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Adiabatic dynamics and numerical simulations of solitons in α-helix proteins

Anjan Biswas; Pablo Suarez; Jacquelyn Gillespie; Fayequa Majid

Department of Mathematical Sciences, Center for Research and Education in Optical Sciences and Applications, Delaware State University, Dover, DE 19901-2277 USA
Department of Mathematical Sciences, Delaware State University, Dover, DE 19901-2277 USA
Department of Science, Wesley College, Dover, DE-19901 USA
Department of Mathematics, Alabama A & M University, Normal, AL-35762

ABSTRACT

The adiabatic dynamics of solitons in α -helix proteins are studied in this paper. The soliton perturbation theory is applied to conduct this research work. The type of nonlinearity that is taken into consideration is the power law nonlinearity. The numerical simulations are also given to support the analytical results.

Key words: solitons; adiabaticity; perturbation; numerics.

INTRODUCTION

The study of the dynamics of solitons in α-helix proteins has been going on for the past few decades [1-10]. There has been a lot of progress that has been made in the past few decades. The governing equation that is studied in this context is the nonlinear Schrödinger's equation (NLSE) which is sometimes referred to as the Davydov model [8]. This is the main equation that describes the inherent dynamics of the solitons. In this paper, NLSE will be used to carry out the adiabatic dynamics of the soliton parameters when perturbation terms are taken into consideration. The soliton perturbation theory will be used

to carry out this investigation. The numerical simulations of the governing NLSE will also be given. This will support the analytical development.

MATHEMATICAL ANALYSIS

The governing equation, in dimensionless form, that will be studied for the solitons in α-helix proteins is given by [1-3]

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

Here in (1), the dimensionless variable $q(x,t)$ represents the wave profile. The independent variables x and t are the spatial and temporal variables while the parameter n is the power law nonlinearity parameter. Generally, the parameter value n is taken to be 1 in the study of Davydov solitons. In this paper, the parameter n is taken into consideration so that it will serve as a generalized approach. Thus, the parameter n dictates the degree of nonlinear regime that the proteins in a biochemical system can be subjected to. It needs to be noted that it is necessary to have

$$0 < n < 2 \tag{2}$$

in order for the Davydov solitons to exist, in particular, $n \neq 2$ to avoid a singularity situation.

The Davydov 1-soliton solution to (1) is given by

$$q(x,t) = A\operatorname{sech}^{\frac{1}{n}}[B(x - vt)]e^{i(-\kappa x - \omega t + \theta)} \tag{3}$$

where

$$\kappa = -v \tag{4}$$

$$\omega = \frac{B^2}{2n^2} - \frac{\kappa^2}{2} \tag{5}$$

$$B = A^n\left(\frac{2n^2}{1+n}\right)^{\frac{1}{2}} \tag{6}$$

Here in (3), the parameter A is the amplitude of the soliton, while the parameter B is the inverse width of the soliton and v is the velocity of the soliton. In the phase component, κ is the soliton frequency while ω is the soliton wave number. One of the many interesting properties of this equation (1) is that it has at least two conserved quantities that are the energy (E) and momentum (M) that are respectively given by

$$E = \int_{-\infty}^{\infty} |q|^2 dx = \frac{A^2\Gamma\left(\frac{1}{n}\right)\Gamma\left(\frac{1}{2}\right)}{B\Gamma\left(\frac{1}{n}+\frac{1}{2}\right)} \tag{7}$$

and

$$M = \frac{i}{2}\int_{-\infty}^{\infty}(q^* q_x - q q_x^*)dx = -\frac{\kappa A^2 \Gamma\left(\frac{1}{n}\right)\Gamma\left(\frac{1}{2}\right)}{B\Gamma\left(\frac{1}{n}+\frac{1}{2}\right)} \tag{8}$$

Also, the velocity of the soliton is given as

$$v = \frac{d}{dt}\left(\frac{1}{E}\int_{-\infty}^{\infty} x|q|^2 dx\right) \tag{9}$$

Perturbation Terms

In presence of perturbation terms that arises in Davydov solitons, the perturbed NLSE is given by [1, 3]

$$iq_t + \frac{1}{2}q_{xx} + |q|^{2n}q = i\epsilon R \tag{10}$$

where ϵ is the perturbation parameter and R represents the perturbation term. Also, here $0 < \epsilon \ll 1$. Now, in presence of perturbation terms, the conserved quantities undergo adiabatic deformation that are given by

$$\frac{dE}{dt} = \epsilon\int_{-\infty}^{\infty}(q^* R + qR^*)dx \tag{11}$$

$$\frac{dM}{dt} = i\epsilon\int_{-\infty}^{\infty}(q_x^* R - q_x R^*)dx \tag{12}$$

Thus equations (11) and (12) leads to the adiabatic deformation of the soliton frequency as

$$\frac{d\kappa}{dt} = \frac{\epsilon}{E}\left[i\int_{-\infty}^{\infty}(q_x^* R - q_x R^*)dx + \kappa\int_{-\infty}^{\infty}(q^* R + qR^*)dx\right] \tag{13}$$

Finally, from (9) and (10), the change in the soliton velocity is

$$v = -\kappa + \frac{\epsilon}{E}\left[\int_{-\infty}^{\infty} x(q^* R + qR^*)dx\right] \tag{14}$$

The specific perturbation terms R are now given by [1, 3]

$$R = \eta q^* q_x^2 + \beta|q_x|^2 q + \gamma|q|^2 q_{xx} + \delta|q|^4 q + \lambda q^2 q_{xx}^* + \nu|q|^2 q_x + \xi q^2 q_x^* + \sigma q_{xxxx} \tag{15}$$

where the perturbation terms given by (15), 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.

