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Terahertz Solitons in Biomolecular Systems and their Excitation by External Electromagnetic Field

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Abstract. Nonlinear dynamics of charge and acoustic excitations in cellular microtubules is considered. Different types of nonlinear solitary waves were studied taking account for dissipation. The mechanism of electro-acoustic pulse excitation by external electromagnetic field of terahertz frequency is recognized.

Keywords: soliton, terahertz oscillations

The frequencies of vibrational, vibrational-rotational and tunneling transitions of biological molecules fall into terahertz range (0.1-10 THz). At the moment there exists a significant number of experiments with terahertz exposure of biological objects [1,2]. On molecular level interaction with terahertz radiation can induce conformational changes in proteins and nucleic acids [1-3], and modify membrane permeability [4]. However, the detailed understanding of underlying mechanisms still remains a problem. There exist several theoretical background for DNA [5,6] and cellular membrane [7]. Let us notice that there is strong interest of theoreticians into another important structural component of cell – microtubules. Despite the great number of works in application to cellular signals and energy transfer [8,9], molecular electronics [10], and even hypothesis of quantum computations [11], there is a lack of theoretical or experimental works regarding interaction of terahertz electromagnetic waves with microtubules. The present theoretical study is devoted to cover this gap.

Microtubules are long hollow cylinders with outer diameter 25nm and inner diameter 15 nm. The length of most extensive microtubules in axons of neural cells may reach up to millimeter. Usually a microtubule consists of 13 polymer proto-filaments. Each protofilament is assembled from alternating monomers of α-tubulin and β-tubulin forming together the heterodimer of tubulin. Microtubules play key role at cellular division, secretion, molecular and signal transport.

Phenomena of signal and energy transfer by various structural distortions in microtubules were thoroughly studied using simple one-component models [8,9]. Here a multi-component model describing ferroelectric and elastic properties of microtubule is proposed. Each dimer within protofilament is characterized by a projection of dipole moment on longitudinal axis of microtubule and by deformation of internal bonds and bonds between nearest dimers. The distribution of internal charge in hydrophobic pocket admits two nondegenerate ground states, which characterize different values of longitudinal components of dipole moment and also defines dimer conformation. The description of charge tunneling is done in terms of quantum mechanics, while displacements of large atom groups (deformation) is described classically. As it is usual for most ferroelectrics, a convenient

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approach here is the application of pseudospin variables with transfer to effective single-particle description using the molecular field approximation [12].
The analysis of dynamical equations of motion shows the existence of soliton and breather solutions set. In continuum approximation it is possible to derive explicit analytic expressions. The solitary waves describe bound transfer of polarization and deformation along microtubule. Different modes of nonlinear wave propagation can be considered as a mechanism of cellular signals and energy transfer. As results from calculation the frequency of charge tunneling fall into terahertz range and the frequency of elastic oscillations fall into sub-terahertz range. Starting from this point different modes of interaction with external resonant electromagnetic field are considered. It happens that interaction is parametric, which demands that external field frequency should be twice as large as resonant frequency. The low-amplitude signals were described analytically, while general case was studied by numerical simulation taking into account for thermal fluctuations.

Sequential consideration of dissipation and external exposure results into conclusion that robust steady state nonlinear solitary waves are dissipative structures. In that case signal properties depend not only on microtubule parameters, but mostly on joint action of external factors. We can suppose that revealed mechanism of electro-acoustic signal excitation plays important role in transfer in cellular information and cell reaction on external electromagnetic fields.

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