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Modified extended tanh-function method and nonlinear dynamics of microtubules

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ABSTRACT

We here present a model of nonlinear dynamics of microtubules (MT) in the context of modified extended tanh-function (METHF) method. We rely on the ferroelectric model of MTs published earlier by Satarić et al. [1] where the motion of MT subunits is reduced to a single longitudinal degree of freedom per dimer. It is shown that such nonlinear model can lead to existence of kink solitons moving along the MTs. An analytical solution of the basic equation, describing MT dynamics, was compared with the numerical one and a perfect agreement was demonstrated. It is now clearer how the values of the basic parameters of the model, proportional to viscosity and internal electric field, impact MT dynamics. Finally, we offer a possible scenario of how living cells utilize these kinks as signaling tools for regulation of cellular traffic as well as MT depolymerisation.

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1. Introduction

Microtubules are major cytoskeletal proteins. They are hollow cylinders formed by protofilaments (PF) representing series of proteins known as tubulin dimers [2,3]. In vivo there are usually 13 longitudinal PFs covering the cylindrical walls of MTs. The inner and the outer diameters of the cylinder are 15 nm and 25 nm, while its length may span dimensions from the order of micrometer to the order of millimetre. Each dimer is an electric dipole whose length and longitudinal component of the electric dipole moment are l = 8 nm [2–4] and p = 337 Debye [5], respectively. The constituent parts of the dimers are α and β tubulins, corresponding to positively and negatively charged sides, respectively [2–4].

In this paper we demonstrate how METHF method [6–10] can be used in the study of nonlinear dynamics of

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MTs. The paper is organized as follows. In Section 2 we explain the well known model for MTs we rely on [1]. The modification of the model presented in this paper is a generalization of the original one and will be referred to as u-model. The model brings about a crucial nonlinear differential equation, describing nonlinear dynamics of MTs. In Section 3 we briefly describe METHF method. Then we solve the basic nonlinear differential equation, mentioned above. We show that its solution is a kink-like solitonic wave. This result is compared with numerical solutions in Section 4. In Section 5 we study some general solutions of the basic equation which may or may not have physical meaning for MT dynamics. Finally, in Section 6, we give concluding remarks. In particular, we emphasize the biological importance of the studied kink-like solitons.

2. U-model of MTs

The model we rely on assumes only one degree of freedom of dimers motion within the PF [1]. This is a longitudinal displacement of a dimer at a position n denoted as u_n

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and thus we call the model as u-model. To be more precise, the u-model assumes an angular degree of freedom, while the coordinate u_n is a projection of the top of the dimer on the direction of PF.

The overall effect of the surrounding dimers on a dipole at a chosen site n can be described by a double-well poten-

$$V_d(u_n) = -\frac{1}{2}Au_n^2 + \frac{1}{4}Bu_n^4 \tag{1}$$

where A and B are positive parameters that should be estimated. As an electrical dipole, a dimer in the intrinsic electric field of the MT acquires the additional potential energy given by [1]

$$V_{el}(u_n) = -Cu_n, \quad C = qE, \tag{2}$$

where E is the magnitude of the intrinsic electric field at the site n, as the dimer n exists in the electric field of all other dimers, and q represents the excess charge within the dipole. It is assumed that q > 0 and E > 0.

The Hamiltonian for one PF is represented as follows

$$H = \sum_{n} \left[\frac{m}{2} \dot{u}_{n}^{2} + \frac{k}{2} (u_{n+1} - u_{n})^{2} + V(u_{n}) \right], \tag{3}$$

where dot means the first derivative with respect to time, m is a mass of the dimer, k is an intra-dimer stiffness parameter and the integer n determines the position of the considered dimer in the PF [1]. The first term represents a kinetic energy of the dimer, the second one is a potential energy of the chemical interaction between the neighbouring dimers belonging to the same PF and the last term is the combined potential

$$V(u_n) = -Cu_n - \frac{1}{2}Au_n^2 + \frac{1}{4}Bu_n^4.$$
 (4)

It is obvious that the nearest neighbour approximation is used. However, this does not mean that the influence of the neighbouring PFs is completely ignored as the value of the electric field E depends also on the dipoles belonging to the neighbouring PFs.

