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Davydov's Soliton in an Inhomogeneous Medium

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Abstract. The damping effect of the interaction of high-frequency amide-I vibrations with the low-frequency acoustic vibrations of the protein is investigated. The phenomena studied phenomonologically by extension of the nonlinear Schrodinger equation. By introducing a local approximation, the damping factor can be expressed as a new term $i\bar{\gamma}\phi$ in the nonlinear Schrodinger equation. The result show that the soliton with damping propagate slower than original one. By introducing a periodic external force, the equation of motion is described by the force-damped nonlinear Schrodinger equation. Solution based on the variational methods show that the Davidov's soliton will be accelerated by a periodic external force.

Keywords: Davydov soliton, inhomogeneous medium, nonlinear Schrodinger equation
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INTRODUCTION

The bio-energy transport is basic mechanism in a life and related to many biological activities. The bio-energy needed are mainly provided by that released in adenosine phosphate (ATP) hydrolysis in living system and the model of the phenomena such as Davydov's, Tekeno's, Yamosa's, Scheitzer's, Cruzeiro-Hansson's, Forner's and Pang's model have been developed [1]. The first model that is called Davydov proposed the mechanism through a nonlinear mechanism from the storage and transfer of vibrational energy (intrapeptide vibration amide-I) in alpha-helical proteins [2]. The interaction of high-frequency amide-I vibrations (vibrations of double C-O bond of peptide groups) with the low-frequency acoustic vibrations of the protein is a self-trapping of the amide-I vibration [2, 3]. The propagation of self-trapping plus the deformational lattice together can travel over macroscopic distances along the molecular chains, retaining the wave shape, energy and momentum. In this way, the bioenergy can be transported as solitary waves or soliton. Soliton is the equilibrium between nonlinear effect and dispersive effect. The other hand,in classical lattices, the anharmonicity gives rise to the occurence of intrinsic localized modes [6]. The measurement of infrared absorption and Raman's scattering of an crystallineacetanilide $(CH_3CONHC_6H_5)_x$ at low temperature shown a new band that closed to amide-I band [7].They interpret that this is a signature of Davidov's soliton. Experiment using femtosecond IR spectroscopy show that a band of amide-I from accetanilide (ACN) and N-methylacetanide (NMA) show absorption spectrum depend on temperature. At high temperature, absorption spectrum will shift to higher frequency [8].

The paper studis the effect of damping and an external force on the propagation of Davydov's soliton. The phenomena studied phenomonologically by extension of the nonlinear Schrodinger equation. The Davydov's model of alpha helix protein is described in sec-2. Derivation of equation of motion describing Davydov's soliton and its behaviour in an inhomogeneous medium is given in sec-3. The paper is ended by a summary.

DAVYDOV'S MODEL

Davydov's model describe a vibrational energy of the C=O stretching (or amide I) oscillator that it localized on the helix chain and act through a phonon coupling mechanism, to deform the structure of the amino acid residue. The deformation of amino acid residues reacts, again through phonon coupling, to trap the amide-I vribational quanta and prevent its dispersion. The Hamiltonian of the system can be written as follow [1],

$$H = H_{ex} + H_{ph} + H_{int}$$

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$$= \sum_n \left[(\varepsilon_0 - D)B_n^+ B_n - J(B_n^+ B_{n+1} + B_{n+1}^+ B_n)\right] + \sum_n \left[\frac{P_n^2}{2M} + \frac{1}{2}w(u_n - n_{n-1})^2\right] + \sum_n \chi(u_{n+1} - u_{n-1})B_n^+ B_n \quad (1)$$

where $\varepsilon_0 = 0.205eV$ is the exciton energy, $B_n + (B_n)$ is the exciton creation (annihilation) operator at the nth site with an energy ε_0, J is resonace (dipole-dipole) interaction, D is the coefficient interaction of the exciton, P_n and u_n are the momentum and coordinate operator of phonon (peptide group) and χ is the coupling constant between the exciton and phonon. By using the trial function $|\psi>=|\Psi>|\Phi>$ in which $|\Psi>=\sum a_n B_n^+|0>_{ex}$ a single of the amide-I excitation and $|\Psi>$ is the coherent phonon state then the average value of H which respect to the product wave function $(<\psi|H|\psi>)$ leads,

$$i\hbar\dot{\phi}_n = \chi(\beta_{n+1} - \beta_n)\phi_n - J(\phi_{n+1} - 2\phi_n + \phi_{n-1}) \quad (2)$$
$$M\ddot{\beta}_n = w(\beta_{n+1} - 2\beta_n + \beta_{n-1}) + Q\chi\left(|\phi|^2 - |\phi_{n-1}|^2\right) \quad (3)$$

