Inter-channel Interaction and Damping Effect on the Dynamics of Energy Transport in Protein

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Abstract. The mechanism of energy transport in alpha-helical protein was modeled by Davydov and Scott. The inter-channel interaction between the three channels of alpha-helical protein and damping effect on the probability amplitude of amide-I energy is investigated in this paper. The study results a set of three coupled non-linear Schrödinger equation. The resulting coupled NLS is analyzed by Hirota bilinear method. The results show that the inter-channel interaction result in the greater amplitude. Meanwhile the damping term has no contribution to the change of soliton amplitude, but it make the soliton propagation slower.

1. Introduction

In biophysicist view, live activity is merely the processes of change, coordination, and incorporation of biomaterial, bioenergy, and bio-information [1]. Meanwhile bioenergy transport is a basic mechanism for live activity, because it is related to many biological activities [2]. The energy required for the live activity mainly provided by the energy released from hydrolysis reaction of Adenosin Triphosphate (ATP).

The mechanism of energy transport in living system for the first time was modeled by Davydov in 1973. Davydov proposed the mechanism by exploiting the regularity of alpha-helical protein structure. In Davydov’s model, the energy released from hydrolysis process is stored in vibrational mode of the peptide group which consists of the C=O stretching known as amide-I. The amide-I vibration then interact with the molecular vibration of phonon from amino-acid. This interaction results exciton excitation on amide-I and molecular deformation on amino-acid. The Excitation and the deformation balance each other and result pulse-like wave called as soliton [3].

The Davydov model of energy transport in alpha-helical protein has become an interesting study for the researchers. Since pioneering by Davydov, many studies relating dynamical properties of Davydov solitons and their formation with various initial condition was investigated in discrete chain and continuum model analytically and numerically. However most of these results have been obtained for an isolated single channel alpha-helical protein. In fact, there are three channels of alpha-helical protein, which interactions between the three of them are possible to happen. The interaction between them was written by adding inter-channel dipole-dipole interaction term [4]. Recent studies about inter-channel interaction were conducted by Veni and Latha. Inter-channel interaction was broken down by them to be several interactions, such as exciton phonon coupling in radial direction and two nearest neighbor interaction. By adding all of those interactions, a set of non-linear Schrodinger (CLNS) equations was obtained. Solving CLNS equations, Veni and Latha got the energy density profile propagated in the
three channels [5]. Moreover in 2014, Veni and Latha added several terms such as: inter-channel exciton-phonon coupling and radial nearest neighbor exciton-phonon coupling. Using tanh method, it resulted dark soliton solution for the difference of energy density propagated in the three channels.

Beside the study relating molecular excitation and its interactions. The Davydov model study of energy transport also concerns about effect of the environment to the soliton propagated in alpha-helical protein channels. Lomdahl and Kerr revealed that there is life time for soliton propagated in the channels, caused by the medium dissipation in a certain temperature \(T \neq 0\). Effect of the environment dissipation was modeled by adding a damping term \((k \frac{\partial u}{\partial t})\) and a stochastic term \((\eta_n(t))\) on the peptide group equation of motion [6]. The result showed that a soliton present in the initial state disappears in a few picoseconds [7]. Sulaiman investigated the thermal and damping effect by contacting Davydov-Scott monomer with thermal bath using open quantum system formalism [8]. The result was found that the environmental effects contribute destructively to the specific heat of the monomer [9]. Sulaiman another study, treat the probability amplitude of amide-I classically, and added a damping \((\gamma \partial a_n / \partial t)\) term and a periodic external force term on the NLS equation resulted. The result showed that Davydov's soliton is accelerated due to external periodic force. Moreover Sulaiman and Mesquita added a loss effect term \((iy\phi)\) on the NLS equation, then the study showed that instead of contribute to soliton amplitude, the effect influence to soliton propagation velocity [2, 10].

Both molecular excitation interaction and medium effect on the soliton are often to be study problems for the researchers relating to Davydov model topic. Therefore this study aims to investigate how the medium affect to the energy transport in alpha-helical protein where inter-channel interactions are taken into account.

2. The Model

Based on Davydov model, the mechanism of energy transport in alpha-helical protein involve amide-I vibration, phonon molecular vibration, and the interactions between them. The original Davydov model was described in Davydov's Hamiltonian including the three parts above [11]. However the interactions part studied in this paper covers inter-channel interaction and nearest neighbor interaction. Amide-I vibration is described by the exciton hamiltonian

\[
H_{ex} = \sum_{n,\alpha} \{E_0 B_{n,\alpha}^\dagger B_{n,\alpha} - J (B_{n,\alpha}^\dagger B_{n+1,\alpha} + B_{n,\alpha}^\dagger B_{n-1,\alpha}) + L (B_{n,\alpha}^\dagger B_{n,\alpha+1} + B_{n,\alpha}^\dagger B_{n,\alpha-1}) \}. \tag{1}
\]

