Physica A 407 (2014) 76–85

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Nonlinear excitations in a disordered alpha-helical protein chain

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HIGHLIGHTS

- The multisoliton interaction in alpha-helical proteins is studied.
- The effect of disorder is investigated using a perturbative technique.
- Inhomogeneity introduces fluctuations in the profile of the solitons.
- Modulation instability occurrence and the stability of soliton is also investigated.

ARTICLE INFO

Article history:
Received 6 November 2013
Received in revised form 7 February 2014
Available online 31 March 2014

Keywords:
Soliton
Nonlinear Schrödinger equation

ABSTRACT

We investigate the dynamics of alpha-helical proteins with dipole and quadrupole type molecular excitations. Performing the symbolic computation on the iterative algorithm of Darboux transformation, we present the multisoliton solutions for the resulting fourth order nonlinear Schrödinger (NLS) equation and study the energy sharing properties. We also study the effect of disorder (inhomogeneity) using the perturbative technique and found that the inhomogeneity in the hydrogen bonding spines introduces fluctuations in the profile of the solitons without affecting their robust nature and the propagation.

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1. Introduction

One of the important secondary structures of protein is the alpha-helical structure in which the basic helix follows the sequence . . .–N–C–C–N–C–C–N–C–C. . . with a pitch of 5.4 Å. Superimposed on this basic structure are three spines which are almost longitudinal with the sequence . . .H–N–C=O. . .H–N–C=O. . . H–N–C=O. . . where C = O represents the locus of the amide-I vibration and the dotted lines denote the longitudinal hydrogen bond that holds the structure in its helical form. In the biological context, the mechanism for transport along alpha-helical proteins of the free energy released by hydrolysis of adenosine triphosphate (ATP) (≈0.42 eV or 3350 cm) continues to be investigated. In 1973, a novel mechanism for the localization and transport of vibrational energy in protein was proposed by A.S. Davydov [1]. According to him, the vibrational energy of the C = O stretching (or Amide-I) oscillators that is localized on the helix acts through a phonon coupling to trap the amide-I oscillation energy and prevents its dispersion in the form of self localized structure called soliton. The seminal properties of Davydov's model continues to encourage intense work on the dynamics of alpha-helical proteins both at the discrete and continuum levels [2–23] considering only a single spine. Moreover Interspine oscillation has been found to arise from the three spine alpha-helical symmetry and the effect of lower order interactions in the three spine structure has also been analyzed at both the levels [24–27]. Very recently the present authors [28,29] have studied

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http://dx.doi.org/10.1016/j.physa.2014.03.087
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the multisoliton interaction in alpha helical proteins with interspine coupling in the discrete level. But as far as we know no work concerning the study of multisoliton interaction in alpha helical proteins at higher order has been presented in the literature. Constructing multisoliton solution is of physical interest since it provides analytic results of solitonic excitations. Hence in this work we study the interaction properties of multisolitons in alpha-helical proteins with higher order molecular excitations and interactions.

In all the works reported earlier, only homogeneous hydrogen bonding spine is considered for analysis. However in nature, the constitution of the alpha-helical protein molecular chain is sequence dependent (inhomogeneous). In alpha-helical proteins, inhomogeneity may arise due to the presence of additional molecules such as drugs in specific sites of the sequence. Also the inhomogeneity in dipole–dipole interactions in proteins may be due to the following reasons, (i) the distance between neighbouring atoms may vary along the lattices, (ii) the atomic wave functions may vary from site to site or (iii) there may be imperfections in the vicinity of bond. Hence we also investigate the effect of inhomogeneity in the dynamics of protein chain. In our present study, we propose a model Hamiltonian with higher order excitations and interactions using the second quantized operators and construct the equations of motion by applying the principles of quantum mechanics. We construct the multisoliton solutions to the resulting higher order NLS equation via the Darboux transformation technique. In case of the inhomogeneous protein chain, we investigate the nature of soliton propagation and the effect of inhomogeneity by using a perturbation technique.

The paper is structured as follows. In Section 2, we consider the model representing the effects of higher order molecular excitations and interactions with its nearest and next nearest neighbours in alpha-helical protein chain. In Section 3, we construct multisoliton solutions for the resulting fourth order NLS equation using a simple but powerful method called Darboux transformation and study the nature of energy transfer along the hydrogen bonding spines of alpha-helical proteins. In Section 4, we propose a model representing inhomogeneous alpha-helical protein chain with dipole and quadrupole type molecular excitations and nearest and next nearest neighbour molecular interactions. We construct the exact travelling wave solution from a perturbative technique in Section 5 and study the effect of inhomogeneity. The results are concluded in Section 6.

2. The model

We consider a homogeneous alpha helical protein chain with dipole and quadrupole type molecular excitations and nearest and next nearest neighbour molecular interactions. The Hamiltonian which consists of six components is written as [15]

$$H = H_1 + H_2 + H_3 + H_4 + H_5 + H_6. \tag{1}$$

In Eq. (1), H_1 stands for the exciton Hamiltonian representing internal molecular excitations. If E_0 is the amide-I excitation energy and $B_n^\dagger$ is an operator for creation of this excitation on the nth peptide group, then H_1 is given by

$$H_1 = \sum_n B_n^\dagger [E_0 B_n - J_0(B_{n+1} + B_{n-1})], \tag{2}$$

where the summation is carried out over all N peptide groups. The first term $E_0 B_n^\dagger B_n$ defines the amide-I excitation energy and the second term describes the resonance dipole–dipole interaction between nearest neighbours. The operators $B_n^\dagger B_{n+1}$ and $B_n^\dagger B_{n-1}$ represent the transfer of amide-I energy from peptide group n to $n \pm 1$ due to the dipole–dipole interaction. The dipole–dipole interaction energy J_0 is given by $2|d|^2/R^3$, which is the usual electrostatic energy associated with two collinear dipoles of moment d separated by the distance R. The energy H_2 associated with displacing the peptide groups away from their equilibrium positions is given in the harmonic approximation by

$$H_2 = \sum_n \frac{1}{2}\left(\frac{p_n^2}{m} + K_1(u_n - u_{n-1})^2 + K_2(u_n - u_{n-2})^2\right), \tag{3}$$

where u_n is the operator for the longitudinal displacement of peptide group parallel to the helical axis from its equilibrium position, p_n is the momentum operator conjugate to u_n, m is the mass of the peptide group, K_1 and K_2 are spring constants or elasticity coefficients of the hydrogen bonds associated with the nearest neighbours and the next nearest neighbours respectively. The first term is the kinetic energy, the second and the third terms represent the potential energy due to the nearest and next nearest neighbour interactions respectively. H_3 is the Hamiltonian for the interaction between the amide-I excitation and the displacements of the peptide groups which takes the form

$$H_3 = \sum_n \chi_1(u_{n+1} - u_{n-1}) B_n^\dagger B_n, \tag{4}$$

where the coupling constant χ_1 represents the change in amide-I energy per unit extension of an adjacent hydrogen bond. The component H_4 represents quadrupole type molecular excitations which can be written as

$$H_4 = \sum_n B_n^\dagger [E_1 B_n B_n^\dagger B_n - J_1(B_{n+1} B_n^\dagger B_{n+1} + B_{n-1} B_n^\dagger B_{n-1})], \tag{5}$$

where E_1 describes the higher order (quadrupole type) excitations of the molecules in each unit cell and J_1 is the quadrupole–quadrupole type coupling between the adjacent unit cells. The energy H_5 for the interaction between the amide-I excitation

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