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Soliton excitations and shape-changing collisions in alpha helical proteins with interspine coupling at higher order

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ABSTRACT

Based on the Lax representation, we solve the three coupled higher order nonlinear Schrödinger equations with the achievement of *N*-soliton solution formula, by means of Darboux transformation. With the involvement of multi-parameters (actually *21* parameters) in the two-soliton solutions, we investigate the soliton excitations and collisions in alpha helical proteins with interspine coupling at higher order, in virtue of multi-parameter management and graphical simulation. It is found that both elastic and inelastic collisions can take place under suitable parametric conditions. Additionally, there exist three kinds of shape-changing collision patterns among the three components, and the inelastic collision of single solitons occur in two different manners: enhancement or suppression of intensity. Our results of multi-parameter management analysis may give theoretical support as well as further impetus in the experimental investigation on soliton excitations, elastic and inelastic collisions in alpha helical proteins with interspine coupling at higher order.

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1. General model

In the 1970s, Davydov proposed a nonlinear mechanism for the storage and transfer of vibrational energy (intrapeptide vibration amide-I) in alpha helical proteins [1], and indicated that the self-trapping of the amide-I vibration takes place due to 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 [1,2]. In the continuum approximation, it has also been demonstrated that the corresponding system of equations for a molecular chain admits a solitonic solution, which describes a constant-velocity self-trapped quasi-particle (a lump of vibrational amide-I energy) accompanied by a self-consistent chain deformation [3,4]. The solitons in protein molecules are generated based on the dynamical balance between the dispersion resulted from the resonant interaction of intrapeptide dipole vibrations and the nonlinearity provided by the interaction of these vibrations with the local displacements of the equilibrium positions of the peptide groups [3]. By giving different initial conditions of the chain, dynamical properties of Davydov solitons and their formation have been investigated in discrete chains and in continuum models [4,5]. Afterwards,

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various properties of such one-dimensional polaronlike self-trapped states have been analytically and/or numerically studied [5,6].

Soliton excitations in discrete and continuum alpha helical proteins have attracted much attention [7–13]. Devoted to Davydov soliton models, investigation was mainly focused on the following aspects, among others, as: (i) higher order molecular excitation/interaction effects and the discreteness effect; (ii) nonlinear molecular excitations along the three hydrogen bonding spines of alpha helical proteins with interspine coupling at the discrete and continuum levels; (iii) generalized Davydov models with higher order molecular interactions and excitations of dipole and quadrupole types with appropriate nonlinear coupling with phonons; (iv) the dynamics of alpha helical proteins with next nearest neighbor interactions and interspine coupling at higher order in the continuum limit; (v) the role of the helical symmetry in the formation, stability, and dynamical properties of Davydov solitons in an alpha helical proteins, and (vi) electron/proton transport in alpha helix sections of proteins.

Generally speaking, the molecular dynamics along the hydrogen bonding spine in alpha helical proteins, with dipole-dipole interactions in the lower order of continuum approximation, is governed by the completely integrable cubic nonlinear Schrödinger (CNLS) equation[1] (see, e.g., Eq. (2.17) in Ref. [7], or Eq. (3.1) in Ref. [10]). It is well known that the CNLS equation possesses bilinear form, Bäcklund transformation, Lax representation and *N*-soliton solution. It can be used to describe the dynamics of spins in an isotropic ferromagnet in the classical continuum limit, and the detailed derivation of its origination in alpha helical proteins can be seen in Refs. [7,10]. In Ref. [15], a possible solitary wave solution of the CNLS equation has been studied in DNA dynamics and it is shown that the wave can be both modulated and nonmodulated depending on a ratio of the envelope and the carrier wave velocities. Moreover, the ratio of these two velocities is a measure of modulation, and the modulated wave is more stable than the nonmodulated one.

