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Dynamics of Energy Distribution in Three Channel Alpha Helix Protein Based on Davydov's Ansatz

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Abstract. An important aspect of many biological processes at molecular level is the transfer and storage mechanism of bioenergy released in the reaction of the hydrolysis of Adenosinetriphosphate (ATP) by biomacromolecule especially protein. Model of Soliton Davydov is a new break-through that could describe that mechanism. Here we have reformulated quantum mechanical the Davydov theory, using least action principle. Dynamical aspect of the model is analyzed by numerical calculation. We found two dynamical cases: the traveling and pinning soliton that we suggest they are related to the energy transfer and storage mechanism in the protein. Traveling and pinning soliton can be controlled by strength of coupling. In 3- channel approach, we found the breather phenomena in which its frequency is determined by interchannel coupling parameter.

Keywords: Least Action Principle, Davydov Soliton, Protein
PACS: 87.15.A-

INTRODUCTION

One of biophysics study in molecular biology is about the function of macromolecule (Protein, DNA, RNA) in living cell. Several biological functions of biomacromolecule are not well understood if just look at chemical structure instead of their dynamical aspects. It was known not only chemical but also physical interaction have shared in determining the function of them. In their activity, biomacromolecule always include transferring and storing process of bioenergy resulted from hydrolysis of ATP (Adenosine Try-phosphate) like in active transport, protein folding, and DNA repairing. Study of an energy transfer model in molecular structure is required to understand such mechanisms in biomacromolecule functioning, and give an answer to next technology challenges, "nanotechnology", in which the technology must be able to transfer information in nanometer scale.

Almost two decades ago, Davydov promotes a model that can describe transferring and storing mechanism of bio-energy in protein. The model proposed by Davydov used solid state theory approach, i.e. exciton concept that was used earlier by Frankel and Landau [1]. In this model, Davydov claims that energy is transferred in protein in solitonic form. Bioenergy resulted from hydrolysis of ATP is

stored as vibration mode of covalent bond C=O. Direct experiment to prove the truth of this theory is still difficult, due to the complexity of protein structure, protein is not really periodic structure and protein is not a single crystal. But even, simple experiments on crystals acetanilida have provided results that verify the model of Davydov's theory.

Now, numerous theoretical and experimental studies of the Davydov's model of protein dynamics have been done. Study of the Davydov model can be classified into several focuses, such as quantum mechanics description of Davydov's soliton, soliton existence in α -helix, lifetime of Davydov's soliton in physiological temperature and confirmation of Davydov's model with experimental studies [5].

In this study, we re-formulated the quantum description of the model Davydov on α -helical protein using least action. Here we considered a protein as α -helical protein with three channels model and in the form of discrete systems as an improvement of one-channel and the continuum approach commonly performed on previous research. Then we study the energy distribution of the protein for various conditions.

DAVYDOV'S MODEL

Alpha-helix structure is the most stable conformation of the polypeptide. Alpha-helix structure formed by the three hydrogen bonds between peptide groups, so it appears that the alpha-helix structure has 3 channels as shown in Figure 1. Alpha-helix structure is right-handed, spinning counter-clockwise, and in one full turn there are 3.6 amino acids. The energy required for the formation of hydrogen bonds between the peptide in the order of 0.21 eV. Nitrogen-peptide works as a hydrogen donor, and the carbonyl-oxygen as hydrogen acceptor. This hydrogen bond has a range optimal for 4.5 Å [1,5].

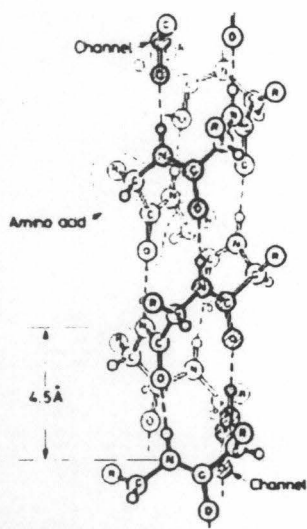


FIGURE 1. Alpha-helix protein structure [5].

