_n is real. The time dependant amplitude can be written in the form

$$a_n^1(t) = \left(\frac{2\omega_b}{3\beta\omega_g^2 + 6\alpha' b^2}\right)^{\frac{1}{2}} \psi_n e^{i\left(\frac{\omega_g^2 - \omega_b^2 + 2k}{2\omega}\right)t}, \tag{5}$$

After solved the length equation we can get,

$$\begin{aligned} &i\frac{d\psi_n}{dt} + P_1(\psi_{n+1} + \psi_{n-1}) + Q_1|\psi_n|^2\psi_n - Q_2[|\psi_{n+1}|^2 \\ &\psi_{n+1} - |\psi_{n-1}|^2\psi_{n-1} + \psi_n^*(\psi_{n+1}^2 - \psi_{n-1}^2) - \\ &\psi_n^2(\psi_{n+1}^* - \psi_{n-1}^*)] = 0. \end{aligned} \tag{6}$$

Equation (6) is a modified discrete nonlinear Schrodinger (MDNLS) equation. it represents one of the simplest equations in which the combinations of dispersive effects with the cubic nonlinearity leads to the localized solutions of soliton type[13]. The interplay between dimensional and the order of nonlinearity has indeed been used in the past as a way to investigate collapse in low-dimensional nonlinear systems [14-15].

Modulational Instability (MI) in DNA Systems: The MI occurs due to the interplay between discreteness and nonlinearity [16]. The MI of waveforms is a fundamental phenomenon in nonlinear media and it's closely associated with the concept of self-localized waves, or solitons. MI involves the exponential growth of weak perturbations through the amplification of sideband frequencies. We investigate the modulational instability of a constant amplitude solution and perform a stability analysis of the solution. The steady –state solution o the above Eq. (6) is given by

$$\psi_n = \psi_0 e^{[i(kn-\omega t)]}, \tag{7}$$

Where ψ_0 the constant amplitude, k is represents the wave number and ω indicates the angular frequency. Satisfying the following dispersion relation

$$\omega = -P_1\cos k - \psi_0^2(Q_1 - Q_2 4\sin k). \tag{8}$$

Now we investigate this solution is stable against small perturbations by performing a linear stability analysis. We consider a small perturbation of the constant amplitude solution (7) is given by

$$\psi_n = (\psi_0 + \delta\psi_n)e^{[i(kn-\omega t)]}, \tag{9}$$

Where, $\delta\psi_n$ is assumed to be a small perturbation in comparison with the carrier wave amplitude ψ_0. The equation which describes the evolution of the perturbation is given by

$$i\delta\psi_n + P[(\delta\psi_n + \delta\psi_{n-1})(e^{ik} - e^{-ik})] + 2Q_1(\psi_0^2\delta\psi_n$$
$$-\psi_0^2\delta\psi_n^*) - Q_2[\psi_0^2\delta\psi_{n+1} - 2\psi_0^2\delta\psi_{n-1} + \delta\psi_n^* \quad (10)$$
$$(\delta\psi_{n+1}^2 - \delta\psi_{n-1}^2) - \delta\psi_n^2(\delta\psi_{n+1}^* - \delta\psi_{n-1}^*)] = 0.$$

We consider a complex plane-wave perturbation

$$\delta\psi_n = \psi_1 e^{i(Qn-\Omega t)} + \psi_2^* e^{-i(Qn-\Omega t)}, \quad (11)$$

where Q and Ω represent the wave number and angular frequency of the perturbation respectively, and ψ_1 and ψ_2^* are the amplitudes of the real and imaginary parts respectively. Substituting Eq. (11) into Eq. (10), we obtain the following system of equations,

$$[\Omega + Q_2 + 2Q_1\cos(Q-K)]\psi_1 - a^2 - b^2 = 0,$$
$$[-\Omega + Q_2 + 2Q_1[\cos(Q+K) - \cos(Q-K)]\psi_2 \quad (12)$$
$$-a^2 - b^2 = 0.$$

We obtain a system of homogeneous equations as represented by

$$\begin{pmatrix} \Omega + a + 2\cos(Q+k) & b \\ b & \Omega - a + 2\cos(Q-k) \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

In order to have a nontrivial solution for the determinate o the coefficient matrix should be zero that leads to

$$\Omega = \frac{-B \pm \sqrt{B^2 - 4C}}{2} \quad (13)$$

Where,

$$B = 2Q_1[\cos(Q+k) - \cos(Q-k)]$$
$$C = -2Q_1\psi_2[\cos(Q+k) + \cos(Q-k)]$$
$$-\cos(Q+k)\cos(Q-k) \quad ,$$
$$a = \omega + 2Q_1\psi_0^2 - \psi_0^2, b = 2Q_1\psi_0^2 - \psi_0^2$$

Naturally Eq. (13) is modulationally in stable for any wave number Q if and only if both Ω_+ and Ω_- are negative. It is evident that for both Ω_+ and Ω_- to be negative, it is necessary that $B^2 - 4C > 0$ and sufficient that 4C is positive. Thus the following inequalities are necessary for modulation stability

$$B^2 - 4C > 0, B^2 < 0, 4C > 0. \quad (14)$$

We then obtain the following criteria for the modulational stability.