Through considering a generalized model Hamiltonian for the alpha helical protein chain with different molecular interactions and excitations, Ref. [10] has derived the dynamical equations in the continuum limit. At different orders of the lattice parameter under continuum approximation, the governing nonlinear dynamical equations are identified to be generalized Davydov models, i.e., Eqs. (3.1), and (3.10) with (3.30) in Ref. [10] and their reductions with suitable transformation and rescalings therein. These equations describe the dynamics of alpha helical proteins internal molecular excitations and interactions with their nearest and next-nearest neighbors, and also nonlinear couplings between lattice vibrations and molecular excitations/interactions. From their perturbed solitons and the perturbation analysis, the nature of nonlinear molecular excitations and the transfer of amide-I energy along the hydrogen bonding spine at different orders (including higher orders) of the lattice parameter can be separately understood.

In the calculations mentioned above, however, the dynamics of a single molecular chain along the hydrogen bonding spine has been considered in the continuum limit, and the interspine coupling with the neighboring hydrogen bonding spines was neglected. Actually, the interspine coupling among unit cells of the neighboring hydrogen bonding spines plays a vital role in real situations, and these macromolecular systems are discrete in nature. The nature of nonlinear molecular excitations along the three hydrogen bonding spines of alpha helical proteins with interspine coupling at the discrete and continuum levels has been studied in Ref. [9], and it is found that the molecular excitations are governed by soliton modes.

On the other hand, having found that the molecular dynamics at the lowest order of lattice parameters, with taking into account of the interspine coupling, is governed by soliton modes, Ref. [11] has considered the alpha helical protein model with interspine coupling (also with next nearest neighbor interactions) and, in the continuum limit, derived the dynamical equations explicitly as follows [16–18]:

$$i\,q_{1,t} + \frac{1}{2}\,q_{1,xx} + \left(|q_1|^2 + |q_2|^2 + |q_3|^2\right)q_1 - i\,\gamma\left[q_{1,xxx} + 3\left(|q_1|^2 + |q_2|^2 + |q_3|^2\right)q_{1,x}\right.$$
$$\left. + \ 3(q_1^* q_{1,x} + q_2^* q_{2,x} + q_3^* q_{3,x})\,q_1\right] = 0,\tag{1a}$$

$$i\,q_{2,t} + \frac{1}{2}\,q_{2,xx} + \left(|q_1|^2 + |q_2|^2 + |q_3|^2\right)q_2 - i\,\gamma\left[q_{2,xxx} + 3\left(|q_1|^2 + |q_2|^2 + |q_3|^2\right)q_{2,x}\right.$$
$$\left. + \ 3(q_1^* q_{1,x} + q_2^* q_{2,x} + q_3^* q_{3,x})\,q_2\right] = 0,\tag{1b}$$

$$i\,q_{3,t} + \frac{1}{2}\,q_{3,xx} + \left(|q_1|^2 + |q_2|^2 + |q_3|^2\right)q_3 - i\,\gamma\left[q_{3,xxx} + 3\left(|q_1|^2 + |q_2|^2 + |q_3|^2\right)q_{3,x}\right.$$
$$\left. + \ 3(q_1^* q_{1,x} + q_2^* q_{2,x} + q_3^* q_{3,x})\,q_3\right] = 0,\tag{1c}$$

where $q_j(x, t)$ $(j = 1, 2, 3)$ represents the amplitude of molecular excitation in the *j*th spine, γ is an arbitrary real parameter, the subscripts *t* and *x* denote the "temporal" and "spatial" partial derivatives and $*$ means the complex conjugate. Via the Hirota bilinear method, Eqs. (1) have been solved with the achievement of one- and two-soliton solutions leading to a study on the dynamic properties of alpha helical proteins with next nearest neighbor interactions and interspine coupling at higher order [11]: (i) the molecular excitations along the three hydrogen bonding spines are governed by soliton modes for specific choices of parameters, and (ii) the solitons propagating along the neighboring spines collide inelastically and share the energy among them. In the context of optical communication, it is also noticeable that Eqs. (1) govern the propagation of light pulses with such

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[1] Additionally, another discrete model which is of nonintegrable classical Ablowitz–Ladik type was reported by Kundu and the analysis of the model was made by using a perturbation method, see Ref. [14] for details.