Conformational transition in protein mediated by 3-Coupled Fourth Order Nonlinear Schrodinger (3-CFONLS) soliton

J. Jacqueline Amelia * and M.M. Latha**

*Govindammal Aditanar College for Women,Tiruchendur, Tamil Nadu, India
**Women's Christian College, Nagercoil- 629001,Tamil Nadu, India

Abstract:

A completely integrable 3-coupled fourth order nonlinear schrodinger(3-CFONLS) equation is taken to explain the protein folding phenomena. One and two soliton solutions are developed by adopting numerical simulation. Caspi -Jacob toy model is introduced to study the folding dynamics mediated by solitons. The interaction of 3-CFONLS soliton with the conformation field provides the energy needed to overcome the barriers for folding, thus avoiding the need for thermal activation. Soliton and the conformation field momentum plots provide a proof for soliton mediated conformational transition (SMCT). The effect of interaction of multisoliton with the conformation field is also analyzed.

Keywords: Soliton,3-coupled fourth order nonlinear schrodinger equation, protein folding

1 Introduction

The Davydov model has been the object of many theoretical studies and it continues to attract the attention of many researches [1-10]. These works include analytical and numerical studies based on the simplest nonlinear model of Davydov incorporating energies corresponding to the internal molecular excitations, displacement of unit cells and interaction between the two. The governing dynamical equation appear as completely integrable soliton possessing cubic NLS equation. The effect of higher order molecular excitations and interactions on the soliton dynamics of alpha helical protein was investigated by Daniel and Deepamala [11] and were governed by fourth order NLS (FONLS) equation. These results have been obtained for a single chain. The dynamics of alpha helical proteins with nearest neighbour interactions and interspine coupling at higher order in the continuum limit were investigated by Daniel and Latha [12] and the molecular excitations along the three hydrogen bonding spines were found to be a set of three-coupled NLS equation (3-CNLS) of third order. Later Latha and Veni [13] proposed a generalized model by including excitations of dipole and quadrupole types, nearest and next nearest-neighbour interactions and interspine coupling at higher order and were governed by completely integrable three-coupled fourth order nonlinear Schrodinger equation (3-CFONLS).
Proteins play major roles in all biological processes. It is a polymer built from twenty

different amonoacids ordered in sequence. This sequence is called the primary structure of that protein. Under normal conditions it folds to a predetermined and rather static structure such as α helices and β-sheets called as native state. Tertiary structure refers to the spatial relationships among all aminoacids in a polypeptide. Since protein folding is a spontaneous process it is clear that the aminoacid sequence of each protein contains the information that specifies both the native structure and the pathway to attain that state [14-17]. Temperatures above or below the range that cells tend to live in will cause proteins to unfold or denature. Incorrectly folded (misfolded) proteins are responsible for the cause of several diseases and some cancers [18]. However, the main mechanisms responsible for a structured folding pathway have not yet been identified.

Conformational transition (i.e. transition from metastable to stable state) in protein is usually treated as being thermally induced. But caspi and Ben Jacob [19] suggested that Davydov's soliton propagating through the backbone of a protein can mediate conformational transition referred as Soliton Mediated Conformational Transition (SMCT) and folding of a protein to its native state termed as Soliton Mediated Folding (SMF) [20-24]. A simple toy model was presented in which the NLS field interacts with another field ϕ corresponding to the conformational angles of the protein. The interaction provided the conformation field with the energy needed in order to overcome energy barriers for folding, thus avoiding the need for thermal activation. The soliton compensates for its energy loss by absorption of the energy gained in the folding process. But the actual equations that describe the energy and charge transport in proteins are probably much more complex than the simple NLS equation. So, recently the authors [25] have taken the FONLS equation to study protein folding. As an extention, we have investigated the soliton mediated protein folding by considering the 3-CFONLS equation.

In this paper, we suggest Caspi-Jacob model to 3-CFONLS soliton that travels along the backbone of the protein. We investigate the propagation and evolution process of one and two solitons using numerical simulation and the details are presented in section 2. Section 3 describes the soliton mediated protein folding by calculating the soliton and conformation field momentum. The results are concluded in section 4.

2 Numerical solution

The solitonic excitation is modeled by a 3-coupled higher order (fourth order) NLS equation. It is a completely integrable one and possesses multisoliton solution [13]. These are in fact, non-topological solitons having a velocity dependent amplitude and can exist at any arbitrarily small energy. The 3-CFONLS equation [13] taken for our model reads as

$$
\begin{aligned}
& iq_{1,T} + q_{1,XX} + 2(|q_1|^2 + |q_2|^2 + |q_3|^2)q_1 + \gamma[q_{1,XXXX} + 2(|q_{1,X}|^2 \\
& + |q_{2,X}|^2 + |q_{3,X}|^2)q_1 + 2(q_1 q_{1,X}^* + q_2 q_{2,X}^* + q_3 q_{3,X}^*)q_{1,X} + 6(q_1^* q_{1,X} \\
& + q_2^* q_{2,X} + q_3^* q_{3,X})q_{1,X} + 4(|q_1|^2 + |q_2|^2 + |q_3|^2)q_{1,XX} + 4(q_1^* q_{1,XX} \\
& + q_2^* q_{2,XX} + q_3^* q_{3,XX})q_1 + 2(q_1 q_{1,XX}^* + q_2 q_{2,XX}^* + q_3 q_{3,XX}^*)q_1 + 6(|q_1|^2 \\
& + |q_2|^2 + |q_3|^2)^2 q_1] = 0,
\end{aligned}
\tag{1}
$$

