

Charge and energy transfer by solitons in low-dimensional nanosystems with helical structure

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Abstract

We study the nonlinear mechanism of the energy and charge transfer in low-dimensional nanosystems with helical structure. We show that the helical symmetry is important for the formation, stability and dynamical properties of the soliton-like self-trapped electron states. We obtain several types of stationary soliton solutions, namely single-band and hybrid two-band solitons which possess different energies. The two-band hybrid soliton spontaneously breaks the local translational and helical symmetries. For the values of the parameters of α -helical proteins this soliton possesses the lowest energy as compared with other types of solitons. This soliton has an inner structure which is manifested by a modulated multi-hump amplitude distribution of excitations on the individual strands of hydrogen bonds, identified in the helix. The displacement of such a soliton along the helix reveals distinctly the complex and composite structure of the soliton and causes oscillations of the energy distributions between the strands of hydrogen bonds. We show that the frequency of these oscillations is proportional to the soliton velocity. The radiative life-time of this hybrid soliton is calculated and shown to exceed by several orders of magnitude the life-time of a soliton excitation in a three-strand macromolecule without helical structure. The other two soliton solutions are formed by single-band states. These solitons preserve the helical symmetry, but in the α -helix they are dynamically unstable: once initially formed, they transform into the ground hybrid soliton state when propagating along the chain.

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1. Introduction

Although the problem of charge and energy transfer in low-dimensional nanosystems such as macromolecular proteins, conducting polymers and recently synthesized nanotubes, has been studied for many years, many open questions remain and several mechanisms of the transfer have been put forward and investigated. The interest in such systems has increased because of their applications in nanotechnologies, microelectronics, information storage devices and biosensors. One of the mechanisms for the

energy storage and charge transport in low-dimensional systems was suggested in the 1970s by Davydov [1] and intensively developed since then (reviews can be found in [2–5]). This mechanism describes the transfer of a quantum of energy or of a charge in the form of the self-trapped soliton state propagating along a molecular chain. Such a state represents a quasiparticle (vibrational excitation, exciton, electron or a hole) which interacts with the deformation of the chain, due to which it is localised within a few lattice sites and, together with a self-consistent distortion of the chain, propagates at a constant velocity. In particular, in proteins, a quantum of energy is released as a result of the hydrolysis of the adenosine triphosphate into adenosinediphosphate. This energy is initially stored in the vibration mode of the double C=O bond of an individual peptide group (PG), called intrapeptide Amid-I vibration,

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and then re-distributed to the nearest neighbouring PGs. Usually molecular systems are modelled by an isolated chain with one exciton (electron) band and one phonon mode corresponding to one atom per unit cell. Real systems have much more complicated structures. Furthermore, some of them, like α -helical proteins, have three such chains (strands or sometimes called spines) of PGs connected by hydrogen bonds along each strand, and possess certain helicity properties. The first attempt to take into account the more complex structure of a protein within such a model has been undertaken by Davydov and Soopron [6], who modelled the α -helix as a three-strand structure with three PGs per cell in a plane perpendicular to the protein axis. Afterwards, the properties of such soliton states were studied analytically in [7,8] and numerically in [9,10]. The model was further improved in [11,12] where a more realistic helical structure of the protein was taken into account. They also found, in an analytical form, the soliton solutions which do not break the chiral symmetry. The detailed numerical study of this problem was carried out by Scott in [11] who has shown that an initial excitation localised on two of the three PGs at the end of the chain, evolves into a soliton which propagates along the protein at a constant velocity with some oscillations of the energy between the strands, which were called ‘interspine oscillations’ (in what follows we will also use this term). Recently in [13] it was shown that in a helix there are several types of solitons, which possess different symmetry properties.

