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Effect of inhomogeneity in energy transfer through alpha helical proteins with interspine coupling

S. Saravana Veni *, M.M. Latha

Department of Physics, Women's Christian College, Nagercoil 629 001, India

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ABSTRACT

The dynamics of homogeneous and inhomogeneous alpha helical proteins with interspine coupling is under investigation in this paper by proposing a suitable model Hamiltonian. For specific choice of parameters, the dynamics of homogeneous alpha helical proteins is found to be governed by a set of completely integrable three coupled derivative nonlinear Schrödinger (NLS) equations (Chen–Lee–Liu equations). The effect of inhomogeneity is understood by performing a perturbation analysis on the resulting perturbed three coupled NLS equation. An equivalent set of integrable discrete three coupled derivative NLS equations is derived through an appropriate generalization of the Lax pair of the original Ablowitz–Ladik lattice and the nature of the energy transfer along the lattice is studied.

1. Introduction

In recent years the problem of energy transport in biological macromolecules has been referred to as a "crisis" owing to the fact that estimates of lifetimes for molecular excitations based on linear dynamics are too short to be reconciled with known features of the biological processes to which they contribute. A resolution of the problem was proposed by Davydov [1], who suggested that the dispersion responsible for the short lifetime of an excitation might be offset by a focusing of the excitation through the nonlinear character of the interatomic forces (e.g., as may arise from hydrogen bonding in polypeptides). He suggested that the amide-I energy could stay localized through the nonlinear interactions of the vibrational excitation with the deformation in the protein structure caused by the presence of the excitation.The excitation and the deformation balance each other to form a soliton. Thus the bio energy can move along the protein molecules in virtue of the motion of the soliton. Since the pioneering work of Davydov [2–7], various properties of Davydov solitons and their formation, given various initial conditions of the chain have been investigated in discrete and continuum models [8–37]. In all the above models only a single spine is considered. However in reality alpha helices contain three strands, each of which contain periodically placed peptide groups connected by hydrogen bonds. A three strand model for an alpha helix was proposed in [38], where the stationary states were studied. This model represents an alpha helix as a three strand structure with three peptide groups per cell in a plane perpendicular to the protein axis. A detailed analytical study on the dynamics of a slightly modified Davydov's model of alpha helical proteins with interspine coupling was also studied both at the discrete and continuum levels giving consideration to the interspine coupling and the dynamics was found to be governed by a set of integrable three coupled perturbed NLS equation [39–43]. Recently studies on the 3D nature of the helix for describing amide-I exciton-mediated energy flow have also been reported [44–48]. In all the above mentioned studies, the alpha helical proteins in homogeneous hydrogen bonding spine is considered for the analysis. However in nature, the presence of different sites along the hydrogen bonding spine makes the molecules site dependent or inhomogeneous. Also defects caused due to

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* Corresponding author. Tel.: +91 9952369860.
E-mail address: veni85s@ymail.com (S.S. Veni).

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the presence of external molecules in the spines lead to inhomogeneity. Thus it has become important and necessary to investigate the internal dynamics of solitons in inhomogeneous alpha helical proteins with interspine coupling. Motivated by this, we propose a model for homogeneous and inhomogeneous alpha helical proteins by including excitations, dipole–dipole interactions between nearest neighbours and next nearest neighbours and interspine coupling. The underlying nonlinear dynamics is investigated by solving the governing equations of motion.

The paper is organized as follows. In Section 2 we propose a model for the homogeneous alpha helical proteins and derive the dynamical equations. We construct the exact travelling wave solutions for the resulting equations by employing the standard extended tanh function analysis and the details are given in Section 3. We introduce a model for inhomogeneous alpha helical proteins with interspine coupling and derive the corresponding equations of motion in Section 4. The effect of inhomogeneity on solitonic excitations is investigated in Section 5 by deriving the exact solutions for the resulting equations. For a specific choice of physical parameters the dynamics is found to be governed by a set of completely integrable three coupled derivative NLS (Chen–Lee–Liu) equations in Section 6. We derive the set of equivalent integrable discrete three coupled derivative NLS equations using the Ablowitz–Ladik formulation and demonstrate the soliton interaction by means of numerical analysis and study the energy sharing properties of the solitons in the discrete alpha helical protein lattices. The results are concluded in Section 7.

