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Fractional unstable patterns of energy in $\alpha-$ helix proteins with long-range interactions

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ABSTRACT

Energy transport and storage in $\alpha-$ helix proteins, in the presence of long-range intermolecular interactions, is addressed. The modified discrete Davydov model is first reduced to a space-fractional nonlinear Schrödinger (NLS) equation, followed by the stability analysis of its plane wave solution. The phenomenon is also known as modulational instability and relies on the appropriate balance between nonlinearity and dispersion. The fractional-order parameter (σ), related to the long-range coupling strength, is found to reduce the instability domain, especially in the case $1 \leq \sigma < 2$. Beyond that interval, i.e., $\sigma > 2$, the fractional NLS reduces to the classical cubic NLS equation, whose dispersion coefficient depends on σ. Rogue waves solution for the later are proposed and the biological implications of the account of fractional effects are discussed in the context of energy transport and storage in $\alpha-$ helix proteins.

1. Introduction

Understanding the biological processes related to energy transport and storage in biomolecules remains one of the biggest challenges in molecular biophysics. A broad range of biological metabolisms need that energy, which is in general transported via proteins, initially released through the hydrolysis of adenosine triphosphate (ATP) [1]. Namely, considering the structure of $\alpha-$ helix proteins, Davydov and Kislukha [2,3] used the exciton formalism to explain the self-trapping of the amide-I oscillations as the consequence of the interaction between the vibrational exciton and the distortion in the protein structure resulting from the presence of the exciton. They established that as a result of the interplay between nonlinearity and dispersion, the self-trapped vibrational amide-I energy, coupled to the protein structure deformation, may travel as a soliton in the protein strand [4,5]. Many studies followed that seminal approach, looking for its detailed confirmation both numerically and analytically [5–7]. Therefore, different aspects of the Davydov model were investigated by Daniel and Deepamala [8] in the presence of higher-order molecular excitations, including competitive effects between first and second-neighbor interactions. Confirmation of solitons propagating in the $\alpha-$ helix chain has also been regarded recently by Tabi and coworkers [9–15], following Daniel and Latha [16] formulation of inter-spine coupling among three hydrogen-bonded protein chains. Some other interactions, such as diagonal and off-diagonal coupling of spines, were considered where the authors discussed the process of energy redistribution among adjacent spines [13]. The Davydov model, in presence of long-range (LR) intermolecular interactions, has also been the concern of Aboringong and Dikandé [17] recently. They came to the conclusion that the finiteness of the interactions range was appropriate to predict efficient energy storage and transport in $\alpha-$ helix proteins. Based on the works of Tarasov and Zaslavsky [18,19], it is also possible to reduce lattice models to their fractional formulation, especially when power-law LR interactions are considered. One of our main objectives in this work is to apply such formulation to the Davydov model. We intend to show that the discrete nonlinear Schrödinger (NLS) equation of the Davydov model for $\alpha-$ helix proteins can be reduced to its space-fractional continuum version without loosing originality. In this context, the theory of modulational instability (MI) [20–24] is used to predict the emergence of molecular solitonic structures, with insistence on their response to fractional-order effect. The suitable balance between nonlinear and dispersive effects can lead to a broad range of solitonic waves, including envelope, breathers and Rogue waves (RWs). In plasma and optical physics [25], investigating the close relationship between the occurrence of RWs and MI has been active research direction that remains fully unexploited when it comes to biological systems. In this paper, we show that beyond a threshold value of the fractional-order parameter, the fractional NLS equation reduces to the cubic NLS equation whose dispersion coefficient depends on the fractional-order pa-

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rameter. RW solutions are presented and discussed for this particular case, including some biological implications. Some concluding remarks end the paper.