By using the generalized coordinates q_n and p_n , defined as $q_n = u_n$ and $p_n = m\dot{u}_n$, applying a continuum approximation $u_n(t) \rightarrow u(x,t)$ and making a series expansion

$$u_{n\pm 1} \to u \pm \frac{\partial u}{\partial x} l + \frac{1}{2} \frac{\partial^2 u}{\partial x^2} l^2$$
 (5)

we can straightforwardly obtain an appropriate dynamical equation of motion. In order to derive a realistic equation, the viscosity of the solvent should also be taken into consideration. This can be achieved by introducing a viscosity force $F_{\nu} = -\gamma \dot{u}$ into the obtained dynamical equation of motion, where γ is a viscosity coefficient [1]. All this brings about the following nonlinear partial differential equation

$$m\frac{\partial^2 u}{\partial t^2} - kl^2 \frac{\partial^2 u}{\partial x^2} - qE - Au + Bu^3 + \gamma \frac{\partial u}{\partial t} = 0.$$
 (6)

It is well known that, for a given wave equation, a travelling wave $u(\xi)$ is a solution which depends upon x and t only through a unified variable ξ

$$\xi \equiv \kappa \mathbf{x} - \omega \mathbf{t},\tag{7}$$

where κ and ω are constants. Substitution of x and t by ξ transforms Eq. (6) into the following ordinary differential equation (ODE)

$$\left(m\omega^2-kl^2\kappa^2\right)u''-\gamma\omega u'-Au+Bu^3-qE=0. \tag{8}$$

By introducing a dimensionless function ψ through the relation

$$u = \sqrt{\frac{A}{R}}\psi,\tag{9}$$

a much more convenient equation can be obtained. This final ODE reads

$$\alpha \psi'' - \rho \psi' - \psi + \psi^3 - \sigma = 0, \tag{10}$$

and contains the following new parameters:

$$\alpha = \frac{m\omega^2 - kl^2\kappa^2}{A},\tag{11}$$

$$\alpha = \frac{m\omega^2 - kl^2\kappa^2}{A},$$

$$\sigma = \frac{qE}{A\sqrt{\frac{A}{B}}},$$
(11)

$$\rho = \frac{\gamma \omega}{A} \tag{13}$$

and $u' \equiv \frac{du}{d\bar{\epsilon}}$.

It was already mentioned that this approach represented a certain improvement of the original model, explained in [1]. If we compare Eq. (10) with the appropriate one in [1] we can see that they are equal for $\alpha = -1$. This approach is more general as our intention is to calculate α . We treat the parameters ρ and σ as an input and will determine values of dynamical parameters of the system, including α . We will see that the final result depends on ρ and σ only, i.e. on the parameters that determine their

The crucial Eq. (10) will be solved in the next section. Before we proceed we want to discuss the potential energy V(u), defined by Eq. (4). This step is very important to understand the physics behind Eq. (10) and its solutions. Using the procedure explained above we can easily obtain the following convenient expression for this potential

$$V(\psi) = \frac{A^2}{B} f(\psi), \tag{14}$$

where

$$f(\psi) = -\sigma\psi - \frac{1}{2}\psi^2 + \frac{1}{4}\psi^4. \tag{15}$$

The function $f(\psi)$ is shown in Fig. 1 for two values of the parameter σ . For σ = 0 the function $f(\psi)$ and, consequently, the potential $V(\psi)$, is symmetric (curve a) while for the increasing σ the right minimum becomes deeper and the left one becomes shallower and elevated. To find the values of ψ for which $f(\psi)$ reaches a maximum and minima we should solve the equation

$$f'(\psi) = -\sigma - \psi + \psi^3 = 0.$$
 (16)

According to the procedure explained in Appendix we can easily obtain the following roots of Eq. (16):

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