The first term expresses exciton excitation with the energy \(E_0\). Second term describes dipole-dipole interaction between two nearest amide-I on the same channel involving the energy \(-J\). The last term states dipole-dipole interaction between the nearest amide-I on the difference channel, involving the energy \(L\). The vibration of peptide group in the longitudinal and radial direction is stated in this hamiltonian

\[
H_p = \sum_{n,\alpha} \left\{ \frac{p_{n,\alpha}^2}{2m} + \frac{1}{2} k (u_{n+1,\alpha} - u_{n-1,\alpha})^2 + \frac{s_{n,\alpha}^2}{2m} + \frac{1}{2} k (v_{n+1,\alpha} - v_{n-1,\alpha})^2 \right\}. \tag{2}
\]

where \(u_n\) and \(v_n\) consecutively are the longitudinal and radial displacement operator. The interaction between amide-I in the three channels and the vibration of peptide group is accommodated by the hamiltonian

\[
H_{int1} = \sum_{n,\alpha} (\chi_1 B_{n,\alpha}^\dagger B_{n,\alpha} + \chi_2 B_{n,\alpha+1}^\dagger B_{n,\alpha+1} + \chi_3 B_{n,\alpha-1}^\dagger B_{n,\alpha-1})(u_{n+1,\alpha} - u_{n-1,\alpha}). \tag{3}
\]

The interaction of two nearest phonon before and after an amide-I in the same channel is governed by the hamiltonian
The equation of motion of vibrational amino acid in radial direction is given by

$$H_{int2} = \sum_{n,\alpha} \{ \chi_4 B^+_{n,\alpha} B_{n+1,\alpha} (u_{n+2,\alpha} - u_{n,\alpha}) + \chi_5 B^+_{n,\alpha} B_{n-1,\alpha} (u_{n,\alpha} - u_{n-2,\alpha}) \}. \quad (4)$$

Meanwhile the similar interaction, but from the other channels phonon is written by the hamiltonian

$$H_{int3} = \sum_{n,\alpha} \left\{ [\chi_6 B^+_{n,\alpha+1} B_{n+1,\alpha+1} + \chi_7 B^+_{n,\alpha-1} B_{n+1,\alpha-1}](u_{n+2,\alpha} - u_{n,\alpha}) \\
+ [\chi_8 B^+_{n,\alpha+1} B_{n-1,\alpha+1} + \chi_9 B^+_{n,\alpha-1} B_{n-1,\alpha-1}](u_{n,\alpha} - u_{n-2,\alpha}) \right\}. \quad (5)$$

The interaction between the helical diameter stretching and the amide-I is stated by

$$H_{int4} = \sum_{n,\alpha} \{ \eta_1 B^+_{n,\alpha} B_{n-1,\alpha} + \eta_2 (B^+_{n,\alpha} B_{n+1,\alpha} - B^+_{n,\alpha} B_{n+1,\alpha}) (v_{n+1,\alpha} - 2v_{n,\alpha} + v_{n-1,\alpha}) \} \quad (6)$$

The statevector of exciton is stated by

$$|\psi\rangle = \Sigma_{n,\alpha} a_{n,\alpha} (t) B^+_{n,\alpha} |0\rangle, \text{ where } \langle \psi | \psi \rangle = 1. \quad (7)$$

Using Schrodinger equation and Ehrenferst theorem, then we can obtain the equation of motion for amide-I vibration, longitudinal vibration and radial vibration of amino-acid. The equation of motion for amide-I can be written as below

$$i \hbar \dot{a}_{n,\alpha} = E_0 a_{n,\alpha} - J (a_{n+1,\alpha} + a_{n-1,\alpha}) + L (a_{n,\alpha+1} + a_{n,\alpha-1}) + a_{n,\alpha} \left[ \chi_1 (b_{n+1,\alpha} - b_{n-1,\alpha}) + \chi_2 (b_{n+1,\alpha-1} - b_{n-1,\alpha-1}) + \chi_3 (b_{n+1,\alpha+1} - b_{n-1,\alpha+1}) \right] + a_{n+1,\alpha} \chi_4 (b_{n+2,\alpha} - b_{n,\alpha}) + \chi_5 (b_{n+2,\alpha-1} - b_{n,\alpha-1}) + \chi_6 (b_{n+2,\alpha+1} - b_{n,\alpha+1}) + \chi_7 (b_{n+2,\alpha-1} - b_{n,\alpha-1}) \right] + a_{n-1,\alpha} \chi_8 (b_{n,\alpha} - b_{n-2,\alpha}) - \chi_9 (b_{n,\alpha+1} - b_{n-2,\alpha+1}) + \eta_1 a_{n,\alpha} + \eta_2 (a_{n,\alpha+1} - a_{n,\alpha-1}) \} (c_{n,\alpha+1} - 2c_{n,\alpha} + c_{n,\alpha-1}) \} \quad (8)$$