2. The model

The Hamiltonian with interspine coupling for a system of three coupled infinite molecular chains with unit cells H—N—C=O characterizing the three hydrogen bonding spines of peptide groups running parallel to the helical axis in an alpha helical protein is given by

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

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

$$H_1 = \sum_{n,\alpha} B^\dagger_{n,\alpha}[E_0 B_{n,\alpha} - J(B_{n+1,\alpha} + B_{n-1,\alpha}) - L(B_{n,\alpha+1} + B_{n,\alpha-1}], \tag{2}$$

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 ($\alpha = 1, 2, 3$). $B^\dagger_n$ and B_n represent the creation and annihilation operators for the internal molecular excitation of the peptide group labelled by n. The first term $E_0 B^\dagger_{n,\alpha} B_{n,\alpha}$ defines the amide-I excitation energy and the second term the resonance dipole–dipole interaction between nearest neighbours. The operator $B^\dagger_{n,\alpha} B_{n+1,\alpha}$ and $B^\dagger_{n,\alpha} B_{n-1,\alpha}$ 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 is given by $2|d|^2/R^3$, which is the usual electrostatic energy associated with two collinear dipoles of moment d (0.3 Debye) separated by the distance R (2.8 Å) and L is the excitation exchange between the spines. The energy H_2 associated with displacing the peptide groups away from their equilibrium positions is given in the harmonic approximation by

$$H_2 = \sum_{n,\alpha} \frac{1}{2}\left(\frac{p^2_{n,\alpha}}{m} + \frac{s^2_{n,\alpha}}{m} + K(u_{n,\alpha} - u_{n-1,\alpha})^2 + I(v_{n,\alpha} - v_{n,\alpha-1})^2\right), \tag{3}$$

where $u_{n,\alpha}$ is the operator for the longitudinal displacement of 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. m is the mass of the peptide group. K and I are the elasticity coefficients relative to changes in helix pitch and helix radius respectively. H_3 is the Hamiltonian for the interaction between amide-I excitation and the displacement of the peptide groups and is given by

$$H_3 = \sum_{n,\alpha}(\chi_1 B^\dagger_{n,\alpha} B_{n,\alpha} + \chi_2 B^\dagger_{n,\alpha+1} B_{n,\alpha+1} + \chi_3 B^\dagger_{n,\alpha-1} B_{n,\alpha-1})(u_{n+1,\alpha} - u_{n-1,\alpha}), \tag{4}$$

where the coupling constant χ_1, χ_2 and χ_3 represent the change in amide-I energy caused by stretching of the helix in the same spine. The energy H_4 for the interaction between amide-I excitation and the displacement of the next nearest peptide groups for same spines is written as

$$\begin{aligned} H_4 = \sum_{n,\alpha}&(\chi_4 B^\dagger_{n,\alpha} B_{n+1,\alpha} + \chi_5 B^\dagger_{n,\alpha+1} B_{n+1,\alpha+1} + \chi_6 B^\dagger_{n,\alpha-1} B_{n+1,\alpha-1})(u_{n+2,\alpha} - u_{n,\alpha}) + (\chi_7 B^\dagger_{n,\alpha} B_{n-1,\alpha} + \chi_8 B^\dagger_{n,\alpha+1} B_{n-1,\alpha+1} \\ &+ \chi_9 B^\dagger_{n,\alpha-1} B_{n-1,\alpha-1})(u_{n,\alpha} - u_{n-2,\alpha}), \end{aligned} \tag{5}$$

where the coupling constants $\chi_4, \chi_5, \ldots, \chi_9$ 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 can be written as