Soliton excitations in a three-spine alpha-helical protein chain with quintic non-linearity

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HIGHLIGHTS

- The dynamics of three-spine alpha-helical proteins with quintic non-linearity is studied.
- The dynamics is studied in the continuum levels.
- The resulting equations are solved analytically.
- The solution supports the propagation of the energy in the form of solitons in alpha-helical proteins.
- The conditions for modulation instability occurrence and the stability of solitons have been found.

ARTICLE INFO

ABSTRACT

We study the dynamics of a three-spine alpha-helical protein chain with quintic non-linearity. The dynamics is found to be governed by a perturbed three-coupled non-linear Schrödinger (NLS) equation. To investigate the solitonic aspects, we identify a completely integrable three-coupled cubic–quintic NLS equation by deriving the Lax pair of operators associated with it. In addition, we study the modulation instability aspects and obtain the conditions for soliton formation.

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1. Introduction

In alpha-helical proteins, a sequence of peptide groups (H–N–C=O) forms the helical structure which is stabilised by three quasi-linear strands of hydrogen bonds between the NH and CO groups of the main chain. Within each peptide group, quantum transitions occur due to the vibrational structure of the C=O double bond (amide-I) in the region of the infrared frequency spectrum. Phonons will propagate through the system from one group to another, thereby introducing dispersive effects. Davydov [1] considered a mathematical model to study the energy transfer in alpha-helical proteins, and he showed that the transport of the hydrolysis energy of adenosine triphosphate (ATP) along alpha-helical proteins is through the formation of solitons moving without loss of energy [2–7]. Soon after this discovery, the non-linear excitations in alpha-helical protein chains were investigated by various authors [8–36]. However, in all the above works, the dynamics of a single molecular spine was considered. Recently analytical studies on the dynamics of a slightly modified Davydov model were also made [37–40], both at the discrete and at the continuum levels, giving consideration to the interspine coupling, and the excitations were found to be governed by soliton modes. However, so far no work on the effect of quintic non-linearity in alpha-helical proteins has been reported in the literature. Hence, in this work we study the effect of quintic non-linearity in the energy transfer in three-spine alpha-helical proteins by proposing a suitable Hamiltonian incorporating higher-order molecular excitations and interactions.

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The article is organised as follows. In Section 2, we consider a three-spine alpha-helical protein model including higher-order molecular excitations, nearest and next-nearest-neighbour interactions which introduce quintic non-linearity in the system. The dynamical equations associated with the model are derived using the Hamilton equations of motion. An integrable equation exhibiting soliton solutions has been identified for a specific choice of parameters. The integrability aspects of the resulting equations have been investigated by deriving a Lax pair of operators through Ablowitz, Kaup, Newell and Segur (AKNS) formalism and the details are given in Section 3. In Section 4, we construct the multi-soliton solutions using the Darboux transformation technique. The modulation instability (MI) aspects of our resultant integrable model are studied in Section 5 and the results are presented in Section 6.

2. The model

We consider a three-spine alpha-helical protein chain with internal molecular excitations, dipole–dipole interactions between nearest and next-nearest-neighbour molecular excitations and interspine coupling. The Hamiltonian, which consists of seven components, is written as

$$H = H_1 + H_2 + H_3 + H_4 + H_5 + H_6 + H_7. \tag{1}$$

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

$$H_1 = \sum_{n,\alpha,\rho} \left[B_{n,\alpha}^\dagger \left(E_0 B_{n,\alpha} - J_0 B_{n+\rho,\alpha} \right) \right]. \tag{2}$$

The summation with respect to n runs over the unit cells (H–N–C=O) along the infinite hydrogen-bonding spines and the summation over α runs over the three hydrogen-bonding spines ($\alpha = 1, 2, 3$) and $\rho = 1$ and -1 represent the nearest-neighbour unit cells of peptides along the hydrogen-bonding spine. The first term $E_0 B_{n,\alpha}^\dagger B_{n,\alpha}$ defines the amide-I excitation energy. The operators $B_{n,\alpha}^\dagger B_{n+1,\alpha}$ and $B_{n,\alpha}^\dagger B_{n-1,\alpha}$ 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 written as