$$iq_{2,T} + q_{2,XX} + 2(|q_1|^2 + |q_2|^2 + |q_3|^2)q_2 + \gamma[q_{2,XXXX} + 2(|q_{1,X}|^2$$
$$+ |q_{2,X}|^2 + |q_{3,X}|^2)q_2 + 2(q_1 q_{1,X}^* + q_2 q_{2,X}^* + q_3 q_{3,X}^*)q_{2,X} + 6(q_1^* q_{1,X}$$
$$+ q_2^* q_{2,X} + q_3^* q_{3,X})q_{2,X} + 4(|q_1|^2 + |q_2|^2 + |q_3|^2)q_{2,XX} + 4(q_1^* q_{1,XX}$$
$$+ q_2^* q_{2,XX} + q_3^* q_{3,XX})q_2 + 2(q_1 q_{1,XX}^* + q_2 q_{2,XX}^* + q_3 q_{3,XX}^*)q_2 + 6(|q_1|^2$$
$$+ |q_2|^2 + |q_3|^2)^2 q_2] = 0, \tag{2}$$

$$iq_{3,T} + q_{3,XX} + 2(|q_1|^2 + |q_2|^2 + |q_3|^2)q_3 + \gamma[q_{3,XXXX} + 2(|q_{1,X}|^2$$
$$+ |q_{2,X}|^2 + |q_{3,X}|^2)q_3 + 2(q_1 q_{1,X}^* + q_2 q_{2,X}^* + q_3 q_{3,X}^*)q_{3,X} + 6(q_1^* q_{1,X}$$
$$+ q_2^* q_{2,X} + q_3^* q_{3,X})q_{3,X} + 4(|q_1|^2 + |q_2|^2 + |q_3|^2)q_{3,XX} + 4(q_1^* q_{1,XX}$$
$$+ q_2^* q_{2,XX} + q_3^* q_{3,XX})q_3 + 2(q_1 q_{1,XX}^* + q_2 q_{2,XX}^* + q_3 q_{3,XX}^*)q_3 + 6(|q_1|^2$$
$$+ |q_2|^2 + |q_3|^2)^2 q_3] = 0. \tag{3}$$

Eqs. (1)-(3) are a set of coupled equations which represents the dynamics of higher order alpha helical proteins with nearest and next nearest neighbour interactions and interspine coupling. They can be solved numerically by properly choosing the initial condition. If the parameter $k_1 = k_2 = $-1-2i is used in the analytic two soliton solution [26-27](Manakov model), the one soliton solution is obtained. Keeping this analytic one soliton solution as initial condition, a well defined numeric one soliton solution is developed and is depicted in fig.1.
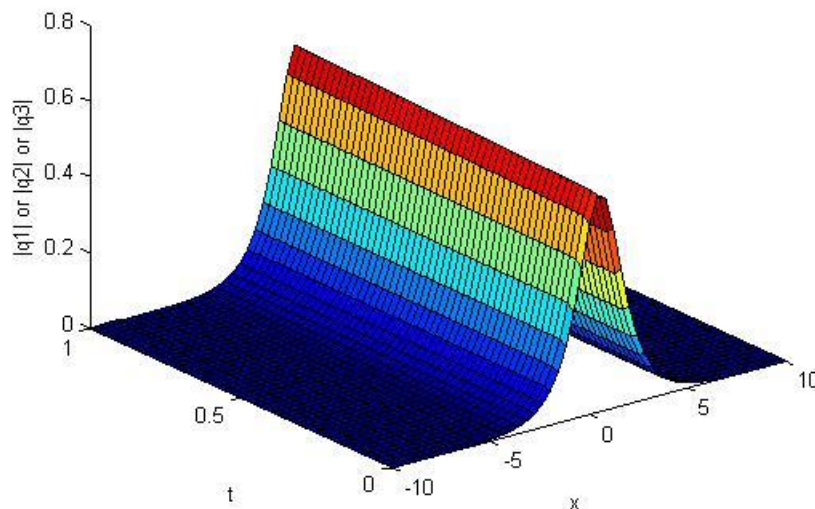

Figure 1: Numerical one soliton solution of 3-CFONLS equation

Similarly by choosing $k_1 = -1-2i$ and $k_2 = 1-1.4i$, the analytic two soliton solution is obtained. One can use this solution as the initial condition, the numeric two soliton solution is developed by writing a suitable program in MATLAB software. The surface plot of the two soliton solution is given in fig.2.
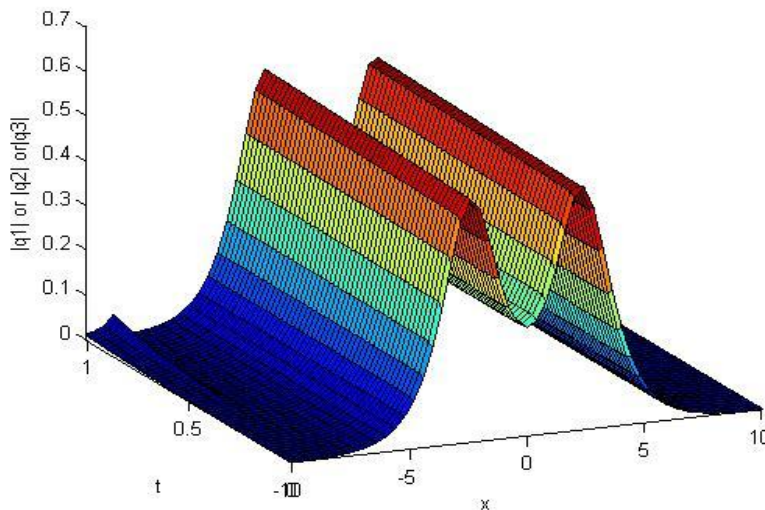

Figure 2: Numerical two soliton solution of 3-CFONLS equation

Obtaining analytic multisoliton solution is very difficult and much complicated. However, the numerical 3,4, ...,N soliton solutions are developed for this 3-CFONLS equation by properly choosing various k_1 and k_2 values in the analytic two-soliton solution. As we are interested to study protein folding rather than developing N-soliton solution, we restrict ourselves to construct one and two soliton solutions. The effect of one and two soliton in protein folding is an important piece of our work, which is postponed in the next section.