2. Model and dynamical equation

2.1. Model

The generalized Hamiltonian for a linear chain of amide-I units that make an $\alpha-$ helix has been proposed by Davydov [1,2]. It considers the coupling between amide-I vibration, and displacements of amino-acid residues, and all the interactions are summarized in the following Hamiltonian [1,2,9,17]:

$$H=\sum_n\left[\hbar\omega_0\beta_n^\dagger\beta_n-\sum_{m\neq n}J_{n-m}(\beta_n^\dagger\beta_m+\beta_n\beta_m^\dagger)-D\beta_n\beta_n^\dagger\beta_{n+1}^\dagger\beta_{n+1}\right], \quad (1)$$

with the subscript n referring to the lattice index along a strand (or chain). The expression of H suggests that an individual amino acid will be identified by the index pair n, such that β_n ($\beta_n^\dagger$) are boson creation (annihilation) operators associated with intramolecular vibrations of the nth peptide group. These operators satisfy the usual commutation relations for bosons, i.e., $[\beta_n,\beta_m^\dagger]=\delta_{m,n}$ and $[\beta_n,\beta_m]=0$. $\hbar\omega_0$ is the local amide-I vibrational energy, and the term $\hbar\omega_0\beta_n^\dagger\beta_n$ is the vibrational energy at the site n. The term $\sum_{m\neq n}J_{n-m}(\beta_n^\dagger\beta_m+\beta_n\beta_m^\dagger)$ is the energy related to the LR interactions between molecular excitations on sites n and m, belonging to the same chain. The coupling parameter J_{n-m} is the LR transfer integral between sites n and m, here considered of the form Etémé et al. [26–29]:

$$J_{n-m}=J_0|n-m|^{-s}, \quad (2)$$

with J_0 being the strength of the transfer integral and s a parameter range whose values are in the interval $[1,+\infty[$. However s covers different physical contexts, depending on its value. For example if $s\to\infty$, the LR interaction reduces to nearest-neighbor couplings. For $s=5$, the LR interaction is of a dipole-dipole type, while for $s=3$, the LR interaction is of the Coulomb type. We should stress that the strongest interaction effects are due to smaller values of s.

We make use of the Heisenberg formulation and obtain the exciton equation in the form

$$i\hbar\frac{\partial\beta_n}{\partial t}=\hbar\omega_0\beta_n-\sum_{m\neq n}J_{n-m}\beta_m-D(\beta_{n+1}\beta_{n+1}^\dagger+\beta_{n-1}^\dagger\beta_{n-1})\beta_n. \quad (3)$$

In order to study coherent states, it will be useful to rewrite Eq. (3) in terms of eigenfunctions of the operators β_n and $\beta_n^\dagger$ so that, if the Glauber coherent states $|\{\gamma_n\}\rangle=\prod_n|\gamma_n\rangle$ and $b_n|\gamma_n\rangle=\gamma_n|\gamma_n\rangle$ are introduced [30], Eq. (3) becomes

$$i\hbar\frac{\partial\gamma_n}{\partial t}=\hbar\omega_0\gamma_n-\sum_{m\neq n}J_{n-m}\gamma_m-D(|\gamma_{n+1}|^2+|\gamma_{n-1}|^2)\gamma_n, \quad (4)$$

which is a discrete nonlinear Schrödinger (DNLS) equation. We can get rid of the term in $\hbar\omega_0\gamma_n$ via the gauge transformation $\gamma_n(t)=u_n(t)e^{-i\omega_0 t}$. This yields the DNLS equation

$$i\frac{\partial u_n}{\partial t}=-\sum_{m\neq n}J_{n-m}u_m-D(|u_{n+1}|^2+|u_{n-1}|^2)u_n, \quad (5)$$

where we have further made the change of variable $t\to t/\hbar$.

