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Short Communication

Modulational instability analysis of neuronal microtubules under the influence of Toda potential

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Abstract

The cytoskeleton of eukaryotic cells is composed of several classes of protein polymers among which neuronal microtubules (NMTs) are the most prominent. The radical control of cellular processes in NMT system, that are cell division, intracellular trafficking, cellular morphogenesis process and also energy moved from one cell to another cell with least loss of energy. We investigate the excitations of soliton with small perturbation along the protofilaments that are governed by Discrete Nonlinear Schrodinger (DNLS) equation. We study the modulational instability analysis on microtubulin system under the influence of electric field with Toda potential. We perform a complete investigation of aninfluence of Toda potential of tubulin dimers in the development of energy localization that has the form of breather-like soliton excitations in the neuronal microtubulinprotofilament. The evolution of the localized wave is expected to explore a very interesting physical phenomenon such as energy transfer mechanism in biological systems.

Keywords: Solitons, rotating wave approximation, discrete nonlinear Schrodinger (DNLS) equation, neuronal microtubules, gain spectrum.

Introduction

Neuronal cells undertake most important developmental variations, such as migrate, synaptic connections, axons and also in dendrites. The formation of neuronal polarity and preserving of axonal integrity functions are most important at the structural organization and dynamic remodeling of the neuronal microtubulin cytoskeleton[1]. Cytoskeleton is responsible for the structural organization of the interior of the neuronal cell. It is made up of microfilaments (MFs), intermediate filaments (IFs) and microtubules (MTs), each having a specific physical property and structure suitable for their role[2]. And without neuron, MTs could not maintain its structural shape of cells[3]. The significant relation of assembly/ disassembly and transport properties in microtubulin systems are the organization of migratory neurons, dendrites, axons and growth cones with the value of intrinsic polarity, such as segregating the chromosomes during cell division and support the motor proteins that are kinesins and dyneinsto which is produce the force essential for cell motions, shape changes and acting as significant targets for anticancer drugs[4].

The microtubules can grow upto 25 nm long and is has the shape of hollow cylinder which is shown in Figure-1. An interior of biological cells are highly arranged in a systematic ways of both structure and dynamics, the NMT cylinder has contain the rich in water molecules and which require the existence of an electric dipoles, static and dynamic electric fields and also the outer surface is bordered by the organization of cytoplasmic water and enzymes. Along the NMT axis, with alternating subunits (α and β) of tubulin hetrodimers are end to end joined to form protofilaments. The wall of NMT is made up of 13 identical protofilaments[4].

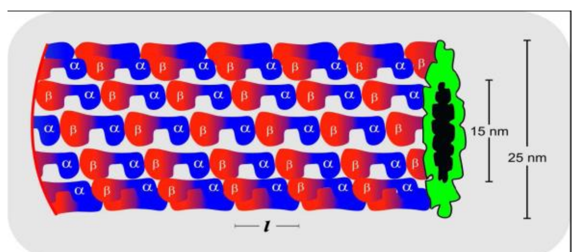

Figure-1: Structural subunits of microtubule.

The neuronal microtubulin system has a strong unidirectional insulator. The periodic arrangement of dimers can be assumed a degree of freedom, it is depend on an angle or longitudinal co-ordinate and the net polarization[5]. The structure of the NMTs is also has the nonlinear nature. Generally, the nonlinear organized systems can produce advanced harmonic components and components with frequency combination and also allow the energy transportation. In this paper we will put theoretical model based on work as follows: we build next section in the model Hamiltonian of the system and develop the DNLS equation that governs the dynamics of MTs. In another section, we carry out the modulational instability (MI) with aid of stability analysis in NMTs under the effect of an internal cell electric field with toda potential and the results are concluded in conclusion section.

The model Hamiltonian and dynamical equation

Thus the n[th] tubulin molecule of a protofilament can be approximately expressed by the following toda potential.

$$\frac{k_2}{b}[(\phi_n-\phi_{n-1})+\frac{1}{b}(\exp(-b(\phi_n-\phi_{n-1})-1))] \qquad (1)$$

Equation (1) represents the toda potential which is described by the overall effect on the *n[th]* site dipoles, here K_2 represents the linear spring constant of a NMTs and *b* stands for the inverse width of a Toda potential well. The total effective Hamiltonian describing the large oscillations of the dimer in a NMT is thus given by

$$H=\sum_{n=1}^{N}\left[\frac{m}{2}\dot{\phi}_n^2+\frac{K_1}{2}(\phi_{n+1}-\phi_n)^2-qlE\cos\phi_n+\frac{K_2}{b}[(\phi_n-\phi_{n-1})+\frac{1}{b}(\exp(-b(\phi_n-\phi_{n-1})-1))]\right]. \qquad (2)$$