In the models, Davydov used solid state approach. This approach was taken based on the existence of periodic structures in biological molecules, especially proteins. In describing the energy transfer in protein structure, the concept of electrons in molecular crystals is often adopted, in this case using the concept of exciton. Exciton concept first introduced by Frenkel (1931) to explain the conversion of light into heat in solids. The energy transfer model proposed by Davydov states that the bio-energy is stored as vibrational energy of the amide-I mode (C = O stretching). This idea departs from the fact that the energy generated from ATP hydrolysis is about 0.42 eV is twice of the quanta energy of vibration C = O, where one quanta of vibrational energy of C = O is about 0,205 eV, this is illustrated in Figure 2. Amide-I vibrational mode are coupled by lattice phonons. Interaction of internal vibrations of C = O as high frequency oscillators (exciton), with lattice vibrations

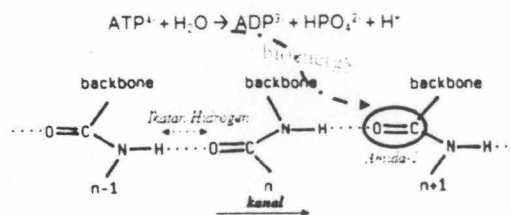


FIGURE 2. Davydov's Model Illustration.

as low frequency oscillators (phonons), and through the nonlinear coupling yield the amide-I vibrational energy that is localized to the helical structures and resist to the dispersion, the phenomenon is commonly referred to as self-localization or self-trapping. Thus the exciton can be viewed as soliton that propagate along the molecular chain [1,2,5].

Hamiltonian of The System

Hamiltonian of the Davydov protein model consists of three components namely exciton, phonon, and interaction term as shown below:

$$\hat{H} = \hat{H}_{ex} + \hat{H}_{ph} + \hat{H}_{int} \quad (1)$$

Excitons energy operator is defined as:

$$\hat{H}_{ex} = \sum_{n,\alpha} [E_0 \hat{B}_{n,\alpha}^\dagger \hat{B}_{n,\alpha} - J (\hat{B}_{n,\alpha}^\dagger \hat{B}_{n+1,\alpha} + \hat{B}_{n,\alpha}^\dagger \hat{B}_{n-1,\alpha}) + L (\hat{B}_{n,\alpha}^\dagger \hat{B}_{n,\alpha+1} + \hat{B}_{n,\alpha}^\dagger \hat{B}_{n,\alpha-1})] \quad (2)$$

where the index n indicates the group of peptides or amino acids (unit or site) in a channel of protein, while the index α indicates a specific channel. $\hat{B}_{n\alpha}^\dagger$ dan $\hat{B}_{n\alpha}$ are the creation and annihilation boson operators for the amide-I oscillators, respectively. E_0 is the energy of exciton, J is the dipole coupling between the nearest unit in one channel, and L states dipole coupling between the nearest units on a different channel. $\hat{B}_{n\alpha}^\dagger \hat{B}_{n\alpha}$ is the number operator that will calculate the amount of excitation in each unit, $\hat{B}_{n\alpha}^\dagger \hat{B}_{n\pm 1,\alpha}$ suggesting the transfer of exciton from peptide - n to $n \pm 1$ and $\hat{B}_{n\alpha}^\dagger \hat{B}_{n,\alpha\pm 1}$ states the transfer of exciton from channel α to $\alpha \pm 1$.

The phonon energy operator is expressed as:

$$\hat{H}_{ph} = \frac{1}{2} \sum_{n,\alpha} \left[\frac{\hat{p}_{n,\alpha}^2}{M} + w(\hat{u}_{n,\alpha} - \hat{u}_{n-1,\alpha})^2 \right] \quad (3)$$

with $\hat{p}_{n\alpha}$ and $\hat{u}_{n\alpha}$ is operator of momentum and position, respectively, M is mass of amino acid and w is spring constant of hydrogen bond.

The last, the interaction energy operator is defined by:

$$\hat{H}_{int} = \sum_{n,\alpha} \chi (\hat{u}_{n+1,\alpha} - \hat{u}_{n-1,\alpha}) \hat{B}'_{n,\alpha} \hat{B}_{n,\alpha} \quad (4)$$

where χ is coupling parameter eksiton-phonon, that define the strength of nonlinearity.