Meanwhile the equation of motion for longitudinal vibration of amino-acid can be stated as

$$m \ddot{b}_{n,\alpha} (t) = k \left[ (b_{n+1,\alpha} - 2b_{n,\alpha} + b_{n-1,\alpha}) + \chi_1 \left( |a_{n+1,\alpha}|^2 - |a_{n-1,\alpha}|^2 \right) + \chi_2 \left( |a_{n+1,\alpha+1}|^2 - |a_{n-1,\alpha+1}|^2 \right) + \chi_3 \left( |a_{n+1,\alpha-1}|^2 - |a_{n-1,\alpha-1}|^2 \right) + \chi_4 (a_{n,\alpha} a_{n+1,\alpha} - a_{n-2,\alpha} a_{n-1,\alpha}) + \chi_5 (a_{n,\alpha+1} a_{n+2,\alpha} - a_{n,\alpha-1} a_{n-2,\alpha+1}) + \chi_6 (a_{n,\alpha} a_{n+1,\alpha+1} - a_{n,\alpha-1} a_{n+1,\alpha-1}) + \chi_7 (a_{n,\alpha+1} a_{n+1,\alpha} - a_{n,\alpha-1} a_{n+1,\alpha-1}) + \chi_8 (a_{n,\alpha} a_{n+2,\alpha+1} - a_{n,\alpha-1} a_{n+2,\alpha-1}) + \chi_9 (a_{n,\alpha} a_{n+2,\alpha} - a_{n,\alpha-1} a_{n+2,\alpha-1}) + \eta_1 a_{n,\alpha} + \eta_2 (a_{n,\alpha+1} - a_{n,\alpha-1}) \} (c_{n,\alpha+1} - 2c_{n,\alpha} + c_{n,\alpha-1}) \} \quad (9)$$

The equation of motion of vibrational amino acid in radial direction is given by

$$m \ddot{c}_{n,\alpha} (t) = \eta_1 \left( c_{n-1,\alpha} - 2c_{n,\alpha} + c_{n+1,\alpha} \right) + \eta_2 \left( |a_{n,\alpha+1}|^2 - 2|a_{n,\alpha}|^2 + |a_{n,\alpha-1}|^2 \right) - \eta_2 (a_{n,\alpha+1} (a_{n+1,\alpha+1} - a_{n-1,\alpha+1}) + a_{n,\alpha-1} (a_{n+1,\alpha-1} - a_{n-1,\alpha-1}) - 2a_{n,\alpha} (a_{n,\alpha+1} - a_{n-1,\alpha})). \quad (10)$$

Assuming the amplitude of lateral displacement in radial direction is slow, then it can be written

$$\dot{c}_{n,\alpha} (t) = \frac{1}{\sigma^2} (c_{n-1,\alpha} - 2c_{n,\alpha} + c_{n+1,\alpha}), \quad (11)$$

where $\sigma$ is a parameter representing small change in $t$ [13]. Using 11, then equation 10 becomes:
\[
\begin{align*}
c_{n-1,\alpha} - 2c_{n,\alpha} + c_{n+1,\alpha} &= A_1 \eta_1 \left( |a_{n,\alpha+1}|^2 - 2|a_{n,\alpha}|^2 + |a_{n,\alpha-1}|^2 \right) + A_1 \eta_2 \left[ a_{n,\alpha+1}^* (a_{n+1,\alpha+1} - a_{n-1,\alpha+1}) + a_{n,\alpha-1}^* (a_{n+1,\alpha-1} - a_{n-1,\alpha-1}) - 2a_{n,\alpha}^* (a_{n,\alpha+1} - a_{n,\alpha-1}) \right] \\
&= \frac{\sigma^2}{\sigma^2_{1-m}}. 
\end{align*}
\]

Making continuum approximation for \( a_{n+1,\alpha} \) and \( b_{n+1,\alpha} \), defining \( \delta_0 = E_0 - 2J \),

\[
y_\alpha = -\varepsilon B_{ax}, \delta_1 = \chi_1 + \chi_4 + \chi_5, \delta_2 = \chi_2 + \chi_6 + \chi_8, \delta_3 = \chi_3 + \chi_7 + \chi_9, \delta_4 = \chi_4 - \chi_5, \delta_5 = \chi_6 - \chi_8, \quad \text{and} \quad \delta_6 = \chi_7 - \chi_9,
\]

and ignoring the \( \varepsilon^2 \) terms beside for the term with \( a_{ax,xx} \), then it can be obtained

\[
iha_{\alpha,t} = \delta_0 a_{\alpha} - J e^2 a_{\alpha,xx} + L (a_{\alpha+1} + a_{\alpha-1}) + A_1 \eta_1^2 \left( |a_{n,\alpha+1}|^2 - 2|a_{n,\alpha}|^2 + |a_{n,\alpha-1}|^2 \right) \\
- 2a_{\alpha} \left( \delta_1 y_{\alpha} + \delta_2 y_{\alpha-1} + \delta_3 y_{\alpha+1} \right) + 2\varepsilon A_1 \eta_1 \eta_2 \left( a_{\alpha} (a_{\alpha+1} a_{\alpha+1,x} + a_{\alpha-1} a_{\alpha-1,x} - 2a_{\alpha}^* a_{\alpha,x}) \right) \\
+ a_{\alpha,x} \left( |a_{n,\alpha+1}|^2 - 2|a_{n,\alpha}|^2 + |a_{n,\alpha-1}|^2 \right).
\]