where a_n is a complex number representing the probability amplitude for finding a quantum of amide-I, $<\Phi|u_n|\Phi>=\beta_n$ and $<\Phi|P_n|\Phi>=\pi_n$ are the average value of the longitudinal displacement and momentum of a phonon. $\phi_n = a_n \exp(it(\varepsilon_0 - D - 2J + w))$ is a gauge transformation. By assuming a stationary solution ($\dot{\beta}_n = 0$) give the discrete nonlinear Schrodinger equation

$$i\frac{\hbar}{J}\frac{\partial\phi_n}{\partial t} + (\phi_{n+1} - 2\phi_n + \phi_{n-1}) + \frac{\chi^2}{2wJ}|\phi_n|^2\phi_n = 0\,, \quad (4)$$

where the corresponding lattice (phonon) distortion is given by,

$$\beta_{n+1} - \beta_n = -\frac{\chi}{2w}|\phi_n|^2\,. \quad (5)$$

In the continuum approximation the equation become,

$$i\frac{\partial\phi}{\partial t} + \frac{J}{\hbar l^2}\frac{\partial^2\phi}{\partial x^2} + \frac{\chi^2}{2w\hbar}|\phi|^2\phi = 0\,, \quad (6)$$

with l is a lattice constant. The single soliton solution is given by [1, 2],

$$\phi(x,t) = \Lambda sech\left[\frac{\Lambda\chi l}{\sqrt{2wJ}}(x - Vt)\right]e^{i(\frac{\hbar l^2 V}{J}x - \omega t)}\,, \quad (7)$$

with the relation $\omega = (\chi^2)/(4w\hbar)\Lambda^2 - (l^2)/(4\hbar)V^2$. If the β is not stationers, the equation of motion in the form of Nonlinear Kline-Gordon equation where have a kink solution. The solution showed that the bio-energy cannot disperse and dissipate in the transport processes.

PROPAGATION OF DAVYDOV SOLITON IN AN INHOMOGENEOUS MEDIUM

The interaction of a system with its environment is given by the dissipation effect in quantum system. The behaviour of the system has attracted many interests in the last decades. The termal effect can be accomodated by adding new term in the Nonlinear Schrodinger equation as follow [9],

$$i\frac{\partial\phi(x,t)}{\partial t} + \frac{J}{\hbar l^2}\frac{\partial^2\phi(x,t)}{\partial x^2} + i\hbar\int_0^L \Gamma(x - x')\phi(x',t)\frac{dx'}{L} + \frac{\chi^2}{2w\hbar}|\phi(x,t)|^2\phi(x,t) = 0\,. \quad (8)$$

Following [9] by introducing a local approximation, that is, neglecting space coordinate correlation, the damping factor can be expressed as $\Gamma(x - x') = \gamma\delta(x - x')$, the equation of Davydov's soliton become,

$$i\frac{\partial\phi(x,t)}{\partial t} + \frac{J}{\hbar l^2}\frac{\partial^2\phi(x,t)}{\partial x^2} + i\hbar\gamma\phi(x,t) + \frac{\chi^2}{2w\hbar}|\phi(x,t)|^2\phi(x,t) = 0\,. \quad (9)$$

The solution of the equation is [9]

$$\phi(x,t) = \Lambda sech\left[\frac{\Lambda\chi l}{\sqrt{2wJ}}(x - Vt)\right]e^{i(\frac{\hbar l^2 V}{J}x - (\omega - i\gamma)t)}\,. \quad (10)$$

The damping coefficient γ is the reciprocal lifetime of excitation. Estimation of soliton velocity is about $V \approx 3x10^4$ cm s^{-1} coresspond with spectral frequency ω =16cm^{-1} [1].

Recents year, there is a new transformation to solve the damped nonlinear Schrodinger equation that proposed by [10]. Let, Eq.(9) can be written as,

$$i\frac{\partial\phi(x,t)}{\partial t} + a\frac{\partial^2\phi(x,t)}{\partial x^2} + i\bar{\gamma}\phi(x,t) + b|\phi(x,t)|^2\phi(x,t) = 0\,, \quad (11)$$

where $a = J/(\hbar l^2)$, $\bar{\gamma} = \hbar\gamma$, and $b = \chi^2/(2w\hbar)$. By using transformation [10],

$$\phi(x,t) = \Phi(x,t)e^{\bar{\gamma}t}\,, \quad (12)$$

the equation become,

$$i\frac{\partial\Phi(x,t)}{\partial t} + a\frac{\partial^2\Phi(x,t)}{\partial x^2} + be^{2\bar{\gamma}t}|\Phi(x,t)|^2\Phi(x,t) = 0\,. \quad (13)$$

By using Taylor expansion in the exponent factor, then Eq. (13) become homogeneous NLS $\Psi(\zeta,\tau)$ with transformation coordinate and fucntion respectively $\zeta = p(t)x$, $\tau = p(t)t$, $p(t) = (1 - 2\bar{\gamma}t)$ and $\Psi = \Phi/\sqrt{p(t)}\exp(-i\bar{\gamma}p(t)x^2/(2a))$ [10].

