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Localized modulated waves and longitudinal model of microtubules

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ABSTRACT

We here study nonlinear dynamics of microtubule (MT). A so-called u - model is explained in detail. A single longitudinal degree of freedom per MT subunits is assumed. It is known that a continuum approximation of a basic discrete dynamical equation of motion enables existence of kink and antikink solitons along MT. In this paper we use semi-discrete approximation for this equation and show that modulated solitonic waves could propagate as well. We suggest possible biological implications of these waves. Also, a detailed parameter analysis is performed.

1. Introduction

MTs are major cytoskeletal proteins. Their structure is well known [1–7]. We here mention only the basic characteristics of MTs. They are hollow cylinders formed by usually 13 longitudinally ordered protofilaments (PFs) aligned in directions that are parallel to the MT axes. The approximate values of the outer and the inner radii of MT cylinder are 25 nm and 15 nm, respectively. PF represents a series of proteins known as tubulin heterodimers. Each dimer is an electric dipole whose length and mass are $l = 8$ nm and $m = 1.8 \times 10^{-22}$ kg, respectively. The component of its electric dipole moment in the direction of PF and charge displacement are: $p = 337$ Debye $= 1.13 \times 10^{-27}$ Cm and $d \approx 4$ nm, respectively [8,9].

MTs in eukaryotic cells are classified in axonemal and cytoplasmic groups. The first group represents very stable MTs in specific structures associated with cell movement (cilia and flagella) with highly ordered bundles of axonemal MTs.

Cytoplasmic MTs are very dynamic and they form the mitotic spindles that are responsible for movement of chromosomes during mitosis. They also contribute to directional movements of vesicles and other organelles by providing the “rails” for cellular traffic exerted by motor proteins (kinesin and dynein).

According to chosen coordinates describing dimers oscillations we can talk of two basic models. A longitudinal one was introduced in Ref. [10]. Its improved version [11] we call as u - model. Hence, u is the longitudinal coordinate. The second model is a radial one [12] and we call it as $\varphi-$ model for short. Notice that both models regard MT as the ferroelectric system.

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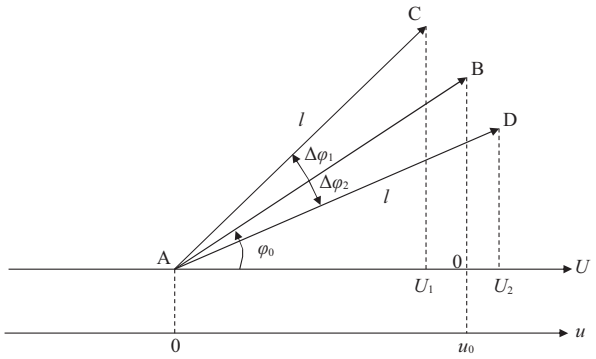

Fig. 1. Demonstration of the u - model of MT.

Two approximations have been used so far to study nonlinear MT dynamics within both models. These are continuum and semi-discrete approximation. The first one has been applied to both models yielding to a conclusion that kink solitons are responsible for energy transfer along MTs. The semi-discrete approximation has been used for the $\varphi-$ model only and completely different result was obtained [13]. This is modulated solitonic wave called breather. Hence, three out of four possible combinations have been studied so far. A logical continuation in this direction of research is the u - model in the context of semi-discrete approximation and this is a topic of this paper.

We assume that the u - model is known [11] and we explain only its basics features in Section 2. In Section 3 the semi-discrete approximation is applied, which is followed by detailed parameter estimations in Section 4. Finally, Section 5 is devoted to some biological explications and concluding remarks.

2. The u - model of MTs

It was mentioned above that the considered model assumes only one degree of freedom per dimer [10]. This is a longitudinal displacement of a dimer at a position n denoted as u_n. In fact, the u - model relies on an angular degree of freedom, while the coordinate u_n is a projection of the top of the dimer on the direction of PF. This is shown in Fig. 1, where a coordinate U belongs to the PF direction. An angle between the PF direction and a ground state of the dimer AB is φ_0. Of course, the dimer performs angular oscillations from AC direction to AD one and the projection of its tip belongs to the interval $U_1 < U < U_2$. An importance of the auxiliary coordinate axis u will be seen later.

A first part of Hamiltonian is

$$H_1 = \sum_n \left[\frac{m}{2}\dot{U}_n^2 + \frac{k}{2}(U_{n+1} - U_n)^2 - CU_n \right], \quad C = QE, \tag{1}$$

where dot means a first derivative with respect to time, m is a mass of the dimer, k is an intra-dimer stiffness parameter, $Q > 0$ represents the excess charge within the dipole, $E > 0$ is internal electric field and the integer n determines the position of the considered dimer in PF. The first term is obviously kinetic energy while the second one shows that the nearest neighboring approximation is used in describing the interaction between the dimers belonging to the same PF. Finally, the last term is potential energy due to the fact that dimers are electric dipoles existing in the field of other dipoles.

Fig. 1 shows only one position, determined by φ_0 and u_0, around which the dimer oscillates. However, it is believed that there is one more [10]. In a symmetric case its position would be determined by a coordinate $-u_0$ (See Fig. 1). These two positions are determined by a well-known double well potential, representing the second part of Hamiltonian, which is [10]

$$H_2 = \sum_n \left[-\frac{1}{2}Au_n^2 + \frac{1}{4}Bu_n^4 \right]. \tag{2}$$

This additional potential energy represents the overall effect of the surrounding dimers on the dipole at a chosen site n [10]. The parameters A and B are positive. Notice capital and small u in Eqs. (1) and (2).

Using an obvious relationship

$$u = u_0 + U, \tag{3}$$

we obtain a usual form of Hamiltonian for one PF [10,11]

$$H = \sum_n \left[\frac{m}{2}\dot{u}_n^2 + \frac{k}{2}(u_{n+1} - u_n)^2 - \frac{1}{2}Au_n^2 + \frac{1}{4}Bu_n^4 - Cu_n \right], \tag{4}$$

where a constant term Cu_0 is neglected.