3 Soliton mediated protein folding

Caspi-Jacob toy model [19] is introduced to the above 3-CFONLS equation. The total energy of the system consists of three parts.

$$H = H_{sol} + H_{conf} + H_{int}, \tag{4}$$

where H_{sol} is the Hamiltonian of the 3-CFONLS equation [13].

$$H_{conf} = \frac{1}{2} m \phi^2 - V(\phi), \tag{5}$$

where ϕ represents the local conformation of the protein. The local potential energy will be simply modeled by an asymmetric ϕ^4 double well potential, namely

$$V(\phi) = \varepsilon(\phi + \delta)^2 \left(\phi^2 - \frac{2}{3} \phi \delta + \frac{1}{3} \delta^2 - 2 \right) \tag{6}$$

where δ is the asymmetry parameter ranging from -1 to +1. The two minima are positioned at $\phi = \pm 1$. The maxima is positioned at $\phi = -\delta$ and its energy is always zero. The interaction energy between the two fields is given by

$$H_{int} = U(q,\phi) = \Lambda(|q_\alpha|^2 + |q_{\alpha+1}|^2 + |q_{\alpha-1}|^2)\phi^2, \tag{7}$$

where Λ is a positive parameter.

The equation of motion can be derived either in the form of Hamilton's equations from the Hamiltonian or in the form of Euler-Lagrange equations from the associated Lagrangian density. We have obtained the equations from the Lagrangian density which represent a coupled system of time dependent, nonlinear partial differential equations. In recent times there are numerous mathematical ideas and techniques to study nonlinear systems. An efficient method best suited for our problem is the numerical method. Thus finite difference method is used to discretize the coupled system of nonlinear partial differential equations. Substitute $q_1 = u_1 + i v_1$, $q_2 = u_2 + i v_2$ and $q_3 = u_3 + i v_3$ and equating the real and imaginary part and rearranging the terms we get the coupled system of equations as

RealPart
*Mode*1 :

$$
\begin{aligned}
v_{1,t} &= u_{1,xx} + 2((u_1^2 + v_1^2) + (u_2^2 + v_2^2) + (u_3^2 + v_3^2))u_1 \\
&+ \gamma(u_{1,xxxx} + 4((u_1^2 + v_1^2) + (u_2^2 + v_2^2) + (u_3^2 + v_3^2))u_{1,xx} \\
&+ 4((u_1^2 + v_1^2)u_{1,xx} + (u_1 u_2 + v_1 v_2)u_{2,xx} - (u_2 v_1 - u_1 v_2)v_{2,xx} \\
&+ (u_1 u_3 + v_1 v_3)u_{3,xx} - (u_3 v_1 - u_1 v_3)v_{3,xx}) + 6(u_1(u_{1,x}^2 - v_{1,x}^2) \\
&+ 2v_1 u_{1,x} v_{1,x} + u_2(u_{1,x}u_{2,x} - v_{1,x}v_{2,x}) + v_2(u_{2,x}v_{1,x} + u_{1,x}v_{2,x}) \\
&+ u_3(u_{1,x}u_{3,x} - v_{1,x}v_{3,x}) + v_3(u_{1,x}v_{3,x} + u_{3,x}v_{1,x})) \\
&+ 2(u_{1,x}^2 + v_{1,x}^2 + u_{2,x}^2 + v_{2,x}^2 + u_{3,x}^2 + v_{3,x}^2)u_1 \\
&+ 2(u_1(u_{1,x}^2 + v_{1,x}^2) + u_2(u_{1,x}u_{2,x} + v_{1,x}v_{2,x}) + v_2(u_{1,x}v_{2,x} - u_{2,x}v_{1,x}) \\
&+ u_3(u_{1,x}u_{3,x} + v_{1,x}v_{3,x}) + v_3(u_{1,x}v_{3,x} - u_{3,x}v_{1,x})) \\
&+ 2((u_1^2 - v_1^2)u_{1,xx} + 2u_1 v_1 v_{1,xx} + (u_1 u_2 - v_1 v_2)u_{2,xx} \\
&+ (u_1 v_2 + u_2 v_1)v_{2,xx} + (u_1 u_3 - v_1 v_3)u_{3,xx} + (u_3 v_1 + u_1 v_3)v_{3,xx}) \\
&+ 6(u_1^2 + v_1^2 + u_2^2 + v_2^2 + u_3^2 + v_3^2)^2 u_1) - \Lambda\phi^2 u_1
\end{aligned}
\tag{8}
$$