Substituting continuum approximation for \( a_{n+1,\alpha} \) and \( b_{n+1,\alpha} \) to equation 9, it leads to

\[
m b_{\alpha,tt} = \frac{\partial}{\partial x} \left\{ 2 \varepsilon \left( \delta_1 |a_{\alpha}|^2 + \delta_2 |a_{\alpha+1}|^2 + \delta_3 |a_{\alpha-1}|^2 \right) \\
+ 2\varepsilon \left( \frac{k}{2} b_{\alpha,xx} - \delta_4 a_{\alpha}^* a_{\alpha} - \delta_5 a_{\alpha+1,x} a_{\alpha+1} - \delta_6 a_{\alpha-1,x} a_{\alpha-1} \right) \right\}.
\]

Multiplying \(-\varepsilon \frac{\partial}{\partial x}\) to equation 14, and using moving frame \((\xi = x - v_1 t)\) then it can be obtained:

\[
\left( k - \frac{mv^2}{2} \right) y_{\alpha,\xi}^2 \\
= \frac{\partial^2}{\partial \xi^2} \left\{ 2 \left( \delta_1 |a_{\alpha}|^2 + \delta_2 |a_{\alpha+1}|^2 + \delta_3 |a_{\alpha-1}|^2 - \frac{k}{2} b_{\alpha,xx} \right) \\
- 2\varepsilon \left( \delta_4 a_{\alpha}^* a_{\alpha} + \delta_5 a_{\alpha+1,x} a_{\alpha+1} + \delta_6 a_{\alpha-1,x} a_{\alpha-1} \right) \right\}.
\]

Defining \( v_0 = \varepsilon \sqrt{\frac{k}{m}} \beta = \frac{1}{k(1-s^2)} \), then 15 can be written as

\[
y_{\alpha} = \beta \left\{ 2 \left( \delta_1 |a_{\alpha}|^2 + \delta_2 |a_{\alpha+1}|^2 + \delta_3 |a_{\alpha-1}|^2 - \frac{k}{2} b_{\alpha,xx} \right) \\
- 2\varepsilon \left( \delta_4 a_{\alpha}^* a_{\alpha} + \delta_5 a_{\alpha+1,x} a_{\alpha+1} + \delta_6 a_{\alpha-1,x} a_{\alpha-1} \right) \right\}.
\]

Substituting the equation above to equation 13, then it can be obtained non-linear Schrodinger equation containing \( a_{\alpha}, a_{\alpha+1}, \text{and} a_{\alpha-1} \) which are coupled each other (CNLS). The CNLS is written as

\[
iha_{\alpha,t} = \delta_0 a_{\alpha} + L (a_{\alpha+1} + a_{\alpha-1}) - \beta_0 a_{\alpha,x} - (\beta_1 |a_{\alpha}|^2 + \beta_2 |a_{\alpha+1}|^2 + \beta_2 |a_{\alpha-1}|^2) a_{\alpha} \\
- (\beta_3 |a_{\alpha}|^2 + \beta_4 |a_{\alpha+1}|^2 + \beta_4 |a_{\alpha-1}|^2) a_{\alpha,xx} \\
- (\beta_5 a_{\alpha}^* a_{\alpha} + \beta_6 a_{\alpha+1,x} a_{\alpha+1} + \beta_7 a_{\alpha-1,x} a_{\alpha-1}) a_{\alpha} \\
- (\beta_3 a_{\alpha}^* a_{\alpha} + \beta_4 a_{\alpha+1,x} a_{\alpha+1} + \beta_4 a_{\alpha-1,x} a_{\alpha-1}) a_{\alpha}.
\]

