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Dynamics of Davydov Solitons in α-Helix Proteins

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Abstract

This paper studies the dynamics of Davydov solitons in α-helix pro-

teins that is governed by the nonlinear Schrödinger's equation. The perturbation terms of this equation are taken into consideration and a stable fixed point is obtained.

1 INTRODUCTION

The α-helical structure is foiund at those sites if protein molecules where the transduction of energy from one end of a molecule to the other takes place and where a protein molecule couples with a few processes, too [1-10]. As an example in a haemoglobin molecule of red blood corpuscles transmitting oxygen, involves 32 helix segments. A bacteriorhodospin molecule incorporated into the membranes of halo-bacteria that live in salty lakes and basins, intersects the cell membrane seven times in the form of α-helix segments. α-helix protein segments incorporate into cytochrome and proteins intersecting inner membranes and mitochondria [6].

The modern investigation of spatial structure of cells demonstrate that a whole cellular interior is spanned by a network of protein microfilaments and microtubes that retains all intracellular organelles in a definite position, determine the shepe of cells, any changes, and all motions inside the cell. Such a network of microfilaments and microtubes is called a *cytoskeleton* [6].

Protein molecules incorporated into cytoskeleton realize the transduction of energy and all intracellular coupling. All these processes expensed the energy released in the hydrogen of ATP molecules. The hydrolysis process takes place with the participation of enzymes and is controlled by a variation of the concentration of calcium ions, in a manner similar to muscle fibers [6].

The existence of contractile proteins, like actine, myosin and troponin, deenium and tubulin, in nonmuscle cells confirm the hypothesis of a unique pathway for

the conversion of chemical energy of hydrolysis of ATP molecules into that of mechanical motion. Intracellular motion also occurs by the pathway of sliding. Nevertheless, this mechanism differs from that which applies to muscle fibers in some details [6].

In muscle fibers, the thick filaments are located at the sarcomer center in the form of parallel rays. The ends of this actin filaments are coupled with the z-th plates separating sarcomers from each other, and are placed in thick filament interior. However, in nonmuscle cells, myosin filaments have no definite position and float in cytoplasma [6].

Helix segments constitute a considerable part of the protein structure of a ctyoskeleton. Besides motion, they transfer energy and information from one cite in a cell to another by means of propagation of soliton excitations [6].

Transmembrane glycoproteins play an important roile in the vitality of a cell, too. Glycoproteins are formed by the covalent binding of proteins with carbohydrate residues, or polysaccharides. Their long protein fraction hasa α-helix structure which spans the whole thickness of the outer cellular membrane. The polysaccharide part is hydrophobic and is located on the outer surface of a cell. The internal parts of glycoproteins are strongly coupled with microfilaments and microtues of the cellular cytoskeleton. Therefore, glycoproteins realize the coupling of the cellular interior and exterior [6].

Glycoproteins determine the cellular individuality, their adhesion, and intercellular interaction. They transmit signals inside cells which are caused by the cellular enviornment through binding of hormones, neurons, immunoglobulins and other molecules [6].

The nonlinear dynamics of solitons can provide a key for the understanding of

the mechanism of transduction of information from the exterior to the interior of a cell.

1.1 GOVERNING EQUATION

The dynamics of solitons in α-helix proteins is governed by the nonlinear Schrödinger's equation (NLSE) that is given by [1-10]

$$iq_t + \frac{1}{2}q_{xx} + |q|^2 q = 0 \tag{1}$$

In equation (1), the dependent variable q represents the excitations corresponding to the dipole intra-peptide vibrations while the independent variables are x and t. The second term represents the dispersion term that arises from the effective mass of the exciton while the third term is the nonlinear term. The exciton type solution, also known as the 1-soliton solution, of (1) that is obtaned by Inverse Scattering Transform is given by [1-10]

$$q(x,t) = \frac{A}{\cosh\left[B(x-\bar{x}(t))\right]} e^{i(-\kappa x + \omega t + \sigma_0)} \tag{2}$$

where

$$\kappa = -v \tag{3}$$

and

$$\omega = \frac{B^2 - \kappa^2}{2} \tag{4}$$

while

$$A = B \tag{5}$$

The the center of mass of the soliton is given by

$$\bar{x}(t) = \frac{\int_{-\infty}^{\infty} x|q|^2 dx}{\int_{-\infty}^{\infty} |q|^2 dx} \tag{6}$$

so that the velocity of the soliton is given by

$$v = \frac{d}{dt}\left(\frac{\int_{-\infty}^{\infty} x|q|^2 dx}{\int_{-\infty}^{\infty} |q|^2 dx}\right) \tag{7}$$

Equation (2) has infinitely many conserved quantities. The first three of them are the energy (E), momentum (M) and the Hamiltonian (H) that are respectively given by

$$E = \int_{-\infty}^{\infty} |q|^2 dx = 2A \tag{8}$$

$$M = \frac{i}{2}\int_{-\infty}^{\infty} (qq_x^* - q^* q_x) dx = -2\kappa A \tag{9}$$

$$H = \frac{1}{2}\int_{-\infty}^{\infty} (|q_x|^2 - |q|^4) dx = \frac{2}{3}A\left(3\kappa^2 - A^2\right) \tag{10}$$

It is to be noted that the value of these conserved quantities are computed by the 1-soliton solution that is given by (2). Also, the center of mass of the soliton is given by

$$v = \frac{d\bar{x}}{dt} = -\kappa + \frac{\epsilon}{E}\int_{-\infty}^{\infty} x\left(q^* R + qR^*\right) dx \tag{11}$$