*Mode*2 :

$$
\begin{aligned}
v_{2,t} &= u_{2,xx} + 2((u_1^2 + v_1^2) + (u_2^2 + v_2^2) + (u_3^2 + v_3^2))u_2 \\
&+ \gamma(u_{2,xxxx} + 4((u_1^2 + v_1^2) + (u_2^2 + v_2^2) + (u_3^2 + v_3^2))u_{2,xx} \\
&+ 4((u_2^2 + v_2^2)u_{2,xx} + (u_1 u_2 + v_1 v_2)u_{1,xx} - (u_1 v_2 - u_2 v_1)v_{1,xx} \\
&+ (u_2 u_3 + v_2 v_3)u_{3,xx} - (u_3 v_2 - u_2 v_3)v_{3,xx}) + 6(u_2(u_{2,x}^2 - v_{2,x}^2) \\
&+ 2v_2 u_{2,x} v_{2,x} + u_1(u_{1,x}u_{2,x} - v_{1,x}v_{2,x}) + v_1(u_{2,x}v_{1,x} + u_{1,x}v_{2,x}) \\
&+ u_3(u_{2,x}u_{3,x} - v_{2,x}v_{3,x}) + v_3(u_{2,x}v_{3,x} + u_{3,x}v_{2,x}))
\end{aligned}
$$

$$+ 2(u_{1,x}^2 + v_{1,x}^2 + u_{2,x}^2 + v_{2,x}^2 + u_{3,x}^2 + v_{3,x}^2)u_2$$

$$+ 2(u_2(u_{2,x}^2 + v_{2,x}^2) + u_1(u_{1,x}u_{2,x} + v_{1,x}v_{2,x}) + v_1(u_{2,x}v_{1,x} - u_{1,x}v_{2,x})$$

$$+ u_3(u_{2,x}u_{3,x} + v_{2,x}v_{3,x}) + v_3(u_{2,x}v_{3,x} - u_{3,x}v_{2,x}))$$

$$+ 2((u_2^2 - v_2^2)u_{2,xx} + 2u_2 v_2 v_{2,xx} + (u_1 u_2 - v_1 v_2)u_{1,xx}$$

$$+ (u_2 v_1 + u_1 v_2)v_{1,xx} + (u_2 u_3 - v_2 v_3)u_{3,xx} + (u_2 v_3 + u_3 v_2)v_{3,xx})$$

$$+ 6(u_1^2 + v_1^2 + u_2^2 + v_2^2 + u_3^2 + v_3^2)^2 u_2) - \Lambda \phi^2 u_2 \qquad (9)$$

Mode 3 :

$$v_{3,t} = u_{3,xx} + 2((u_1^2 + v_1^2) + (u_2^2 + v_2^2) + (u_3^2 + v_3^2))u_3$$

$$+ \gamma(u_{3,xxxx} + 4((u_1^2 + v_1^2) + (u_2^2 + v_2^2) + (u_3^2 + v_3^2))u_{3,xx}$$

$$+ 4((u_3^2 + v_3^2)u_{3,xx} + (u_1 u_3 + v_1 v_3)u_{1,xx} - (u_1 v_3 - u_3 v_1)v_{1,xx}$$

$$+ (u_2 u_3 + v_2 v_3)u_{2,xx} - (u_2 v_3 - u_3 v_2)v_{2,xx}) + 6(u_3(u_{3,x}^2 - v_{3,x}^2)$$

$$+ 2v_3 u_{3,x}v_{3,x} + u_1(u_{1,x}u_{3,x} - v_{1,x}v_{3,x}) + v_1(u_{3,x}v_{1,x} + u_{1,x}v_{3,x})$$

$$+ u_2(u_{2,x}u_{3,x} - v_{2,x}v_{3,x}) + v_2(u_{3,x}v_{2,x} + u_{2,x}v_{3,x}))$$

$$+ 2(u_{1,x}^2 + v_{1,x}^2 + u_{2,x}^2 + v_{2,x}^2 + u_{3,x}^2 + v_{3,x}^2)u_3$$

$$+ 2(u_3(u_{3,x}^2 + v_{3,x}^2) + u_1(u_{1,x}u_{3,x} + v_{1,x}v_{3,x}) + v_1(u_{3,x}v_{1,x} - u_{1,x}v_{3,x})$$

$$+ u_2(u_{2,x}u_{3,x} + v_{2,x}v_{3,x}) + v_2(u_{3,x}v_{2,x} - u_{2,x}v_{3,x}))$$

$$+ 2((u_3^2 - v_3^2)u_{3,xx} + 2u_3 v_3 v_{3,xx} + (u_1 u_3 - v_1 v_3)u_{1,xx}$$

$$+ (u_3 v_1 + u_1 v_3)v_{1,xx} + (u_2 u_3 - v_2 v_3)u_{2,xx} + (u_2 v_3 + u_3 v_2)v_{2,xx})$$

$$+ 6(u_1^2 + v_1^2 + u_2^2 + v_2^2 + u_3^2 + v_3^2)^2 u_3) - \Lambda \phi^2 u_3 \qquad (10)$$

Imaginary part Mode 1 :

$$u_{1,t} = -v_{1,xx} - 2((u_1^2 + v_1^2) + (u_2^2 + v_2^2) + (u_3^2 + v_3^2))v_1$$

$$- \gamma(v_{1,xxxx} + 4((u_1^2 + v_1^2) + (u_2^2 + v_2^2) + (u_3^2 + v_3^2))v_{1,xx}$$

$$+ 4((u_1^2 + v_1^2)v_{1,xx} + (u_1 u_2 + v_1 v_2)v_{2,xx} + (u_2 v_1 - u_1 v_2)u_{2,xx}$$

$$+ (u_1 u_3 + v_1 v_3)v_{3,xx} + (u_3 v_1 - u_1 v_3)u_{3,xx}) + 6(-v_1(u_{1,x}^2 - v_{1,x}^2)$$

$$+ 2u_1 u_{1,x}v_{1,x} - v_2(u_{1,x}u_{2,x} - v_{1,x}v_{2,x}) + u_2(u_{2,x}v_{1,x} + u_{1,x}v_{2,x})$$

$$- v_3(u_{1,x}u_{3,x} - v_{1,x}v_{3,x}) + u_3(u_{1,x}v_{3,x} + u_{3,x}v_{1,x}))$$

$$+ 2(u_{1,x}^2 + v_{1,x}^2 + u_{2,x}^2 + v_{2,x}^2 + u_{3,x}^2 + v_{3,x}^2)v_1$$