$$H_2 = \sum_{n,\alpha} \frac{1}{2} \left[\frac{p_{n,\alpha}^2}{m} + \frac{s_{n,\alpha}^2}{m} + L(u_{n,\alpha} - u_{n-1,\alpha})^2 + I(v_{n,\alpha} - v_{n,\alpha-1})^2 \right], \tag{3}$$

where $u_{n,\alpha}$ is the operator for the longitudinal displacement of the peptide group parallel to the helical axis from its equilibrium position in each hydrogen-bonding spine and $v_{n,\alpha}$ that for the displacement along the helical radius. $p_{n,\alpha}$ and $s_{n,\alpha}$ are the momentum operators conjugate to $u_{n,\alpha}$ and $v_{n,\alpha}$, respectively. H_3 is the Hamiltonian for the interaction between amide-I excitation and the displacement of the peptide groups, which is given by

$$H_3 = \sum_{n,\alpha} \left[B_{n,\alpha}^\dagger \left(\chi_1 B_{n,\alpha} + \chi_2 B_{n,\alpha+1}^\dagger B_{n,\alpha+1} + \chi_3 B_{n,\alpha-1}^\dagger B_{n,\alpha-1} \right) (u_{n+1,\alpha} - u_{n-1,\alpha}) \right], \tag{4}$$

where the coupling constants χ_1, χ_2 and χ_3 represent the change in amide -I energy per unit extension of an adjacent hydrogen bond. We write the energy H_4 for the interaction between amide-I excitation and the displacement of the next-nearest peptide groups for same spines as

$$H_4 = \sum_{n,\alpha} [(\chi_4 B_{n,\alpha}^\dagger B_{n+1,\alpha} + \chi_5 B_{n,\alpha+1}^\dagger B_{n+1,\alpha+1} + \chi_6 B_{n,\alpha-1}^\dagger B_{n+1,\alpha-1})(u_{n+2,\alpha} - u_{n,\alpha})$$
$$+ (\chi_7 B_{n,\alpha}^\dagger B_{n-1,\alpha} + \chi_8 B_{n,\alpha+1}^\dagger B_{n-1,\alpha+1} + \chi_9 B_{n,\alpha-1}^\dagger B_{n-1,\alpha-1})(u_{n,\alpha} - u_{n-2,\alpha})] \tag{5}$$

where the coupling constants χ_4, χ_5, ..., χ_9, represent the change in amide-I energy caused by stretching of the helix between two nearest neighbours as well as next-nearest neighbours of the same spine. The Hamiltonian H_5 for the interaction between the amide-I excitation and the displacement of the peptide groups in the nearest neighbouring spines takes the form

$$H_5 = \sum_{n,\alpha,\rho} [B_{n,\alpha-1}^\dagger [\eta_1 B_{n,\alpha} + \eta_2 (B_{n+1,\alpha} - B_{n-1,\alpha})][v_{n,\alpha+\rho} - 2v_{n,\alpha}]]. \tag{6}$$

The internal molecular excitations with quadrupole–quadrupole-type coupling between the adjacent unit cells with the amide-I excitation energy are represented by H_6. It is written as

$$H_6 = \sum_{n,\alpha,\rho} [B_{n,\alpha}^\dagger (E_1 B_{n,\alpha} B_{n,\alpha}^\dagger B_{n,\alpha} - J_1 B_{n,\alpha} B_{n+\rho,\alpha}^\dagger B_{n+\rho,\alpha} - J_2 [B_{n+1,\alpha} B_{n,\alpha+1}^\dagger B_{n+1,\alpha+1} - B_{n-1,\alpha} B_{n,\alpha+1}^\dagger B_{n-1,\alpha+1}]$$
$$- J_3 [B_{n+1,\alpha} B_{n,\alpha-1}^\dagger B_{n+1,\alpha-1} - B_{n-1,\alpha} B_{n,\alpha-1}^\dagger B_{n-1,\alpha-1}] - J_4 [B_{n+1,\alpha} B_{n+1,\alpha+1}^\dagger B_{n,\alpha+1} - B_{n-1,\alpha} B_{n-1,\alpha+1}^\dagger B_{n,\alpha+1}]$$
$$- J_5 [B_{n+1,\alpha} B_{n+1,\alpha-1}^\dagger B_{n,\alpha-1} - B_{n-1,\alpha} B_{n-1,\alpha-1}^\dagger B_{n,\alpha-1}])], \tag{7}$$