where we already defined new constants: \( \beta_0 = J e^2, \beta_1 = 2(2\beta (\delta_2^2 + \delta_5^2 + \delta_7^2) + A_1 \eta_1^2), \beta_2 = 4\beta (\delta_1 \delta_2 + \delta_2 \delta_3 + \delta_3 \delta_4) - A_1 \eta_1^2, \beta_3 = 4\beta A_1 \eta_1 \eta_2, \beta_4 = -2\varepsilon \eta_1 \eta_2, \beta_5 = 4\beta (\delta_1 \delta_4 + \delta_2 \delta_5 + \delta_3 \delta_6), \beta_6 = 4\beta (\delta_1 \delta_5 + \delta_2 \delta_6 + \delta_3 \delta_4), \text{and} \beta_7 = 4\beta (\delta_1 \delta_6 + \delta_2 \delta_4 + \delta_3 \delta_5). \]
Using transformation for $t \rightarrow T = \frac{1}{\hbar} t$, and $a_\alpha \rightarrow \zeta_\alpha = a_\alpha e^{-\frac{i}{\hbar} \delta_0 a_\alpha}$, then the equation above can be rewritten as:

$$
i \zeta_{\alpha,T} - L(\zeta_{\alpha+1} + \zeta_{\alpha-1}) + \beta_0 \zeta_{\alpha,XX} + (\beta_1 |\zeta_\alpha|^2 + \beta_2 |\zeta_{\alpha+1}|^2 + \beta_2 |\zeta_{\alpha-1}|^2) \zeta_\alpha + (\beta_3 |\zeta_\alpha|^2 + \beta_4 |\zeta_{\alpha+1}|^2 + \beta_4 |\zeta_{\alpha-1}|^2) \zeta_{XX}$$

$$+ (\beta_5 \zeta_{\alpha,X} \zeta_\alpha + \beta_6 \zeta_{\alpha+1,X} \zeta_{\alpha+1} + \beta_7 \zeta_{\alpha-1,X} \zeta_{\alpha-1}) \zeta_\alpha$$

$$- (\beta_3 \zeta_\alpha \zeta_{XX} + \beta_4 \zeta_{\alpha+1,X} \zeta_{\alpha+1} + \beta_4 \zeta_{\alpha-1,X} \zeta_{\alpha-1}) \zeta_\alpha + i \gamma \zeta_\alpha = 0. \quad (18)$$

### 3. Hirota Bilinear Method

The solution of CNLS equations is obtained by using Hirota bilinear method. This method requires a non-linear equation to be transformed into a bilinear equation. Therefore the CNLS equations above are transformed into bilinear equations with these transformations [16]:

$$\zeta_1(x,T) = \frac{g_1(x,T)}{f(x,T)}, \quad \zeta_2(x,T) = \frac{g_2(x,T)}{f(x,T)}, \quad \zeta_3(x,T) = \frac{g_3(x,T)}{f(x,T)},$$

where $g_1(x,T), g_2(x,T), \text{ and } g_3(x,T)$ are complex functions while $f(x,T)$ is a real function.

Substituting the transformations above to equation 18, then it can be obtained

$$f [(D_T + \beta_0 D_X^2 + i \gamma)(g_{\alpha,f}) - L(g_{\alpha+1,f} + g_{\alpha-1,f})] - g_\alpha \beta_0 D_X^2 (f,f) - (\beta_1 |g_\alpha|^2 + \beta_2 |g_{\alpha+1}|^2 + \beta_2 |g_{\alpha-1}|^2) +$$

$$\{\beta_5 (D_X g_{\alpha,f}) g_{\alpha} + \beta_6 (D_X (g_{\alpha+1,f})) \ast g_{\alpha+1} + \beta_7 (D_X (g_{\alpha-1,f})) \ast g_{\alpha-1}\} g_{\alpha} +$$

$$\{\beta_3 g_\alpha (D_X (g_{\alpha,f})) + \beta_4 g_{\alpha+1} (D_X (g_{\alpha+1,f})) + \beta_4 g_{\alpha-1} (D_X (g_{\alpha-1,f}))\} g_{\alpha} = 0, \quad (19)$$

where $D_x$ and $D_T$ are Hirota bilinear operators, which are defined as

$$D_X f^n (g_{\alpha,f}) (x,T) = \left( \frac{\partial}{\partial x} - \frac{\partial}{\partial x'} \right)^n \left( \frac{\partial}{\partial T} - \frac{\partial}{\partial T'} \right) g_{\alpha,f} (x,T). f(x',T) \bigg|_{x=x',T=T}.$$

The equation 19 above can be separated into three equations. These equations are

$$(iD_T + \beta_0 D_X^2 + i \gamma)(g_{\alpha,f}) = L(g_{\alpha+1,f}), \quad (20a)$$

$$\beta_0 D_X^2 (f,f) = (\beta_1 |g_\alpha|^2 + \beta_2 |g_{\alpha+1}|^2 + \beta_2 |g_{\alpha-1}|^2), \quad (20b)$$

$$D_X (g_{\alpha,f}) \beta_3 |g_\alpha|^2 + \beta_4 |g_{\alpha+1}|^2 + \beta_4 |g_{\alpha-1}|^2 + \beta_5 (D_X (g_{\alpha,f})) \ast g_{\alpha} +$$

$$\beta_6 (D_X (g_{\alpha+1,f})) \ast g_{\alpha+1} + \beta_7 (D_X (g_{\alpha-1,f})) \ast g_{\alpha-1} + \beta_3 g_{\alpha} (D_X (g_{\alpha,f})) +$$

$$\beta_4 g_{\alpha+1} (D_X (g_{\alpha+1,f})) + \beta_4 g_{\alpha-1} (D_X (g_{\alpha-1,f})) g_{\alpha} = 0. \quad (20c)$$