$$+ 2(v_1(u_{1,x}^2 + v_{1,x}^2) + v_2(u_{1,x}u_{2,x} + v_{1,x}v_{2,x}) - u_2(u_{1,x}v_{2,x} - u_{2,x}v_{1,x})$$

$$+ v_3(u_{1,x}u_{3,x} + v_{1,x}v_{3,x}) - u_3(u_{1,x}v_{3,x} - u_{3,x}v_{1,x}))$$

$$+ 2(-(u_1^2 - v_1^2)v_{1,xx} + 2u_1 v_1 u_{1,xx} - (u_1 u_2 - v_1 v_2)v_{2,xx}$$

$$+ (u_1 v_2 + u_2 v_1)u_{2,xx} - (u_1 u_3 - v_1 v_3)v_{3,xx} + (u_3 v_1 + u_1 v_3)u_{3,xx})$$
$$+ 6(u_1^2 + v_1^2 + u_2^2 + v_2^2 + u_3^2 + v_3^2)^2 v_1) + \Lambda\phi^2 v_1 \tag{11}$$

*Mode*2 :

$$u_{2,t} = -v_{2,xx} - 2((u_1^2 + v_1^2) + (u_2^2 + v_2^2) + (u_3^2 + v_3^2))v_2$$
$$- \gamma(v_{2,xxxx} + 4((u_1^2 + v_1^2) + (u_2^2 + v_2^2) + (u_3^2 + v_3^2))v_{2,xx}$$
$$+ 4((u_2^2 + v_2^2)v_{2,xx} + (u_1 u_2 + v_1 v_2)v_{1,xx} + (u_1 v_2 - u_2 v_1)u_{1,xx}$$
$$+ (u_2 u_3 + v_2 v_3)v_{3,xx} + (u_3 v_2 - u_2 v_3)u_{3,xx}) + 6(-v_2(u_{2,x}^2 - v_{2,x}^2)$$
$$+ 2u_2 u_{2,x} v_{2,x} - v_1(u_{1,x} u_{2,x} - v_{1,x} v_{2,x}) + u_1(u_{2,x} v_{1,x} + u_{1,x} v_{2,x})$$
$$- v_3(u_{2,x} u_{3,x} - v_{2,x} v_{3,x}) + u_3(u_{2,x} v_{3,x} + u_{3,x} v_{2,x}))$$
$$+ 2(u_{1,x}^2 + v_{1,x}^2 + u_{2,x}^2 + v_{2,x}^2 + u_{3,x}^2 + v_{3,x}^2)v_2$$
$$+ 2(v_2(u_{2,x}^2 + v_{2,x}^2) + v_1(u_{1,x} u_{2,x} + v_{1,x} v_{2,x}) - u_1(u_{2,x} v_{1,x} - u_{1,x} v_{2,x})$$
$$+ v_3(u_{2,x} u_{3,x} + v_{2,x} v_{3,x}) - u_3(u_{2,x} v_{3,x} - u_{3,x} v_{2,x}))$$
$$+ 2(-(u_2^2 - v_2^2)v_{2,xx} + 2u_2 v_2 u_{2,xx} - (u_1 u_2 - v_1 v_2)v_{1,xx}$$
$$+ (u_2 v_1 + u_1 v_2)u_{1,xx} - (u_2 u_3 - v_2 v_3)v_{3,xx} + (u_2 v_3 + u_3 v_2)u_{3,xx})$$
$$+ 6(u_1^2 + v_1^2 + u_2^2 + v_2^2 + u_3^2 + v_3^2)^2 v_2) + \Lambda\phi^2 v_2 \tag{12}$$

*Mode*3 :

$$u_{3,t} = -v_{3,xx} - 2((u_1^2 + v_1^2) + (u_2^2 + v_2^2) + (u_3^2 + v_3^2))v_3$$
$$- \gamma(v_{3,xxxx} + 4((u_1^2 + v_1^2) + (u_2^2 + v_2^2) + (u_3^2 + v_3^2))v_{3,xx}$$
$$+ 4((u_3^2 + v_3^2)v_{3,xx} + (u_1 u_3 + v_1 v_3)v_{1,xx} + (u_1 v_3 - u_3 v_1)u_{1,xx}$$
$$+ (u_2 u_3 + v_2 v_3)v_{2,xx} + (u_2 v_3 - u_3 v_2)u_{2,xx}) + 6(-v_3(u_{3,x}^2 - v_{3,x}^2)$$
$$+ 2u_3 u_{3,x} v_{3,x} - v_1(u_{1,x} u_{3,x} - v_{1,x} v_{3,x}) + u_1(u_{3,x} v_{1,x} + u_{1,x} v_{3,x})$$
$$- v_2(u_{2,x} u_{3,x} - v_{2,x} v_{3,x}) + u_2(u_{3,x} v_{2,x} + u_{2,x} v_{3,x}))$$
$$+ 2(u_{1,x}^2 + v_{1,x}^2 + u_{2,x}^2 + v_{2,x}^2 + u_{3,x}^2 + v_{3,x}^2)v_3$$
$$+ 2(v_3(u_{3,x}^2 + v_{3,x}^2) + v_1(u_{1,x} u_{3,x} + v_{1,x} v_{3,x}) - u_1(u_{3,x} v_{1,x} - u_{1,x} v_{3,x})$$
$$+ v_2(u_{2,x} u_{3,x} + v_{2,x} v_{3,x}) - u_2(u_{3,x} v_{2,x} - u_{2,x} v_{3,x}))$$
$$+ 2(-(u_3^2 - v_3^2)v_{3,xx} + 2u_3 v_3 u_{3,xx} - (u_1 u_3 - v_1 v_3)v_{1,xx}$$
$$+ (u_3 v_1 + u_1 v_3)u_{1,xx} - (u_2 u_3 - v_2 v_3)v_{2,xx} + (u_2 v_3 + u_3 v_2)u_{2,xx})$$
$$+ 6(u_1^2 + v_1^2 + u_2^2 + v_2^2 + u_3^2 + v_3^2)^2 v_3) + \Lambda\phi^2 v_3 \tag{13}$$