2.2. The NLS equation with fractional derivative

In order to derive the fractional-derivative version of Eq. (5), we introduce the functions [18,19,31]

$$\phi(k,t)=\sum_{m=-\infty}^{+\infty}e^{-iknd}u_n(t) \text{ and } J(k)=\sum_{m=-\infty}^{+\infty}e^{-iknd}J_n, \quad (6)$$

where the parameter k is a wavenumber, d is the lattice spacing and J_n is given by Eq. (2). Inversely, the function $u_n(t)$ is related to $\phi(k,\ t)$ through the formula

$$u_n(t)=\int_{-\pi}^{\pi}e^{iknd}\phi(k,t)dk. \quad (7)$$

In the continuum approximation, i.e., $u_n(t)\to u(x,\ t)$, with $x=nd$, when $k\to 0$, relations (6) and (7) become

$$\phi(k,t)=\int_{-\infty}^{+\infty}e^{-ikx}u(x,t)dx \text{ and}$$
$$u(x,t)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{ikx}\phi(k,t)dk. \quad (8)$$

Applying all the above to Eq. (5) in the continuum approximation leads to

$$i\frac{\partial u(x,t)}{\partial t}=-J(0)u(x,t)-\int_{-\infty}^{+\infty}dydxK(x-y)\frac{\partial u(x,t)}{\partial x} -2D|u(x,t)|^2u(x,t), \quad (9)$$

where the Kernel $K(x)$ is given by

$$K(x)=\frac{1}{\pi}\int_{-\infty}^{+\infty}e^{ikx}\frac{G(k)}{k^2}dk, \quad (10)$$

with $G(k)=J(0)-J(k)$, $J=\zeta(s)^{-1}$, with the $\zeta-$ function being given by $\zeta=\sum_{1=1}^{\infty}n^{-s}$. For the specific case, where $2\le s<3$, the function $G(k)$ is in the form

$$G(k)=\frac{\pi J_0}{\Gamma(\sigma+1)\sin\left(\frac{\pi\sigma}{2}\right)}|k|^\sigma, \quad (11)$$

where where $\Gamma(\sigma)$ is the $\Gamma-$ function, with $\sigma=s-1$ and $\Gamma(\sigma+1)=\sigma\Gamma(\sigma)$. Therefore, given the possible values of s, the values of σ will be found between 1 and 2. Under such considerations, the continuum Eq. (9) takes the form

$$i\frac{\partial u(x,t)}{\partial t}=-J(0)u(x,t)-P_\sigma\frac{\partial^\sigma}{\partial|x|^\sigma}u(x,t)-2D|u(x,t)|^2u(x,t), \quad (12)$$

where the coefficient P_σ is given by

$$P_\sigma=\frac{\pi J_0}{\Gamma(\sigma+1)\sin\left(\frac{\pi\sigma}{2}\right)}. \quad (13)$$

The Riesz fractional derivative is given by Uchaikin [32,33]

$$\frac{\partial^\sigma}{\partial|x|^\sigma}u(x,t)=-\frac{1}{2\pi}\int_{-\infty}^{+\infty}|k|^\sigma\phi(k,t)dk. \quad (14)$$

By making use of the gauge transfomation $u(x,t)\to u(x,t)e^{iJ_0t}$, we finally find the equation

$$i\frac{\partial u(x,t)}{\partial t}=-P_\sigma\frac{\partial^\sigma}{\partial|x|^\sigma}u(x,t)-Q|u(x,t)|^2u(x,t), \quad (15)$$

which is the NLS equation with space fractional derivative term. We have also fixed $Q=2D$, which is the nonlinearity parameter. Obviously, the dispersion term P_σ is a function of the fractional-order parameter σ. However, the Riesz fractional derivative is also expressed as [32,33]

$$\frac{\partial^\sigma}{\partial|x|^\sigma}u(x,t)=-\left(-\frac{\partial^2}{\partial|x|^2}\right)^{\sigma/2}u(x,t) =-\frac{1}{2\cos\left(\frac{\pi\alpha}{2}\right)}\left[\mathcal{D}_+^\sigma u(x,t)+\mathcal{D}_-^\sigma u(x,t)\right], \quad (16)$$

where $\mathcal{D}_+^\sigma u(x,t)$ and $\mathcal{D}_-^\sigma u(x,t)$, are the left- and right-side Riemann–Liouville fractional derivatives of order σ, that are respectively given by [32,33]