The first term in Equation (2) denotes longitudinal displacement of dimers represented as kinetic energy term, here *m* and *n* represent as mass of each dimer and position of the protofilament. The overdotis atime derivative order one. The followed second term represents the restoring strain forces in between the adjacent dimers in the protofilament and this force term describe the potential energy appear attribute to chemical interaction among nearest two dimers, K_1 represent an intra-dimer stiffness. The third term represents as intrinsic electric field ($\vec{E}$) in dimers with the electric dipole at NMT cylinder, it having the potential energy $(U=-\vec{p}.\vec{E}=qlE\cos\phi_n)$. By the third term *q* denotes the extra charge inside the electric dipole,*l* denotes the dimer length and here *E > 0,q > 0*. For large oscillations using Hamiltonian in NMT, the Hamilton's equation of motion will directly yield,

$$\ddot{\phi}_n-\frac{K_1}{m}(\phi_{n+1}+\phi_{n-1}-2\phi_n)+\frac{qlE}{m}(\phi_n-\frac{\phi_n^3}{6})-\frac{K_2}{m}[\frac{1}{b}(\phi_n-\phi_{n-1})-(\phi_n-\phi_{n-1})^2-\frac{K_2b}{2m}(\phi_n-\phi_{n-1})^3]=0, \qquad (3)$$

In Equation (3) is very hard to solve because of its discreteness and nonlinearity and it has various nonlinear phases and different nonlinear couplings. So, we analyzing system behavior through the Rotating Wave Approximation (RWA) with our model equation of motion[6-9].

$$\phi_n=\phi_n e^{-i\omega_0 t}+\phi_n^{*}e^{-i\omega_0 t}, \qquad (4)$$

where ω_0 stands for linear frequency of oscillation. Thus, we could call upon RWA to the discrete equation of motion in Equation (4).

$$\dot{\phi}_n+\varepsilon_1(\phi_{n+1}+\phi_{n-1}-2\phi_n)+\beta|\phi_n|^2\phi_n+\frac{\alpha}{2}\phi_n+\gamma(\phi_n-\phi_{n-1})=0, \qquad (5)$$

where,

$$\alpha=-(\frac{qlE}{\omega_0 m}-\omega_0),\beta=\frac{qlE}{4\omega_0 m},\gamma=\frac{K_2}{2\omega_0 bm},\varepsilon_1=\frac{K_1}{2\omega_0 m}.$$

The obtained Equation (5) is often called as a DNLS equation, it is very fascinating role in modern science and technology. The DNLS equation is a well-known non integrable model which has a number of applications in molecular Physics, nonlinear optics, and in other fields[10,11]. Generally, DNLS equation is one of the easily understanding soliton type equation at the combined effects of dispersion and nonlinearity. Therefore, DNLS equation is exhibits the chaotic dynamics in the certain regimes, continuous translational symmetry and integrable nature brooked at the simultaneously due to discretization effect. Here, we have studied in the present section fordynamics of NMTs structure which can be described by the DNSLS equation and further, from which we paid to study thediscrete modulational instability analysisin the next section.

Modulational Instability Analysis in NMTs

Using finite difference method in Equation (5). The constant amplitude solution[12,13].

$$\phi_n=\phi_0 e^{i(k_1 n-\omega t)} \qquad (6)$$

In above equation manifests MI is most important plane wave solution of Equation (5). Here ϕ_0 is amplitude which treated as a constant, ω is an angular frequency and$k_1$is wave number. In order to substituting Equation (6) into Equation (5), gives appropriate nonlinear dispersion relation,

$$\omega=-2\varepsilon[\cos k_1-2]-\beta\phi_0^2-\frac{\alpha}{2}-\gamma[1-\cos k_1+i\sin k_1] \qquad (7)$$

To the initially solution is little perturbed and learn small perturbation grows with propagation are the essential thought of linear stability analysis. The perturbed amplitude slightly small associated with the initial plane wave, is suitable for linear stability analysis. This analysis is provide the small perturbation amplitude with the early wave amplitude. So, we adopt initial plane wave to investigate in MI. For the stability properties of small perturbation inserted into initial plane wave solution, we have

$$\phi_n=(\phi_0+\delta\phi_n)e^{i(k_1 n-\omega t)}. \qquad (8)$$

Where $\delta\phi_n$ as small perturbation is compared to ϕ_0. We substitute the above solution into Equation (5), and keeping only linear terms, then, we obtain the first-order differential equation as,

$$\omega\delta\phi_n+i\delta\dot{\phi}_n+\varepsilon\delta\phi_{n+1}e^{ik_1}+\varepsilon\delta\phi_{n-1}e^{-ik_1}-2\delta\phi_n+2\beta\phi_0^2\delta\phi_n+\beta\phi_0^2\delta\phi_n^{*}+\frac{\alpha}{2}\delta\phi_n \qquad (9)$$
$$+\gamma\delta\phi_n-\gamma\delta\phi_{n-1}e^{-ik_1}=0.$$