The forward difference formula used for u_t, u_x, u_{xx} and u_{xxxx} are given below:

$$u_t = \frac{u_{i,j+1} - u_{i,j}}{k} \tag{14}$$

$$u_x = \frac{u_{i+1,j} - u_{i,j}}{h} \tag{15}$$

$$u_{xx} = \frac{u_{i+1,j} + u_{i-1,j} - 2u_{i,j}}{h^2} \tag{16}$$

and

$$u_{xxxx} = \frac{u_{i+1,j} + 6u_{i-1,j} - 4u_{i,j} - 4u_{i-2,j} + u_{i-3,j}}{h^4} \tag{17}$$

where h and k are usual interval of differencing for distance and time respectively. Similar expression holds good for v_t, v_x, v_{xx} and v_{xxxx} also. Substitute the above expressions in equations (8 - 13) and solving we get $q_1 = abs(u_1 + iv_1)$ etc. When $\Lambda = 0$, the same one soliton solution as in fig.1 is obtained for q_1, q_2 and q_3. Similarly the two soliton solution same as fig.2. is obtained for the above three modes. Note that the initial conditions given to solve the above equations are already mentioned in section 2. Similarly the conformation field solution for Caspi-Jacob model takes the form

$$\phi_{i,j} = \phi_{i,j-1} + \frac{k^2}{2m + \Gamma k}[-4\varepsilon(\phi_{i,j-1} + \delta)(\phi_{i,j-1}^2 - 1)$$

$$- 2\Lambda(|q1_{i,j-1}|^2 + |q2_{i,j-1}|^2 + |q3_{i,j-1}|^2)\phi_{i,j-1}]. \tag{18}$$

The solution $\phi_{i,j}$ is developed initially for $\Lambda = 0$.

Soliton mediated protein folding can be explained by calculating the momentum. The soliton momentum for q_1 mode and the conformation field momentum are defined by

$$P_{soliton} = -i\int_{-\infty}^{\infty}(q_1^* q_{1,x} - q_{1,x}^* q_1)dx \tag{19}$$

and

$$P_{conf} = -\int_{-\infty}^{\infty}\phi\dot{\phi}_x dx. \tag{20}$$

Once the solution q_1 and ϕ are known the momentum can be calculated. Since we are using the elastic collision the same solution as that of q_1 is obtained for q_2 and q_3 and hence the soliton momentum is same for all the three modes. As inelastic collision does not play a significant role

in folding dynamics, we restrict ourselves to elastic collision. The interaction parameter Λ best suited for this 3-CFONLS equation is 70. Note that such a large interaction parameter is required if we consider the higher order coupled equation. For $\Lambda = 0$ and $\Lambda = 70$ the one soliton solution for q_1 mode and ϕ are developed and their momenta are calculated. The soliton momentum and the corresponding conformation field momentum are depicted in fig.3. and fig.4. respectively.
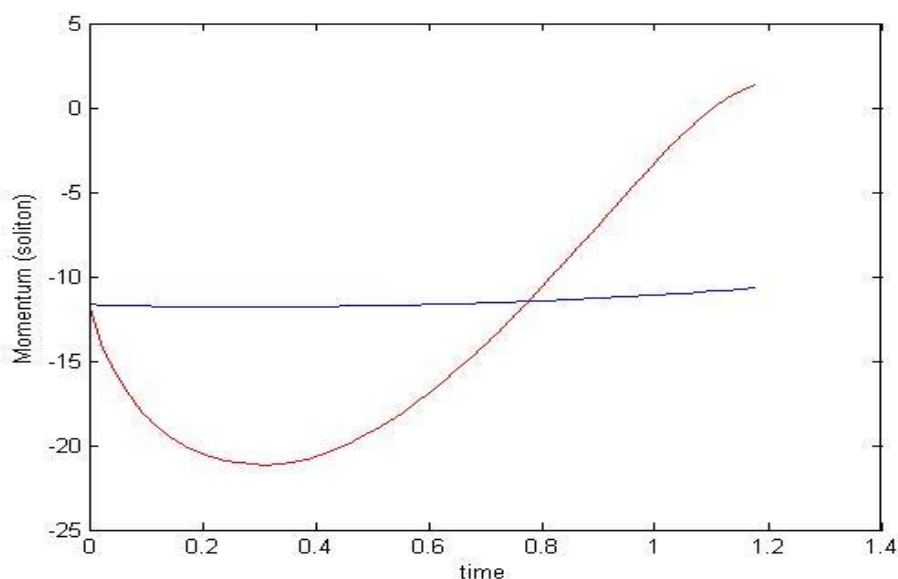