In this paper we show that these stationary soliton states are formed in the helical macromolecule by a single-band or by collectivised two-band excitations. The single-band solitons preserve the helical symmetry, while the two-band hybrid soliton spontaneously breaks the local translational and helical symmetries. The dynamical properties of these solitons are different, and depend on the relations between the parameters of the system, including the degree of the helicity. The hybrid soliton has an inner structure which is manifested by a modulated multi-hump amplitude distribution of excitations on individual strands of hydrogen bonds. We show that the propagation of this soliton is accompanied by oscillations of the energy distribution between the three strands of hydrogen bonds. These interspine oscillations are caused by the system helicity and their frequency depends on the soliton velocity. We also calculate the radiative life-time of the hybrid soliton and show that it is several orders of magnitude larger than the life-time of a soliton excitation in a three-strand macromolecule without helicity.

2. Hamiltonian and energy spectrum of a helix

As an example of a helical nanosystem we consider the α -helical macromolecule. The polypeptide chain of such a macromolecule is rolled into a helix which is stabilized by the intra-chain hydrogen bonds between the hydrogen atom of the l -th PG and the oxygen atom of the $l \pm 3$ -th

PG along the chain so that there are 3.6 PGs per helix turn (here l runs over the $3N$ values along the polypeptide chain). The nearest neighbours along the macromolecule are bound together by the rigid valence bonds, while hydrogen bonds between the PGs are relatively soft. The corresponding structure is shown in Fig. 1, where the solid line corresponds to the chain of chemical bonds, and three different dashed lines correspond to the three strands of hydrogen bound molecules. In α -helical proteins these molecules are PGs, and the three strands are also rolled in a superhelix of a large period. These superhelicity can be essential for the interaction of proteins with external electromagnetic fields, but does not affect the properties of the electronic excitations studied in the present paper.

In view of the difference in the softness of the chemical and hydrogen bonds, we can assume that the distances between the l -th and $(l \pm 1)$ -th molecules are fixed, while molecules can displace from their equilibrium positions due to the softness of the hydrogen bonds and free rotation around the single-valent bond. Introducing the double index j, n , where n enumerates sites in the j -th hydrogen bound chain (so called strain or spine) and runs from 1 to N , instead of the number $l = 1, \dots, 3N$ of the site along the polypeptide chain, we can write down the radius-vector in the form:

$$\vec{R}_{j,n} = \vec{R}_{j,n}^{(0)} + \vec{u}_{j,n}. \quad (1)$$

Here $\vec{u}_{j,n}$ is the vector for the displacement of the (n, j) -th site

$$\vec{u}_{j,n} = \vec{e}_{j,n} u_{j,n}. \quad (2)$$

The constraint equations determine the unit vector $\vec{e}_{j,n}$ as the direction of small displacements of the amplitude $u_{j,n}$ without changing the valence bond length.

Therefore, the total Hamiltonian of the helix can be written in the form

$$H = H_q + H_v + H_{\text{int}} \quad (3)$$

where H_q , H_v , and H_{int} are the Hamiltonians which describe the quasiparticle, lattice vibrations and the interaction of the quasiparticle with vibrations, respectively.

The first term can be chosen in the following form:

$$H_q = \sum_l \left(E_0 A_l^\dagger A_l + \sum_m L_m (A_l^\dagger A_{l-m} + A_{l-m}^\dagger A_l) \right). \quad (4)$$

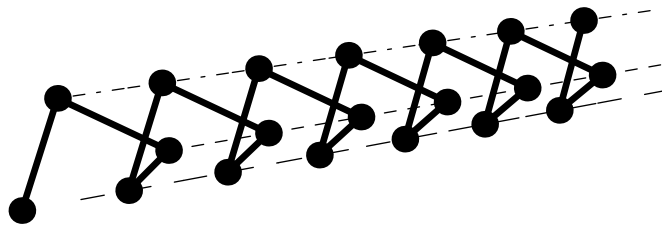


Fig. 1. A schematic model of a nanosystem with helical structure. Solid line corresponds to chemical bonds between the molecules shown by circles, dashed lines correspond to the three strands of hydrogen bonds.

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