The perturbed wave solution written from the Equation (9), we get

$$\delta\phi_n = \phi_1 e^{i(Qn-\Omega t)} + \phi_2^* e^{-i(Qn-\Omega^* t)}. \qquad (10)$$

Where * means complex conjugate, Q is the perturbation wave vector and Ω represent the perturbation frequency. Inserting Equation (10) into Equation (9) provides a linear homogeneous system for ϕ_1 and ϕ_2^*

$$\Omega\phi_1 + \omega\phi_1 + 2\varepsilon\phi_1\cos(Q+k_1) - 2\phi_1 + 2\beta\phi_0^2\phi_1 + \frac{\alpha}{2}\phi_1 + \gamma\phi_1 - \gamma(\cos(Q+k_1) - i\sin(Q+k_1)) + 2\beta\phi_0^2\phi_2 = 0, \qquad (11)$$

$$-\Omega\phi_2 + \omega\phi_2 + 2\varepsilon\phi_2\cos(Q-k_1) - 2\phi_2 + 2\beta\phi_0^2\phi_2 + \frac{\alpha}{2}\phi_2 + \gamma\phi_2 - \gamma\phi_2(\cos(Q-k_1) - i\sin(Q-k_1)) + 2\beta\phi_0^2\phi_1 = 0, \qquad (12)$$

Now, we can write the coefficients of the 2 × 2 matrix as followed by

$$\begin{pmatrix} \Omega + A_1 + 2\varepsilon\cos(Q+k_1) - \gamma(\cos(Q+k_1) - i\sin(Q+k_1)) & \beta\phi_0^2 \\ \beta\phi_0^2 & -\Omega + A_1 + 2\varepsilon\cos(Q-k_1) - \gamma(\cos(Q-k_1) + i\sin(Q-k_1)) \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

where, (13)

$$A_1 = \omega - 2 + 2\beta\phi_0^2 + \frac{\alpha}{2} + \gamma$$

Equations (11 & 12) has the nontrivial solution of linear homogeneous system and its determinant vanishes. This gives second order equation condition

$$\Omega^2 + \Omega B_1 + C_1 = 0, \qquad (14)$$

Where,

$$B_1 = -2\varepsilon\cos(Q-k_1) + \gamma\cos(Q-k_1) + i\gamma\sin(Q-k_1) + 2\varepsilon\cos(Q+k_1) - \gamma(\cos(Q+k_1) + i\gamma\sin(Q+k_1)$$

$$C_1 = A_1^2 + A_1[2\varepsilon\cos(Q-k_1) - \gamma\cos(Q-k_1) - i\gamma\sin(Q-k_1) + 2\varepsilon\cos(Q+k_1) - \gamma(\cos(Q+k_1) + i\gamma\sin(Q+k_1)] + 4\varepsilon^2\cos(Q+k_1)\cos(Q+k_1) - 2\varepsilon\cos(Q+k_1)\cos(Q-k_1) - 2i\varepsilon\gamma\cos(Q+k_1)\sin(Q-k_1) - 2\gamma\varepsilon\cos(Q+k_1)\cos(Q-k_1) + \gamma^2\cos(Q+k_1)\cos(Q-k_1) + i\gamma^2\cos(Q+k_1)\sin(Q-k_1) + 2i\varepsilon\gamma\cos(Q-k_1)\sin(Q+k_1) - \gamma^2\cos(Q-k_1) + \gamma^2\sin(Q+k_1) - \beta\phi_0^4$$