In second quantization form, the Hamiltonian above can be represented as shown below:

$$\begin{aligned} \hat{H}_{ex} &= \sum_{n,\alpha} [E_0 \hat{B}'_{n,\alpha} \hat{B}_{n,\alpha} - J(\hat{B}'_{n,\alpha} \hat{B}_{n+1,\alpha} + \hat{B}'_{n,\alpha} \hat{B}_{n-1,\alpha}) + \\ &\quad L(\hat{B}'_{n,\alpha} \hat{B}_{n,\alpha+1} + \hat{B}'_{n,\alpha} \hat{B}_{n,\alpha-1})] \\ \hat{H}_{ph} &= \sum_{\alpha,k} \hbar \omega_{\alpha,k} \left[\hat{b}_k^\dagger \hat{b}_k + \frac{1}{2} \right], \\ \hat{H}_{int} &= \sum_{n,\alpha,k} B_{n,\alpha,k} (\hat{b}_k + \hat{b}_k^\dagger) \hat{B}'_{n,\alpha} \hat{B}_{n,\alpha}, \end{aligned} \quad (5)$$

Davydov's Ansatz

Davydov's trial wave function (ansatz) chosen for the protein model is the multiplication of two wave functions namely exciton and phonon (wave function of phonon represent as coherent state of harmonics oscillator) [2,3].

$$|D\rangle = |\psi\rangle_{ex} |\varphi\rangle_{ph}$$

$$\text{With } |\psi\rangle_{ex} = \sum_{n,\alpha} A_{n,\alpha}(t) \hat{B}'_{n,\alpha} |0\rangle_{ex},$$

$$|\varphi\rangle_{ph} = \hat{U}_{na} |0\rangle_{ph} = \exp \left[\sum_{n,\alpha,k} (b_{n,\alpha,k}(t) \hat{b}_k^\dagger - b_{n,\alpha,k}^*(t) \hat{b}_k) \right] |0\rangle_{ph}$$

and the ansatz chosen has the form:

$$|D\rangle = \sum_{n,\alpha} A_{n,\alpha}(t) \hat{U}_{n,\alpha} \hat{B}'_{n,\alpha} |0\rangle_{ex,ph} \quad (6)$$

EQUATION OF MOTION

The equations of motion of Davydov's model can be obtained by using Euler-Lagrange equation below

with regard to the chosen ansatz satisfy the Schrödinger equation.

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\phi}_j} \right) - \frac{\partial L}{\partial \phi_j} = 0 \quad (7)$$

Lagrangian for Schrodinger equation can be obtained by using least action principle, so that we get the Lagrangian in Hamiltonian average representation for the Schrodinger equation:

$$L = \left\langle D \left| \frac{i\hbar}{2} \frac{\partial}{\partial t} \right| D \right\rangle - \langle D | H | D \rangle \quad (8)$$

With $|D\rangle = \sum_j \phi_j D_j$, we get:

$$\begin{aligned} \left[\frac{d}{dt} \frac{\partial}{\partial \dot{\phi}_j} - \frac{\partial}{\partial \phi_j} \right] \left\langle D \left| \frac{i\hbar}{2} \frac{\partial}{\partial t} \right| D \right\rangle = \\ - \frac{\partial \langle D | H | D \rangle}{\partial \phi_j} \end{aligned} \quad (9)$$

By substituting the Davydov's ansatz (6) into Euler-Lagrange equation (9), with $A_{n,\alpha}$ and $b_{n,\alpha,k}$ as ϕ_j , we obtain two equation of motion that describe the dynamics of exciton (10) and phonon (11), respectively.

$$\begin{aligned} i\hbar \dot{A}_{n,\alpha}(t) + \\ \frac{i\hbar}{2} \sum_k A_{n,\alpha}(t) (b_{n,\alpha,k}^\dagger(t) b_{n,\alpha,k}^*(t) - b_{n,\alpha,k}(t) b_{n,\alpha,k}^\dagger(t)) = \\ \frac{\partial \langle H \rangle}{\partial A_{n,\alpha}^*(t)} \end{aligned} \quad (10)$$

and

$$\begin{aligned} i\hbar \sum_{n,\alpha} |A_{n,\alpha}(t)|^2 (b_{n,\alpha,k}^\dagger) = \\ - \frac{i\hbar}{2} \sum_{n,\alpha} (b_{n,\alpha,k}^\dagger(t) A_{n,\alpha}(t) - A_{n,\alpha}^*(t) b_{n,\alpha,k}(t)) b_{n,\alpha,k} + \frac{\partial \langle H \rangle}{\partial b_{n,\alpha,k}^*(t)} \end{aligned} \quad (11)$$