Figure 3: Soliton momentum in q_1 mode for one soliton solution of 3-CFONLS equation
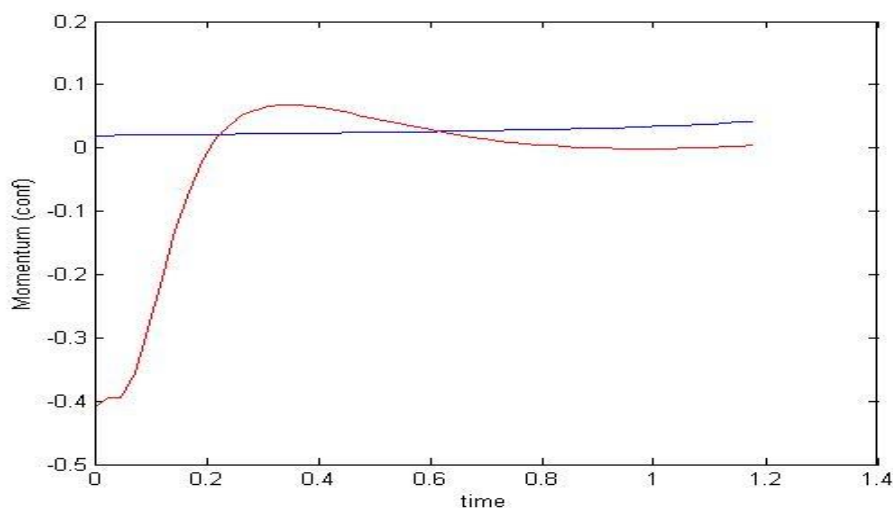(Λ = 0 and Λ = 70)

Figure 4: Conformation field momentum for one soliton solution of 3-CFONLS equation
(Λ = 0 and Λ = 70)

The outcome of the numerical result may be summarized as follows. The conformation field momentum is nearly zero and the soliton momentum is almost constant before interaction. Hence no conformation transition takes place initially. According to our model the interaction parameter (Λ) between soliton and the conformation field plays an important role. If Λ is too small the soliton will not be able to transfer enough energy to take ϕ from one state to another over energy barrier. Thus by slightly increasing the Λ value the required interaction parameter to undergo conformational transition is fixed as 70. When the interaction ($\Lambda = 70$) is turned on, the soliton slows down due to the transfer of momentum and hence energy to the conformation field. The interaction may be in such a way that the conformation field gets enough energy from the soliton and crosses the potential barrier. Depending upon the magnitude of interaction the conformation field is raised to a particular higher energy state (metastable state). Then it causes transition from metastable to stable state. Since the conformation transition process are exothermic, the soliton gets back some of the energy and hence momentum of the soliton increases. Thus the soliton extract the energy in a single event of local conformational transition and transfering it to a distant location. Fig.4 shows a single SMCT(Soliton Mediated Conformational Transition) event occured in protein folding. Similarly it may be used to activate another transition and the energy released in that process could be extracted again. Similar transition takes place continuously and hence large sections of a protein can fold very fast. After the folding process is completed the soliton reaches a steady state finite velocity as discussed by the author [19]. Thus the momentum graph obtained for this model reflects the folding process mediated by 3-CFONLS soliton.

4 Effect of soliton interaction on protein folding

Instead of a single soliton if two solitons travel along a single hydrogen bonded spine, after some time these two solitons will interact among themselves. And also we have three hydrogen bonded spines which will produce additional interaction. The effect of these interactions on protein folding may be analyzed by calculating the momentum as before for two soliton solution of 3-CFONLS equation. The same interaction parameter is chosen for this two soliton interaction case also. The other parameters used to solve equations(8 - 13 and 18) are m=1, ε =2, δ =-0.5, Γ =1 and γ =.001. By developing the solution q_1 and ϕ, the soliton momentum in q_1 mode and the conformation field momentum are evaluated using Eqs. (19) and (20). The momentum figures are depicted in figs.5 and 6.
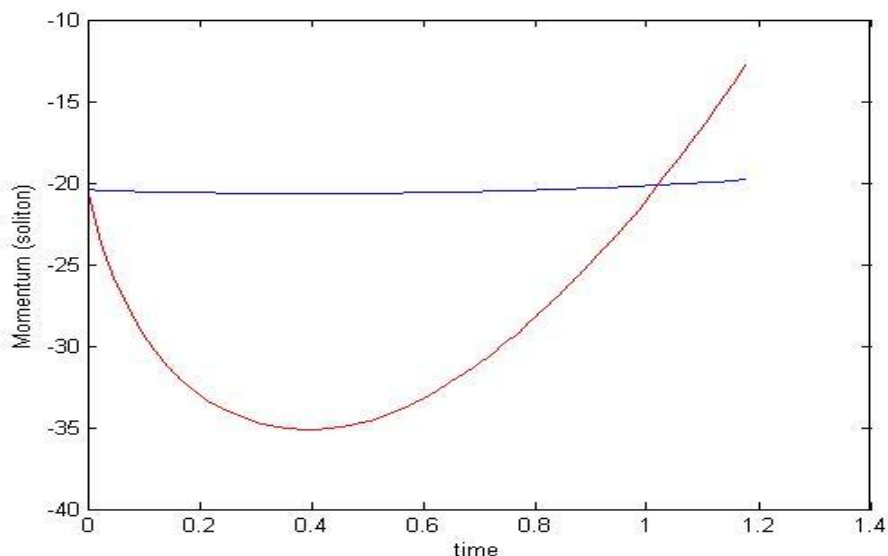
Figure 5: Soliton momentum in q_1 mode for two soliton solution of 3-CFONLS equation
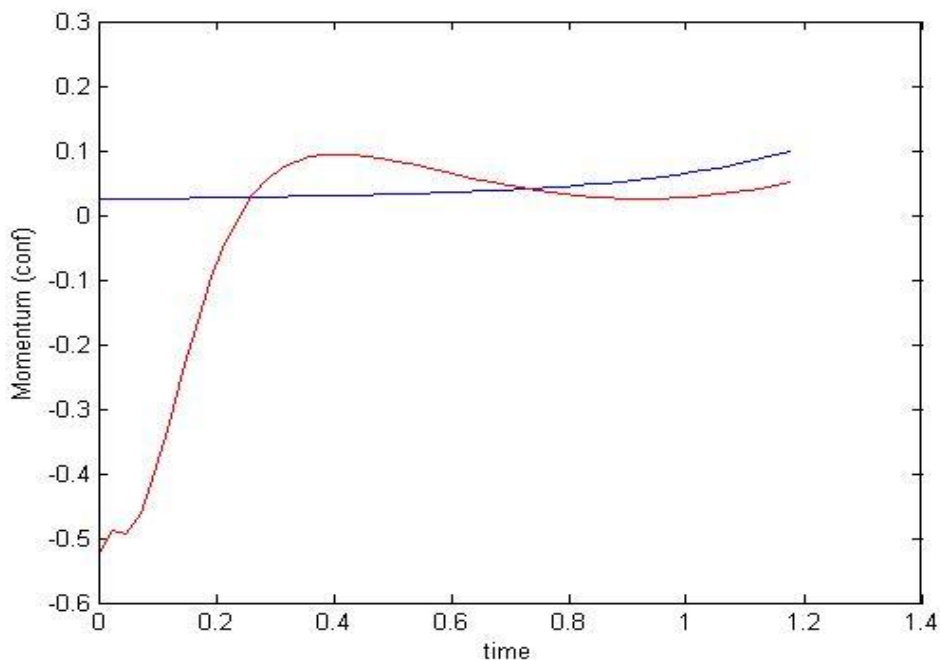($\Lambda = 0$ and $\Lambda = 70$)