The adiabatic dynamics of the soliton energy (E) and the frequency (κ) in presence of the perturbation terms given by (15), is

$$\frac{dE}{dt}=\frac{2\epsilon A^4}{n^2 B}\left[\{n^2\kappa^2(\beta-\eta-\gamma-\lambda)+B^2(\eta+\beta-3\gamma-3\lambda)\}\frac{\Gamma\left(\frac{2}{n}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{2}{n}+\frac{1}{2}\right)}\right. \\ \left. +\{n^2\delta A^2-B^2(\eta+\beta-3\gamma-3\lambda)\}\frac{\Gamma\left(\frac{3}{n}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{3}{n}+\frac{1}{2}\right)}\right] \tag{16}$$

$$\frac{d\kappa}{dt}=0 \tag{17}$$

and the change in the velocity of the soliton is given by

$$v=-\kappa-\frac{\epsilon(\xi+\nu)A^4}{2BE}\frac{\Gamma\left(\frac{2}{n}\right)\Gamma\left(\frac{1}{2}\right)}{\Gamma\left(\frac{2}{n}+\frac{1}{2}\right)} \tag{18}$$

Thus, the dynamical system given by (16) and (17) have a fixed point, namely a node, that is given by $(\bar{E},\bar{\kappa})$ where $\bar{\kappa}=\kappa_0$ with κ_0 being a constant and

$$\bar{E}=\frac{\bar{A}^2}{\bar{B}} \tag{19}$$

while $\bar{A}$ and $\bar{B}$ are obtained from the relations

$$\{n^2\kappa_0^2(\beta-\eta-\gamma-\lambda)+\bar{B}^2(\eta+\beta-3\gamma-3\lambda)\}\frac{\Gamma\left(\frac{2}{n}\right)}{\Gamma\left(\frac{2}{n}+\frac{1}{2}\right)} \\ =\{\bar{B}^2(\eta+\beta-3\gamma-3\lambda)-n^2\delta\bar{A}^2\}\frac{\Gamma\left(\frac{3}{n}\right)}{\Gamma\left(\frac{3}{n}+\frac{1}{2}\right)} \tag{20}$$

and (6).

Numerical Simulations

In this section we study the numerical solution of the perturbed and unperturbed NLSE. For solving numerically these equations we follow the approach in [11] and let $(x,t)=u(x,t)+iv(x,t)$. By making this substitution the modulus in the right and left hand side of the equation are eliminated. The

$$u_t + \frac{1}{2} v_{xx} + v(u^2 + v^2) = \epsilon \, ImR \quad (21)$$

$$v_t - \frac{1}{2} u_{xx} - u(u^2 + v^2) = \epsilon \, ReR \quad (22)$$

These equations have initial data $u(x,0) = Re(q(x,0))$ and $v(x,0) = Im(q(x,0))$. Weideman *et. al.* showed in [12] that good results can be obtained by using spectral methods when solving nonlinear PDE systems. In particular in that work the authors solved the Sine-Gordon equation using Fourier, Sinc and Hermite spectral collocation method. For purposes of this work the best suited method is the Fourier spectral collocation method.

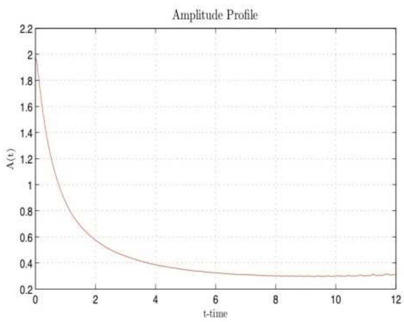

Figure 1(a) Amplitude of Soliton

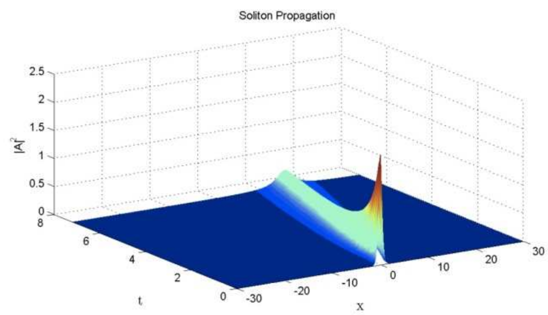

Figure 1(b) Soliton Propagation

Numerical Example

For a numerical example we let the initial condition $q(x,0) = \sqrt{2} e^{2xi} \text{sech}(\sqrt{2}x)$. We let the perturbation n=1, $\epsilon = 0.01, \eta = 1, \beta = \lambda = \gamma = 1$ and $\nu = 2$. The choice of these parameters avoid any singularities when solving the related amplitude equation (16). The numerical solution can be obtained by using the *dmsuite* package used developed by Weideman (see [12] for details).

The related amplitude equation predicts that we have a decaying amplitude. The decay in amplitude can be seen in figure 1(a). This matches with the soliton's numerical solution seen in figure 1(b).

CONCLUSION

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 the solitons amplitude and the frequency leads to a fixed point that is actually a node. Therefore the solitons travel with a fixed amplitude and frequency.

The numerical simulations of the solitons in presence of perturbation terms for the perturbed NLSE are obtained. Finally, the adiabatic dynamics of the soliton amplitude is also obtained when the perturbation terms are turned on. These numerical simulations give a clear picture of the biological phenomena that is going on with the proteins.

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