By resolving last term on the right side of both equation (10,11) we get nonlinear equation of exciton and phonon

$$i\hbar \dot{A}_{n,\alpha}(t) = E_0 A_{n,\alpha}(t) - \frac{i\hbar}{2} \sum_l A_{n,\alpha}(t) (b_{n,\alpha}^*(t) b_{n,\alpha}^*(t) - b_{n,\alpha}(t) b_{n,\alpha}(t)) - J(A_{n-1,\alpha}(t) \tilde{U}_{n,n-1} + A_{n+1,\alpha}(t) \tilde{U}_{n,n+1}) + L(A_{n,\alpha+1}(t) \tilde{U}_{n,\alpha,n+1} + A_{n,\alpha-1}(t) \tilde{U}_{n,\alpha,n-1}) + \sum_l A_n(t) \hbar \omega_{\text{cvt}} \left[b_{n,\alpha}^*(t) b_{n,\alpha}(t) + \frac{1}{2} \right] + \sum_l B_{n,\alpha}(t) (b_{n,\alpha}(t) + b_{n,\alpha}^*(t)) A_n(t)$$

and

$$i\hbar \dot{b}_{n,\alpha}(t) = J \left[\frac{A_{n+1,\alpha}(t)}{A_n(t)} (b_{n+1,\alpha}(t) - b_{n,\alpha}(t)) \tilde{U}_{n,n+1} + \frac{A_{n-1,\alpha}(t)}{A_n(t)} (b_{n-1,\alpha}(t) - b_{n,\alpha}(t)) \tilde{U}_{n,n-1} \right] + L \left[\frac{A_{n,\alpha+1}(t)}{A_{n,\alpha}(t)} (b_{n,\alpha+1}(t) - b_{n,\alpha}(t)) \tilde{U}_{n,\alpha,n+1} + \frac{A_{n,\alpha-1}(t)}{A_{n,\alpha}(t)} (b_{n,\alpha-1}(t) - b_{n,\alpha}(t)) \tilde{U}_{n,\alpha,n-1} \right] + \hbar \omega_{\text{cvt}} b_{n,\alpha}(t) + B_{n,\alpha}$$

with $B_{n,\alpha} = -2i\chi \left(\frac{\hbar}{2Nm\omega_{\text{cvt}}} \right)^{1/2} \sin(kl) e^{-i\omega_{\text{cvt}} t}$ and

$$\omega_{\text{cvt}} = 2 \left(\frac{W}{m} \right)^{1/2} |\sin kl / 2|$$

RESULT AND DISCUSSION

Energy distribution on Davydov's model based on equation (12) and (13) is evaluated numerically using Runge-Kutta method. Several parameter on the equation are given by the following table:

TABLE 1. Parameters value of alpha-helix protein [3,5]

| Parameter | Description | Value | Unit |
|-----------|---|------------------------|------|
| W | Spring constant of Hydrogen bond | 13-40 | N/m |
| M | Mass of amino acid | 1.9×10^{-25} | Kg |
| J | Dipole-dipole coupling between site in a channel | 1.55×10^{-22} | J |
| χ | Exciton-phonon coupling | 20-60 | pN |
| l | Lattice Constant | 4.5×10^{-10} | m |
| L | Dipole-dipole coupling between site inter channel | 2.46×10^{-22} | J |

In the simulation of energy distribution in a protein channel, we found two cases, namely traveling soliton and pinning soliton. Traveling and pinning cases can be control by strength of exciton-phonon coupling (χ). When χ is small enough or weak coupling i.e $\chi=40$ pN, the energy move site to site along protein chain but dispersed as shown at Figure 3. With increasing χ i.e

$\chi=50$ pN, the dispersed energy will be reduced as shown at Figure 4. But when χ is big enough or strong coupling i.e $\chi=150$ pN, the energy going to be trapped on a site, like as Figure 5.