The one soliton solution of Hirota bilinear method is provided by Hirota perturbation for $g_\alpha$ and $f$ as below

$$g_{\alpha} = \chi g_{\alpha}^{(1)} \text{ and } f = 1 + \chi^2 f^{(2)}. \quad (21)$$

Using the perturbation above and substituting it into equation 19, then collecting all of the terms with same orders of $\chi$, we have

$$\chi^0: \beta_0 D_X^2 (1.1) = 0, \quad (22a)$$

$$\chi^1: (iD_T + \beta_0 D_X^2 + i \gamma)(g_{\alpha,f}) = L([g_{\alpha+1,f} + g_{\alpha-1,f}]), \quad (22b)$$

$$\chi^2: \beta_0 D_X^2 (f + f.1) = (\beta_1 |g_\alpha|^2 + \beta_2 |g_{\alpha+1}|^2 + \beta_2 |g_{\alpha-1}|^2), \quad (22c)$$

$$\chi^3: (iD_T + \beta_0 D_X^2 + i \gamma)(g_{\alpha,f}) = L([g_{\alpha+1,f} + g_{\alpha-1,f}]), \quad (22d)$$

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\[\begin{align*}
D_x(g_{\alpha+1})(\beta_2 g_a + \beta_4 |g_{\alpha+1}|^2 + \beta_4 |g_{\alpha-1}|^2) + \{\beta_5(D_x(g_{\alpha+1}))^* g_a + \\
\beta_5(D_x(g_{\alpha-1}))^* g_{\alpha-1}\}g_a + \{\beta_5(D_x(g_{\alpha+1}))^* g_{\alpha+1}\}g_{\alpha+1} + \\
+ \{\beta_5(D_x(g_{\alpha-1}))^* g_{\alpha-1}\}g_{\alpha-1}\}g_a + \{\beta_5 g_a(D_x(g_{\alpha+1})) + \\
\beta_4 g_a(D_x(g_{\alpha+1}))\}g_{\alpha+1} + \{\beta_5 g_a(D_x(g_{\alpha-1})) + \\
\beta_4 g_a(D_x(g_{\alpha-1}))\}g_{\alpha-1}\}g_a = 0, \quad (22c)
\end{align*}\]

\[\chi^4: \beta_0 D_x^2(\cdot, f) = 0, \quad (22f)\]

\[\chi^5: D_x(g_a)(\beta_2 g_a + \beta_4 |g_{\alpha+1}|^2 + \beta_4 |g_{\alpha-1}|^2) + \{\beta_5(D_x(g_{\alpha+1}))^* g_a + \\
\beta_5(D_x(g_{\alpha-1}))^* g_{\alpha-1}\}g_a + \{\beta_5(D_x(g_{\alpha+1}))^* g_{\alpha+1}\}g_{\alpha+1} + \\
+ \{\beta_5(D_x(g_{\alpha-1}))^* g_{\alpha-1}\}g_{\alpha-1}\}g_a + \{\beta_5 g_a(D_x(g_{\alpha+1})) + \\
\beta_4 g_a(D_x(g_{\alpha+1}))\}g_{\alpha+1} + \{\beta_5 g_a(D_x(g_{\alpha-1})) + \\
\beta_4 g_a(D_x(g_{\alpha-1}))\}g_{\alpha-1}\}g_a = 0. \quad (22g)\]

The solution for order of \(\chi^0\) in the equation 22a is trivial. Meanwhile for order of \(\chi^4\), operating the D Hirota operator, we obtain

\[i \frac{\partial g_a}{\partial T} + \beta_0 \frac{\partial^2 g_a}{\partial x^2} = L(g_{\alpha+1} + g_{\alpha-1}) - i\gamma g_a. \quad (23)\]

The equation 23 can be simplified with transformation \(g_a \rightarrow G_a = g_a e^{\gamma T}\), then it can be written as

\[i \frac{\partial G_a}{\partial T} + \beta_0 \frac{\partial^2 G_a}{\partial x^2} = L(G_{\alpha+1} + G_{\alpha-1}). \quad (24)\]

If the right hand side of equation 24 is zero, then the solution will have a form of exponential function [16, 17]. Assuming \(G_a\) solution for equation 24 also takes a form of exponential function, then

\[\left(i \frac{\partial}{\partial T} + \beta_0 \frac{\partial^2}{\partial x^2}\right)G_a = \Lambda G_a,\]

where \(\Lambda\) is a complex constant. Therefore equation 23 can be stated as

\[\Lambda G_a = L(G_{\alpha+1} + G_{\alpha-1}). \quad (25)\]