Figure 6: Conformation field momentum for two soliton solution of 3-CFONLS equation
($\Lambda = 0$ and $\Lambda = 70$)

Figure shows that conformational transition takes place quickly for one soliton solution. If we take two soliton solution, some interaction takes place and hence slightly larger time is required to undergo conformational transition. As a consequence, the two soliton momentum is

slightly lesser than the momentum obtained for one soliton solution. Similar results are obtained for q_2 and q_3 modes also. When solitons propagate along the three hydrogen bonded spines they will collide among themselves either elastically or inelastically and during collision there will be a change in the distribution of energy in the neighbouring spines but the total energy of the system is conserved. Hence there won't be much change in the conformation field momentum. So, we restrict ourselves to calculate the momentum for elastic collision alone.

5 Conclusion

In this paper a very complicated 3-coupled higher order (fourth order) nonlinear Schro dinger equation was taken to study protein folding. By means of systematic simulation the one soliton solution was obtained. Though developing multisoliton solution for such complicated system by analytic method is a herculian task, that could be achieved easily by numerical method. Caspi-Jacob toy model was introduced to this 3-CFONLS equation and the Soliton Mediated Folding(SMF) was explained by calculating the momentum. The inclusion of soliton interaction along the same spine and also with the adjacent spines does not affect the overall picture. Transition from a metastable to a stable conformation state (SMCT event) is usually treated as being thermally induced. We suggested and proved that conformational transition of this sort was mediated by solitons that travel along the backbone of the protein.

References

[1] Scott A C, *Phys. Rev. A*, **26**, 578 (1982).

[2] Eilbeck J C, Lomdahl P S and Scott A C, *Phys. Rev.B*, **30**, 4703 (1984).

[3] Xiav J X and Yang, *Phys. Rev.A*, **44**, 8375 (1991).

[4] Schweitzer J W, *Phys. Rev.A*, **45**, 8914 (1992).

[5] Forner W, *J. Phys. Condensed Matter*, **5**, 823 (1993).

[6] Peyrard M, *Nonlinear Excitations in Biomolecules*, Springer, Berlin,1995.

[7] Daniel M and Latha M M, *Physica A*, **240**, 526 (1997).

[8] Caspi S and Ben Jacob E, *Europhysics Lett.*, **47**, 522 (1999).

[9] Keba C Biswas and Jacquelyn Gillespie, Advanced studies in Biology, **1**, 1 (2009).

[10] Latha M M and Merlin G, *Phys. Rev.A*, **376**, 938 (2012).

[11] Daniel M and Deepamala K, *Physica A*, **221**, 241 (1995).

[12] Daniel M and Latha M M, *Phys. Lett. A*, **252**, 92 (1999).

[13] Saravana Veni S and Latha M M, *Phys. Scr.*, **86**, 025003 (2012).

[14] Pauling L, Corey R R B and Hayward R, *Sci. Am.*, **191**, 51 (1954).

[15] Stryer L, *Biochemistry*, Freeman W H and Company, New York, 1995.

[16] Narayanan P, *Essentials of Biophysics*, New Age International Publishers, New Delhi,1995.

[17] Schulz G E and Schirmer R H, *Principles of Protein Folding*, Springer, New York, 1979.

[18] Dobson C M, *Nature*, **426**, 884 (2003).

[19] Caspi S and Ben Jacob E, *Phys. Lett. A*, **272**, 124 (2000).

[20] Frauenfelder H, Parak F and Young R D, *Ann. Rev. Biophys. Chem.*, **17**, 451 (1988).

[21] Olsen O H, Samuelsen M R, Petersen S B and Norskov L, *Phys. Rev. A*, **3964**, 3130 (1989).

[22] Shakhnovich E I, *Phys. Rev. Lett.*, **72**, 3907 (1994).

[23] Natalia G. Berloff , *Phys. Lett. A*, **337**, 391(2005).

[24] Brown T A, *Genomes*, Wiley, New York, 1999.

[25] Jacqueline Amelia J and Latha M M, *International Journal of Advanced Scientific and Technical Research*, **4**, 86(2014).

[26] Manakov S V, *Sov. Phys. JETP*, **38**, 248 (1974).

[27] Daniel M and Latha M M, *Phys. Lett. A*, **302**, 94 (2002).