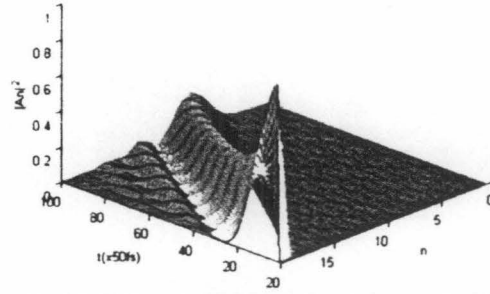


FIGURE 3. Energy distribution in a protein channel with $\chi=40$ pN.

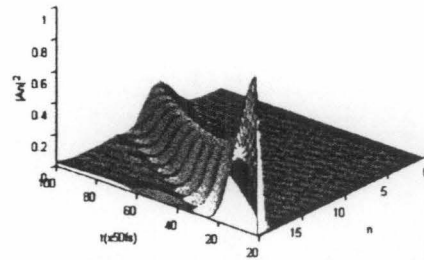


FIGURE 4. Energy distribution in a protein channel with $\chi=50$ pN.

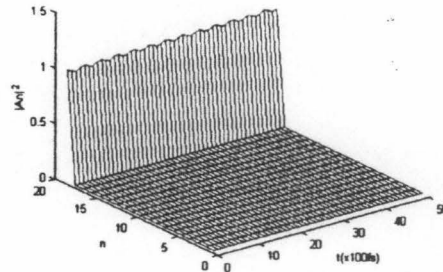


FIGURE 5. Energy distribution in a protein channel with $\chi=150$ pN.

In three channel view, we found breather phenomena, that is figure how energy move from site to site through different channel. Figure 6 and Figure 7 describes how the energy oscillates with a specific frequency from site to site across the channel. The frequency of oscillation depend on the strength of inter channel dipole-dipole coupling parameter (L).

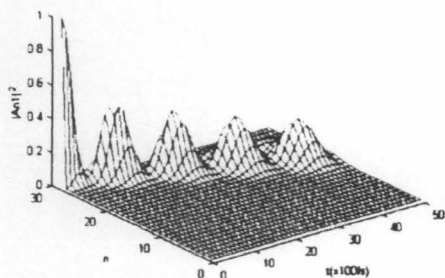


FIGURE 6. Energy breather in three channel protein with $L=2.4e-22$ J.

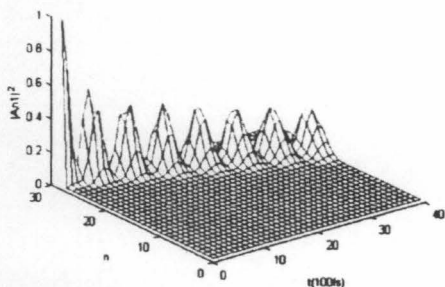


FIGURE 7. Energy breather in three channel protein with $L=4.8e-22$ J.

From the simulation result, we found at least three feature that is traveling, pinning, and breather energy. What is the correlation of them to the functioning of protein? It is a question arise. We suggest that traveling and pinning energy related to mechanism of transferring dan storing energy in protein that can be controlled by the strength of exciton-phonon coupling (χ). With inter channel coupling (L), energy can move site to site through different channel, without it energy just move through single channel. The greater inter channel coupling (L), the greater frequency of inter channel energy switching ($f \sim L$). But, how the influence of the frequency to the efficiency of energy transfer in relation to the length of protein chains need further review.

CONCLUSION

Davydov model can be derived quantum mechanically use least action principle. Based on the model we found that the energy is transferred in protein chain in solitonic form. By adjusting the physical parameter of protein we can control portion or balancing of dispersion and nonlinearity degree, so that we get traveling soliton and pinning soliton case. In three channel approach, breathers of energy between channels appear, in which the frequency of breather depend on the physical of protein also. We

suggest that traveling, pinning, and breather of energy of protein have correlation to the functioning of protein such as energy transfer, storage, and efficiency.

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