If the system drive by an external force such as electromagnetic for example, the equation of motion can be written as,

$$i\frac{\partial\phi(x,t)}{\partial t}+a\frac{\partial^2\phi(x,t)}{\partial x^2}+i\bar{\gamma}\phi(x,t)$$
$$+\delta\phi(x,t)+b|\phi(x,t)|^2\phi(x,t)=E_0\mathrm{e}^{-i\Omega t}\ . \quad (14)$$

By using transformation,

$$\phi(x,t)=\Psi(x,t)\mathrm{e}^{-i\Omega t}\ , \quad (15)$$

Eq. (14) become,

$$i\frac{\partial\Psi(x,t)}{\partial t}+a\frac{\partial^2\Psi(x,t)}{\partial x^2}+\kappa^2\Psi(x,t)$$
$$+i\bar{\gamma}\Psi(x,t)+\bar{b}|\Psi(x,t)|^2\Psi(x,t)=E_0\ , \quad (16)$$

where $\kappa^2=\Omega+\delta$. The equation has interested of many scientist and they studied its stability, bifucrcation and their bound state of propagation of soliton [11]. The equation can be written in the better form by transformation $t'=\kappa^2 t$, $x'=\kappa x$, $\bar{E_0}=-E_0/\kappa^3$, $\tilde{\gamma}=\bar{\gamma}/\kappa^2$, and $\Psi=\kappa\psi$ [11],

$$i\frac{\partial\psi}{\partial t'}+\frac{\partial^2\psi}{\partial x'^2}+\psi(x,t)+2|\psi(x,t)|^2\psi=\bar{E_0}\ . \quad (17)$$

In the term of traveling wave soliton $z=x'-Vt'$, the partial differential equation become the ordinarry differential equation. By assuming stationary solution then we can get the driving strength $\bar{E_0}$ as follow [11],

$$\bar{E_0}=\frac{\sqrt{2}\cosh^2\bar{\gamma}}{(1+2\cosh^2\bar{\gamma})^{3/2}}\ . \quad (18)$$

By using numerical methods of an ordinary differential equation, the parameter $\bar{E_0}$ can be used as a studies of an initial conditions. We use widely accepted values for the physical parameters for the alpha helix protein molecules [2, 1], J=1.55 $\times$ 10^{-22}, w=(13-19.5) N/m, M=(1.17-1.91) $\times$ 10^{-25} kg, χ=62$\times 10^{-12}$ N and l=4.5 $\times$ 10^{-10} m. The solution of Eq.(10) is depicted in Fig.1. The result show that the soliton with damping propagate slower than without damping effect. The solution Eq.(10) show that the damping effect does not contribute into the amplitude of soliton. The dissipation effect in the term of $i\gamma\phi$ can be viewed as driving (forcing) or damping of the soliton solution.

Interestingly, suppose if we consider a propagation of Davydov's soliton in a viscous medium. If we treat the medium is a classical object then it can be done by replace the term of $i\bar{\gamma}\phi$ by $\gamma\partial\phi/\partial t$ in Eq.(14) with $\delta=0$. We get the equation as follow,

$$i\frac{\partial\phi(x,t)}{\partial t}+a\frac{\partial^2\phi(x,t)}{\partial x^2}+\bar{\gamma}\frac{\partial\phi(x,t)}{\partial t}$$
$$+b|\phi(x,t)|^2\phi(x,t)=E_0\mathrm{e}^{-i\Omega t}\ . \quad (19)$$

This is called the forced damped nonlinear Schrodinger equation (FDNLS). The solution of the FDNLS can be found by means of variational methods based on the Lagrangian formulation [12]. Based on the corresponding variational methods to solve the damped-forced nonlinear Schroedinger equation, one can use the single soliton solution as the related basic form and considering its amplitude, width, phase velocity and the position of the soliton to be time dependent [12]. Let us write the 1-soliton in the following form,

$$\phi(x,t)=\eta(t)\mathrm{sech}[\eta(x+\zeta(t))]\exp\left(-i[\theta(t)x+\varphi(t)]\right)\ . \quad (20)$$