For \(\alpha = 1, 2,\) and 3, it leads to:

\[\frac{\Lambda}{L} = \frac{(G_{\alpha+1} + G_{\alpha-1})}{G_a} = \frac{G_2 + G_3}{G_1} = \frac{G_1 + G_3}{G_2} = \frac{G_1 + G_2}{G_3}. \quad (26)\]

Consequently, the \(G_1, G_2,\) and \(G_3\) relation satisfying 26

\[G_1 + G_2 + G_3 = 0. \quad (27)\]

Using the above relation, equation 24 can be written as

\[i \frac{\partial G_a}{\partial T} + \beta_0 \frac{\partial^2 G_a}{\partial x^2} + LG_a = 0. \quad (28)\]

Therefore solution for \(G_1, G_2,\) and \(G_3,\) satisfying equation 28 can be written as below

\[G_1 = e^{\eta}, G_2 = e^{\eta+\sigma}, G_3 = e^{\eta+\epsilon}\]

when \(\eta = k_1 x + \omega t + \eta_0,\) with \(k_1, \omega, \eta_0, \sigma\) and \(\eta\) are complex constants. From equation 27, we obtain

\[e^\epsilon = -(1 + e^\sigma). \quad (30)\]
Separating the real and the imaginary components of the parameters in equation 37, we obtain

\[
\omega_R = -2\beta_0 k_1 R k_{1f} \quad \text{and} \quad \omega_I = \beta_0 (k_1 R - k_{1f}^2) + L.
\]  

Then we obtain the solution for \( g_\alpha \) are

\[
g_1 = e^{\eta - \tau r}, \quad g_2 = e^{\eta + \sigma - \tau r}, \quad \text{and} \quad g_3 = e^{\eta + \varepsilon - \tau r}.
\]

Order of \( \chi^2 \) in equation 22c, for \( \alpha = 1, 2, \) and 3 requiring the condition of \( \beta_1 = \beta_2, \) then

\[
2 \frac{\partial^2 f^{(2)}}{\partial x^2} = \frac{\beta_1}{\beta_0} (|g_1|^2 + |g_2|^2 + |g_3|^2).
\]

Substituting \( g_1, g_2, \) and \( g_3 \) in equation 32 into 33, we have

\[
f(x, T)^{(2)} = \frac{\beta_1 e^{(\eta - \tau r)}}{2 \beta_0 (k_1 + k_{1f}^2)} \left( 1 + e^{(\sigma + \sigma')} + e^{(\varepsilon + \varepsilon')} \right) + f(T).
\]

The equation 22d and equation 22f give us \( f(T) = 0, \) then we get

\[
f = 1 + \frac{\beta_1 e^{(\eta - \tau r)}}{2 \beta_0 (k_1 + k_{1f}^2)} \left( 1 + e^{(\sigma + \sigma')} + e^{(\varepsilon + \varepsilon')} \right).
\]

The equation 22e and 22g require the condition of these constants relations

\[
6\beta_4 + \beta_5 - \beta_6 = 0; \beta_6 = \beta_7.
\]

Therefore we have the solutions of our CNLS equations

\[
\zeta_1 = \frac{e^{(\eta - \tau r)}}{1 + \frac{\beta_1 e^{(\eta - \tau r)}}{2 \beta_0 (k_1 + k_{1f}^2)} \left( 1 + e^{(\sigma + \sigma')} + e^{(\varepsilon + \varepsilon')} \right)}.
\]

\[
\zeta_2 = \frac{e^{(\eta + \sigma - \tau r)}}{1 + \frac{\beta_1 e^{(\eta + \sigma - \tau r)}}{2 \beta_0 (k_1 + k_{1f}^2)} \left( 1 + e^{(\sigma + \sigma')} + e^{(\varepsilon + \varepsilon')} \right)}.
\]

\[
\zeta_3 = \frac{e^{(\eta + \varepsilon - \tau r)}}{1 + \frac{\beta_1 e^{(\eta + \varepsilon - \tau r)}}{2 \beta_0 (k_1 + k_{1f}^2)} \left( 1 + e^{(\sigma + \sigma')} + e^{(\varepsilon + \varepsilon')} \right)}.
\]

