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Non-symmetrical W-potential in nonlinear biophysics of microtubules

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Microtubules (MTs) are long structures, representing a main part of cytoskeleton. They are also a road network for motor proteins. Their structure is shown in Fig. 1. A key point is that a heterodimer, or dimer for short, is an electric dipole. This means that MT behaves as ferroelectric [1]. Some more information about MT structure and function, including a few models and used mathematical procedures, can be found in Refs. [2,3]. The structure of the dimer is shown in Fig. 2.

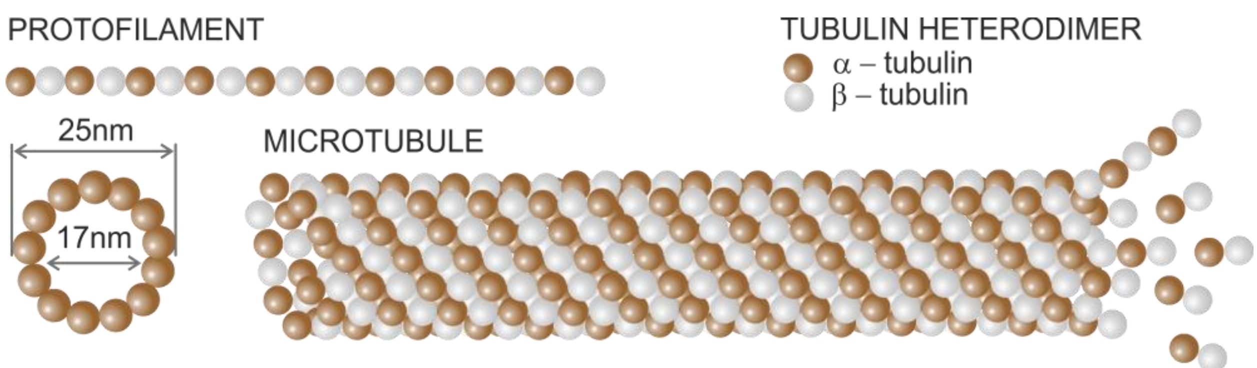
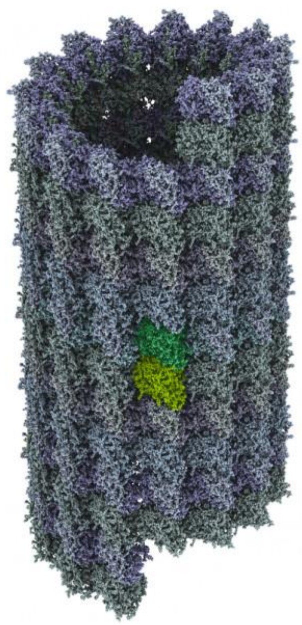


Fig. 1. Microtubule



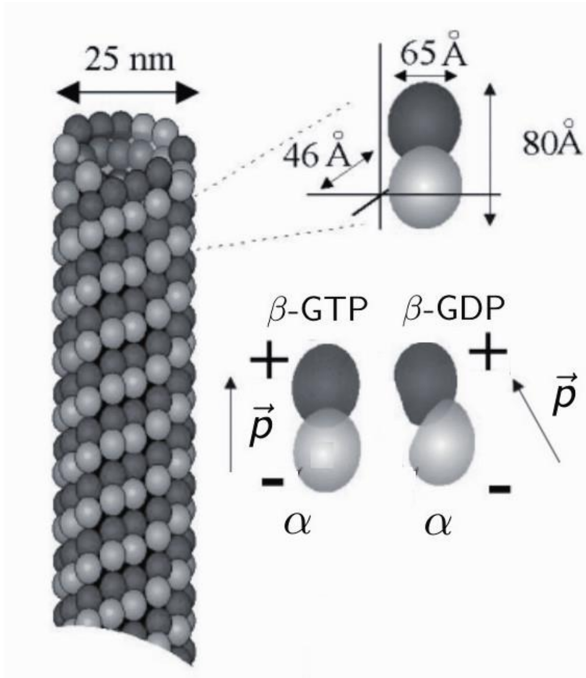


Fig. 2. Microtubule

To study nonlinear dynamics of MT, we start with Hamiltonian, which is [4]

$$H = \sum_n \left[\frac{I}{2} \dot{\varphi}_n^{\ 2} + \frac{k}{2} \left(\varphi_{n+1} - \varphi_n \right)^2 + W(\varphi_n) - pE \cos \varphi_n \right]. \tag{1}$$