$$\Omega = -(\frac{1}{2})\{[2(a\cos(Q-k) + \cos(Q+k))] \pm$$
$$[2(a^2\cos^2(Q-k) + \cos^2(Q+k) + 2a\cos(Q-k) \quad ,$$
$$\cos(Q+k)) - 4a\cos(Q+k)\cos(Q-k) + 2(a^2+b^2)]^{\frac{1}{2}}\}$$

The perturbation that grows exponentially with the intensity given by the growth rate or the modulational instability gain g(Ω) defined by

g (Ω)=I_m(Ω),

where I_m denotes the imaginary part and existence of localized structures are possible only when the constant-amplitude solution is unstable. The gain shows more interesting dependence of Ω on the parameters ψ_1, ψ_2 and ω. Above equation determines the stability and instability of a plane wave with wave number Q in the discrete DNA system and the instability gain spectrum is portrayed for the choices of parameters ψ_o=0.3, h=5, γ=0.1×10^{-10}, d=0.1×10^{-19}, m=5.1×10^{-25}, k=8, Q=1.6×10^{-19}, K=0.8 shown in Figs. () depict the regions of stability/instability and the corresponding influence of the parameters and Morse potential with stretching are explored pictorially. In the figures, the dark bluish area corresponds to a region where the nonlinear plane waves are stable with respect to modulation of any wave number Q and the region with bright yellowish orange represent the exponential growth. While increasing the value of the Morse potential and stretching parameters the stable domain is increasing ie while increasing the growth rate of the DNA system driven to highly instable nature of the modulated wave. Also we did the discrete breathers.

Conclusion: Nonlinear localization phenomenons in biological lattices have attracted a steadily growing interest and their existence has been predicted in a wide range of physical settings. We describe the nonlinear dynamical equation governing the dynamics of DNA using the semi-discrete approximation method. We suggest a possible localization mechanism of nucleotides interaction in a DNA system through modulation instability analysis. We present a detailed analysis on modulational instability and the role of Morse potential on the process of bio-energy localization is notably pointed out. While doing MI the amplitude of the soliton with increasing the Morse potential and increasing the stretching, Fourier transformation gives the stability for short and long time period. We perform numerical simulation such as molecular dynamical simulations which gives the possible existence of long-lived excitations in DNA system that move on to nonlinear regime. We employ symbolic computation to solve the associated DNA dynamical equation and exhibit the solitonic structure. The nonlinear behavior of DNA macromolecular system can be understood by the evolutionary plots which are in the form of solitary profile. This soliton is most important for the transcription and translation process and also from the simulation results the effect of the stretching is playing a major role in functions of DNA.

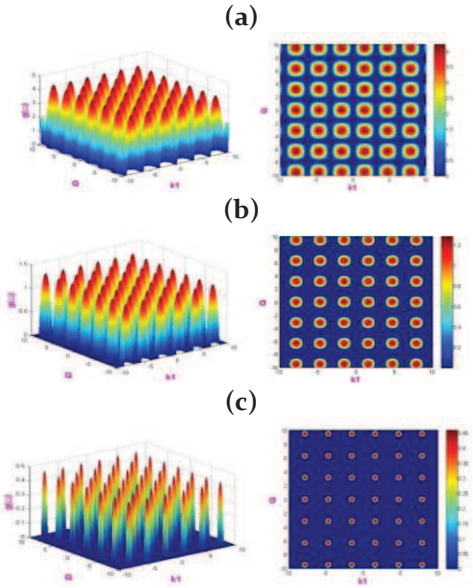

Fig.3: Stability/Instability Region in the (Q,K_1) Plane, MI Gain Profile for (A)$S=1\times10^{9}m^{-1}$,'(B) $S=4\times10^{9}m^{-1}$,'(C) $S=7\times10^{9}m^{-1}$ And All Plots $\Psi_o=0.3$, $H=5$, $\Gamma=0.1\times10^{-10}$, $D=0.1\times10^{-19}$, $M=5.1\times10^{-25}$, $K=8$, $Q=1.6\times10^{-19}$, $K=0.8$

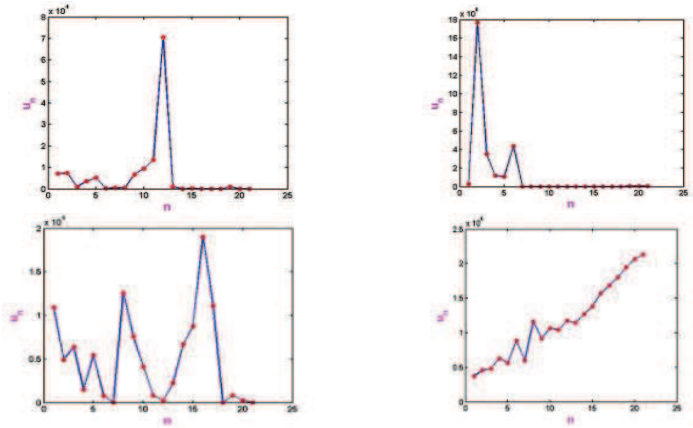

Fig.4: Snapshots of DBs profile for Parametric Values $a=0.2$ to 0.5, $k=8Nm^{-1}$, $\lambda=0.009$, $P=1.2$,$q=0.5\times10^{-19}c$

Acknowledgment: This work would not have been possible without the assistance and support of my guide Dr.L. Kavitha, Associate Professor of Physics, CUTN, BRNS,India in the form of Young Scientist Research Award and ICTP, Italy in the form of junior Associateship.

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