Separating the real and the imaginary components of the parameters in equation 37, 38, and 39 such as \( k_1, \omega, \eta_0, \sigma, \) and \( \varepsilon, \) then we can change the form of the solutions above into

\[
\zeta_1 = A \exp \left[ i (k_1 x + \omega R T + \eta_0) \right] \sech(k_1 R x + (\omega R - \gamma) T + \theta_0),
\]

\[
\zeta_2 = A \exp [\sigma R] \exp \left[ i (k_1 x + \omega R T + \eta_0 + \sigma_I) \right] \sech(k_1 R x + (\omega R - \gamma) T + \theta_0),
\]

\[
\zeta_3 = A \exp [\varepsilon R] \exp \left[ i (k_1 x + \omega R T + \eta_0 + \varepsilon_I) \right] \sech(k_1 R x + (\omega R - \gamma) T + \theta_0),
\]

\[
A = k_1 R \left( \frac{2 \beta_0}{\beta_1 (1 + e^{(\sigma + \sigma')} + e^{(\varepsilon + \varepsilon')})} \right) \frac{1}{2}, \quad \text{and} \quad \theta_0 = \eta_0 R \frac{1}{2} \ln \left( \frac{\beta_1 (1 + e^{(\sigma + \sigma')} + e^{(\varepsilon + \varepsilon')})}{2 \beta_0 (k_1 + k_{1f}^2)} \right).
\]
4. Nonlinear Dynamics of Energy Transport in Alphahelical Protein

The solutions of our CNLS equations are $\zeta_1$, $\zeta_2$, and $\zeta_3$. These variables can be transformed back to be $a_1, a_2,$ and $a_3$ which mean the probability amplitude of the excitation energy in amide-I. Meanwhile the quantity of $|a_1|^2$ characterizes the distribution of the amide-I energy over the individual peptide group of a channel [3]. From our solutions we get the profiles of $|a_d|^2$ as below.

![Graph](image1)

**Figure 1.** Comparison of energy density distributed in; a) $|a_1|^2$, b) $|a_2|^2$, and c) $|a_3|^2$ for $k_1 = 1 - 0.4i$, $\sigma = 0.5 + 0.5i$, $\eta_0 = -15 + 2i$ at $t = 10s$.

Figure 1 shows energy distribution propagated in every channels of alpha-helical protein. It is shown that the energy propagated in the form of soliton. The distribution for the three channels has the same pattern ($|a_1|^2$, $|a_2|^2$, and $|a_3|^2$), but they have different amplitude.

![Graph](image2)

**Figure 2.** Comparison of energy density distributed in; a) $|a_1|^2$, and b) $|a|^2$ for $k_1 = 1 - 0.4i$, $\sigma = 0.5 + 0.5i$, $\eta_0 = -15 + 2i$ at $t = 10s$.

Figure 2 shows that when the inter-channel interaction taken into account, its soliton has greater amplitude than the soliton without inter-channel interaction. Therefore the inter-channel interaction contribute to the addition of the energy propagating in each channels. Furthermore it is observed that the two solitons has a different phase. But the phase difference is resulted by the difference in initial phase angle ($\theta_0$). If we look to the solution, we can see that inter-channel interactions affect to the initial
phase angle. Therefore the soliton's initial phase angle with inter-channel interaction greater than the soliton's initial phase angle without it.

![Figure 3. Soliton in channels 1, 2, 3, and soliton without inter-channel interaction propagate in the same velocity, for $k_1 = 1 - 0.4i$, $\sigma = 0.5 + 0.5i$, $\eta_0 = -15 + 2i$.](image)

Nevertheless the two soliton has the same envelope velocity. It is shown from the figure 3, that all of the soliton propagate with the same speed. Therefore there is none soliton left behind in propagation.

![Figure 4. Soliton propagation in channel $\alpha = 1$, when there is no damping (black) and when the damping is taking into account (red), for for $k_1 = 1 - 0.4i$, $\sigma = 0.5 + 0.5i$, $\eta_0 = -15 + 2i$ and $\gamma = 0.5$.](image)

In figure 4, it is shown that the damping term has no contribution to the change of the soliton amplitude. It means the damping term does not make the energy propagating through the channels decrease. However it is observed that the damping term affect to the envelope velocity of the soliton, which means the damping term makes soliton propagate slower. This study has the same result with the study of [2]. Instead of contributes to the change of soliton amplitude the damping term makes the soliton propagation slower, although his study did not consider the inter-channel interactions.
5. Conclusions
The nature of dynamics of energy transport in alpha-helical protein with inter-channel interaction and damping effect was investigated. The dynamics is governed by a set of CNLS equations. Solving the CNLS equations by using Hirota bilinear method, we have the solution of the probability amplitude \( a_d \) for the three channels of alpha-helical protein. The one soliton solution resulting the solution of the distribution of energy transported in the three channels \( |a_d|^2 \) has the similar shape, which is the bell-shaped soliton with the amplitude difference. The soliton amplitude of the three channels differ due to energy sharing between the three different channels. The amplitude differences are found to be depended on the choice of the parameters of \( k_\lambda \), \( \eta_0 \), and \( \sigma \) or \( \epsilon \). The inter-channel interactions result in greater amplitude and initial phase angle of the soliton in the three channels. Meanwhile the damping term represented by \( i\gamma \zeta_d \) has no contribution to the change of the soliton amplitude, nevertheless it affects to the decrease in envelope velocity of soliton.

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