An angle φ_n describes the dimer`s oscillation and *n* is its position. We recognize a kinetic and potential energy of the interaction of the two neighbouring dimers belonging to the same protofilament (PF). A term $W(\varphi)$ represents the interaction of a single dimer with all other ones that do not belong to the same PF. It is called W-potential energy, or potential for short, as it looks like a letter W. The very last term is coming from the fact that the electric dimer is in a field of all other ones. For this paper, the most important is the W-potential. We study the following three cases:

Case 1. W-potential is a symmetric function:

$$W = -\frac{A}{2} \varphi_n^{\ 2} + \frac{B}{4} \varphi_n^{\ 4}, \quad A > 0, \quad B > 0. \tag{2}$$

Case 2. W-potential is a non-symmetric function:

$$W_1 = -\frac{A}{2} \varphi_n^{\ 2} + \frac{B}{4} \varphi_n^{\ 4} + C\varphi_n. \tag{3}$$

Case 3. W-potential is a non-symmetric function:

$$W_3 = -\frac{A}{2}\varphi_n^{\ 2} + \frac{B}{4}\varphi_n^{\ 4} + D\varphi_n^{\ 3}. \tag{4}$$

We use a continuum approximation $\varphi_n(t) \Rightarrow \varphi(x,t)$ and obtain dynamical equations of motion. They are:

Case 1. $$\alpha\psi'' - \rho\psi' + \psi - \psi^3 = 0, \tag{5}$$

Case 2. $$\alpha\psi'' - \rho\psi' + \psi - \psi^3 + \sigma = 0, \tag{6}$$

and

Case 3. $$\alpha\psi'' - \rho\psi' + \psi - \psi^3 + \sigma K^2\psi^2 = 0. \tag{7}$$

Here

$$\varphi = \pm\sqrt{\frac{A - pE}{B - pE/6}}\,\psi \equiv K\psi, \quad \alpha = \frac{I\omega^2 - kl^2\kappa^2}{pE - A}, \quad \rho = \frac{\Gamma\omega}{pE - A}, \quad \sigma = \frac{C}{K(pE - A)} \tag{8}$$

and

$$\varphi(x,t) = \varphi(\xi), \qquad \xi = \kappa x - \omega t, \qquad \varphi' \equiv \mathrm{d}\varphi/\mathrm{d}\xi, \tag{9}$$

where κ and ω are constants.

There are many mathematical procedures for solving Eqs. (5)-(7). One of the simplest is a tangent hyperbolic function (THF) method. According to THF method, we expect the solution ψ as

$$\psi = a_0 + a\Phi, \tag{10}$$

where Φ is the solution of the well-known Riccati equaton

$$\Phi' = b + \Phi^2 \tag{11}$$

and the parameters a_0, a and b should be determined. After rather tedious mathematics, we obtain the final solutions for Eqs. (5)-(7). For Case 1, the solution is

$$\varphi(\xi) = \frac{K}{2}\left[1 + \tanh\left(\frac{3}{4\rho}\xi\right)\right], \qquad \alpha > 0. \tag{12}$$

This is a kink soliton shown in Fig. 3. The solutions for Eqs. (6) and (7) will be explained in a more elaborate version of this work, i.e. in a conference proceeding.

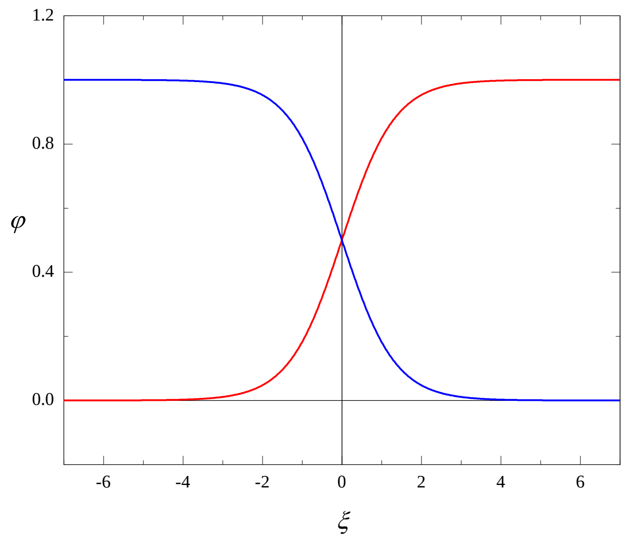


Fig. 3. Kink soliton (blue, $\rho = -1$) and antikink soliton (red, $\rho = 1$) for $K = 1$.

It might be interesting to study a special case when viscosity in neglected, that is for $\rho = 0$. For Case 1, the solution is

$$\varphi_0 = K \tanh(\xi/a), \qquad \alpha = a^2/2 > 0, \tag{13}$$

where a is an arbitrary constant introduced in Eq. (10). This function is similar to the one shown in Fig. 3 but it goes from $-K$ to K.

References

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