Obviously, equation (14) has the solution

$$\Omega = \frac{-B_1 \pm i\sqrt{B_1^2 - 4C_1}}{2}. \qquad (15)$$

the perturbation growth rate written as

$$g(\Omega) = 2\,\mathrm{Im}(\Omega) = \pm i\sqrt{B_1^2 - 4C_1}, \qquad (16)$$

Relation (16) represents the MI gain for plane waves in the system of NMT lattices which is described by the DNLS equation. In this equation, *Im* is the imaginary part and if unstable amplitude solution begins to arise the localized structures else not possible it. The gain Ω depend on the α, β, γ, ε_1 which is play essential role of MI, also occur stability in imaginary part and controls the stability/instability of a perturbation of wave number (Q) in Equation (16). Figure-2 shows that instability gain spectrum with to set the suitable parameters q=0 in the.1 C, l=1 m, m=1.1 kg m^{-2}, K_1=0.1 Nm^{-1}, K_2=10 Nm^{-1}, E=5 × 10^{-5} Nm^{-1}, ω_0 =5.01 and b=0.1. In the inverse width of the toda potential, stability and instability area has been explored clearly in Figures-2, here dark bluish region represented as stable in the modulated any wave number (Q) and also in the nonlinear plane wave and the reddish region represented as the unstable in the amplitude of modulated wave, it is estimated to abruptly exhibit an exponential like growth. Figures-2, clearly shows from domains of MIappears to be better as the value of inverse width of toda potential increases from b=0.1 to b=0.8, thus decreasing the instable nature of propagating plane wave in neuronal microtubules. In Figure-2, shows the instability region initially maximum of perturbed wave after that this region significantly changes with *b* increasing in the NMT and eventually strong stability appear in the modulated plane waves. It is revealed from Figures-2 that, the play-role of inverse width of toda potential leads to the stability and succeeding arrangement of intrinsic localized structures.

Conclusion

Exploring the nonlinear excitations in biological system still attracts deep interest. It contributes to illustrate biomolecular processors, such as the vibrational energy transport in dimers, energy localization and replication phenomenon in NMTs. The neuronal microtubulincytoskeleton has peripheral shape and the division of neurons that are structured and carry out its cytoplasm to motile and metabolic behavior of necessary life. In the between of dipole-dipole along neuronal microtubule protofilament, we formulated Hamiltonian using the toda potential. By using the Rotating wave approximation (RWA) technique, we derive the nonlinear dynamical equation into Discrete Nonlinear Schrodinger (DNLS). In viamodulational instability analysis, we get soliton localization of dipole oscillations in a NMT protofilament. According to acquired graphical analysis, we have discussed the process of bioenergy localizationin the role of essential cell electric field with toda potential.

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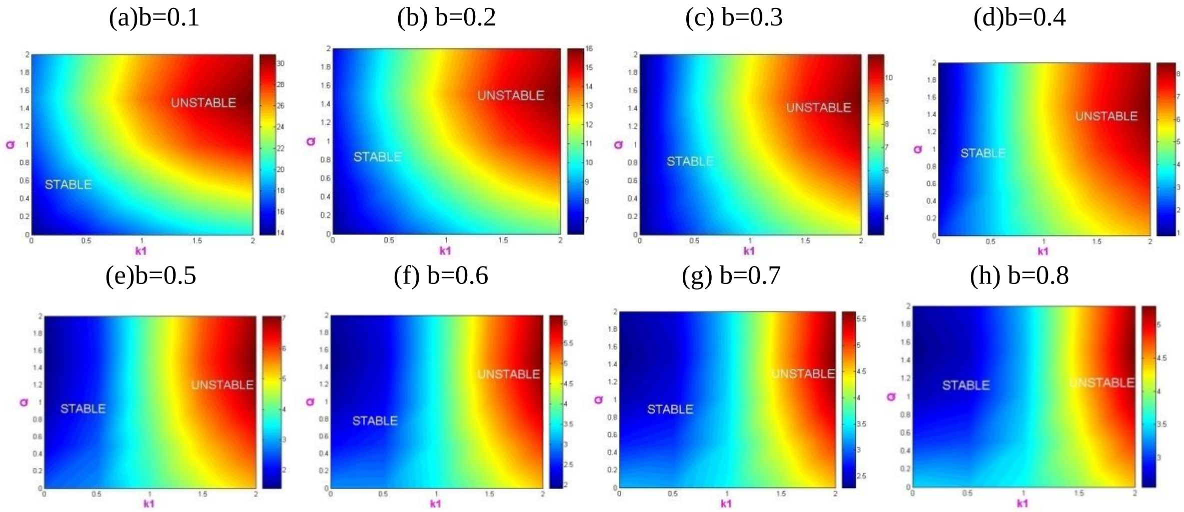

Figure-2: The variation of Q with k_1 for different values of b with to set the suitable parameters q=0.1 C, l=1 m, m=1.1 kg m^{-2}, K_1=0.1 Nm^{-1}, K_2=10 Nm^{-1}, E=5 × 10^{-5} $Nm^{-1}$and ω_0 =5.01.

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