The dynamics of η, θ, ζ and ϕ function can be obtained by using the variational methods. By construction of the Lagrangian,

$$\begin{aligned}\mathscr{L} \quad &= \frac{i}{2}(\phi_t\phi^*-\phi_t^*\phi)-a\mid\phi_x\mid^2+b\mid\phi\mid^4\\ &+\bar{\gamma}(\phi_t\phi^*-\phi_t^*\phi^*)-(f\phi^*+f^*\phi).\end{aligned} \quad (21)$$

where $f=E_0\mathrm{e}^{-i\Omega t}$ and substituting into the Euler-Lagrange equation using $L=\int_{-\infty}^{\infty}\mathscr{L}d\xi$, $\int_{-\infty}^{\infty}\mathrm{sech}(a\xi)d\xi=\pi/a$ and $\int_{-\infty}^{\infty}\mathrm{sech}^2(a\xi)\tanh(a\xi)d\xi=0$ yields,

$$(1+i\bar{\gamma})\eta\dot{\zeta}-4a\theta \quad = \quad 2\eta\frac{\partial F}{\partial\eta}-\frac{\partial F}{\partial\theta} \quad (22)$$

$$(1+i\bar{\gamma})\dot{\varphi}-4(a\theta^2-b\eta^2)=\zeta\frac{\partial F}{\partial\zeta}-\eta\frac{\partial F}{\partial\eta}-F \quad (23)$$

where

$$F=\int_{-\infty}^{\infty}\left(f\mathrm{e}^{i[\theta x+\varphi]}+f^*\mathrm{e}^{-i[\theta x+\varphi]}\right)\mathrm{sech}[\eta(x-\zeta]dx. \quad (24)$$

Numerical methods by using Runge-Kutta methods is used to study this equation. Soliton solution of Eq.(19) by using variational method is depicted in Fig.2. The result show that Davidov's soliton accelerate by an periodic external force. Study of propagation of Davydov's soliton have been studied by montecarlo simulation [1]. The thermal reservoir at temperature T is done by added a damping force and noise force ($F_n=-m\Gamma\beta_n+\eta_n$). This extension converts the dynamics equation of the molecular displacement to Langevin equations. The effect is to bring the system to thermal equilibrium [1]. The study of thermal equlibrium can be done only in the term of statistical mechanics approach. It's still in progress.

SUMMARY

The propagation of Davydov's soliton in an inhomogeneous medium is investigated. By introducing a local

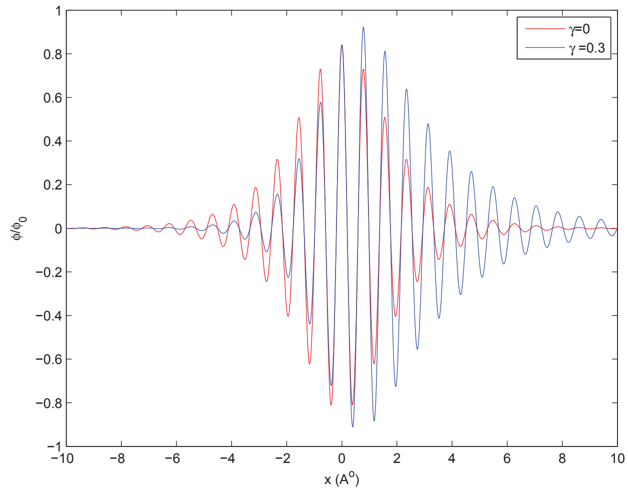

FIGURE 1. Davydov's soliton with dissipation effect.

approximation,the damping factor can be expressed as a new term $i\overline{\gamma}\phi$ in the nonlinear Schrodinger equation. The result show that the soliton with damping propagate slower than without damping effect. It's mean that the damping effect does not contribute into the amplitude of soliton. This term can be viewed as a driving (forcing) or a damping of the soliton solution. Studies of Davydov's soliton in a viscous medium can be done by treating a classical object i.e. replace the term of $i\overline{\gamma}\phi$ by $\gamma\partial\phi/\partial t$. By introducing a periodic external force, the equation of motion is described by the force-damped nonlinear Schrodinger equation. Solution based on the variational methods show that the Davidov's soliton will be accelerated by a periodic external force.

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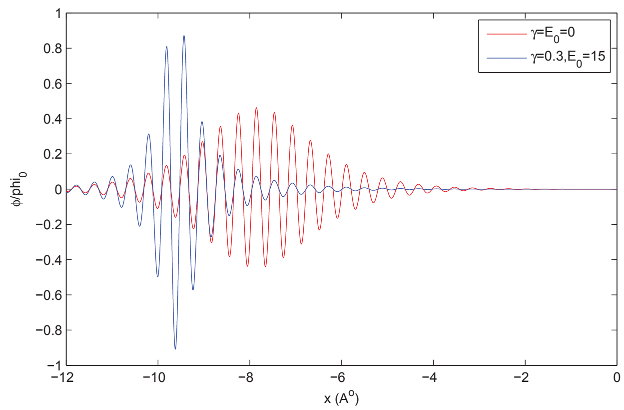

FIGURE 2. Davydov's soliton with dissipation effect and an external force.