1.2 PERTURBATION TERMS

The perturbed NLSE that is going to be studied in this subsection is given by

$$iq_t + \frac{1}{2}q_{xx} + |q|^2 q = i\epsilon R \tag{12}$$

where in (12), R represents the perturbation terms and ϵ represents the perturbation parameter. In presence of perturbation terms, the energy, momentum and the Hamiltonian are no longer conserved. Instead they undergo an adiabatic deformation that leads to the adiabatic deformation of the soliton parameters. The laws of these adiabatic deformation of the soliton parameters are given by

$$\frac{dA}{dt} = \frac{dB}{dt} = \frac{\epsilon}{2}\int_{-\infty}^{\infty} (q^* R + qR^*) dx \tag{13}$$

$$\frac{d\kappa}{dt} = \frac{\epsilon}{2A}\left[i\int_{-\infty}^{\infty} (q_x^* R - q_x R^*) dx - \kappa\int_{-\infty}^{\infty} (q^* R + qR^*) dx\right] \tag{14}$$

The change in the velocity, in presence of the perturbation terms is given by

$$v = \frac{d\bar{x}}{dt} = -\kappa + \frac{\epsilon}{E}\int_{-\infty}^{\infty} x\left(q^* R + q R^*\right) dx \tag{15}$$

In this paper, the following perturbation terms that are considered, are all studied in the context of solitons in α-helix proteins.

$$\begin{aligned} R = {} & \eta q^* q_x^2 + \beta \left|q_x\right|^2 q + \gamma \left|q\right|^2 q_{xx} \\ & + \delta \left|q\right|^4 q + \lambda q^2 q_{xx}^* + \nu \left|q\right|^2 q_x + \xi q^2 q_x^* + \sigma q_{xxxx} \end{aligned} \tag{16}$$

Thus (12), with the perturbation terms given by (16), represents the dynamics of α-helix proteins with internal molecular excitations and interactions with their nearest and next-nearest neighbors and also nonlinear couplings between molecular excitations and interactions [4, 5].

In presence of these perturbation terms and using the 1-soliton solution that is given by (16), the adiabatic variation of the soliton amplitude and frequency are given by

$$\begin{aligned} & \frac{dA}{dt} = \frac{dB}{dt} = \\ & \quad \frac{4\epsilon A^3}{15}\left[\eta\left(A^2 - 5\kappa^2\right) + \left(A^2 + 5\kappa^2\right) - (\gamma + \lambda)\left(11A^2 + 5\kappa^2\right) + 4\delta A^2\right] \end{aligned} \tag{17}$$

$$\frac{d\kappa}{dt} = 0 \tag{18}$$

while the change in the soliton velocity is given by

$$v = -\kappa + \frac{\epsilon A^2}{6}\left(\xi + \nu\right) \tag{19}$$

The fixed point of the Dynamical System given by (17) and (18) is

$$\left(\bar{A}, \bar{\kappa}\right) = \left(\kappa_0 \sqrt{\frac{\eta - \beta + \gamma + \lambda}{\eta + \beta - 11(\gamma + \delta) + 4\delta}}, \kappa_0\right) \tag{20}$$

eherre κ_0 is the constant frequency. This fixed point is a node and therefore the solitons in α-helix proteins travel with a fixed amplitude and frequency that is given in (20) and the velocity of the soliton is given in (19).

2 CONCLUSIONS

In this paper, the adiabatic parameter dynamics of the solitons in α-helix proteins are studied in presence of the perturbation terms. The Dynamical System of thesolitons amplitude andthe frequency leads to a fixed point that is actually a node. Therefore the solitons travel with a fixed amplitude and freequency.

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References

[1] E. A. Bartnik, J. A. Tuszynski & D. Sept. "Effects of distance dependence of exciton hopping on the Davydov soliton". *Physics Letters A*. Volume 204, Issues 3-4, 263-268. (1995).

[2] S. Caspi, E. Ben-Jacob. "Conformation changes and folding of proteins mediated by Davydov solitons". *Physics Letters A*. Volume 272, Issues 1-2, 124-129. (2000).

[3] P. L. Christiansen, J. C. Eilbeck, V. Z. Enolskii & J. B. Gaididei. "On ultrasonic Davydov solitons and the Henon-Heiles system". *Physics Letters A*. Volume 166, Issue 2, 129-134. (1992).

[4] M. Daniel & K. Deepmala. "Davydov soliton in alpha helical proteins: higher order and discreteness effects". *Physica A*. Volume 221, Issues 1-3, 241-255. (1995).

[5] M. Daniel & M. M. Latha. "A generalized Davydov soliton model for energy transfer in alpha helical proteins". *Physica A*. Volume 298, Issues 3-4, 351-370. (2001).

[6] A. S. Davydov. *Solitons in Molecular Systems*. Kluwer Academic Publishers, Norwell, MA. USA. (1991).

[7] W. Forner. "Effects of temperature and interchain coupling on Davydov solitons". *Physica D*. Volume 68, Issue 1, 68-82. (1993).

[8] B. Tan & J. P. Boyd. "Davydov soliton collisions". *Physics Letters A*. Volume 240, Issue 6, 282-286. (1998).

[9] Y. Xiao. "One more reason why the Davydov soliton may be thermally stable". *Physics Letters A*. Volume 243, Issue 3, 174-177. (1998).

[10] S. Zekovic & Z. Ivic. "Damping and modification of the multiquanta Davydov-like solitons in molecular chains". *Bioelectrochemistry and Bioenergetics*. Volume 48, Issue 2, 297-300. (1999).

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