SOLITONS IN MICROTUBULES

Beata Trpisova
University of Alberta
Department of Physics
412 Avadh Bhatia Physics Laboratory
Edmonton, Alberta
CANADA T6G 2J1

1. The Biological Cell

Eucaryotic cells consists of membranes, organelles, nuclei and the bulk medium called cytoplasm. Cytoplasm is comprised of a network of protein fibres called cytoskeleton in which the space between the fibres is filled with a water solution. The cytoskeleton is built from microtubules (MTs), actin filaments and microtrabecular lattice. The dynamical changes in the cytoskeleton are the basis for fundamental cellular processes, e.g. changing the shape of the cell, cell movement, positioning of organelles, cell division, processing of information within the cell, internal transport.

2. Microtubule Structure

MTs are hollow cylinders formed of tubulin protofilaments. The number of protofilaments varies between $n = 12$ and $n = 17$, typically $n = 13$. Tubulin is a dimer molecule that consists of two protein monomers - α and β. The weight of each monomer is approximately 55 kilodaltons, its length and diameter $4\,nm$. Due to an asymmetric charge distribution each tubulin

dimer posseses a dipole moment $\vec{p}$ which projection on the vertical axis is $+p$ (α state) or $-p$ (β state). Flipping the dipole from the α state to the β state is associated with a conformational change - tilting the dimer by 29$\circ$ with respect to the vertical axis.

3. Kink-like Solitons in a MT Protofilament

MTs either form stable patterns or continuously grow and shrink. In the process of growth molecules of tubulin are attached to the growing end of a MT and energy of about 0.9 kcal/mol is released due to hydrolysis of GTP to GDP. It has been suggested that it can contribute to coherent lattice excitations leading to kink-like reorientation of dimer dipoles. If the lateral interactions are neglected this process can be studied in one MT protofilament. The kink is a domain wall that separates two sections of the protofilament where the dipoles are oriented in the opposite directions. The dipole dynamics of this system is described by the hamiltonian

$$H = \sum_{n=1}^{N} [\frac{1}{2} M (\frac{du_n}{dt})^2 + \frac{1}{2} K (u_{n+1} - u_n)^2 - (\frac{A}{2} u_n^2 - \frac{B}{4} u_n^4) - q_{eff} E u_n], \quad (1)$$

where u_n is the displacement of the dimer at site n, M is the mass, K, A, B are constants, $q_{eff} = 2 \times 18e = 36e$. $E = \frac{Q_{eff}}{4\pi\epsilon_0 r^2}$ is the electric field produced by the MT when the dipoles are oriented in the same direction. $Q_{eff} = 26 \times 36e$, r is the MT length.

The water surrounding the MT produces damping force $-\gamma \frac{du_n}{dt}$. Based on this and the hamiltonian (1) the equation of motion of one dimer in the continuous limit is

$$M \frac{\partial^2 U}{\partial t^2} - K R_0^2 \frac{\partial^2 U}{\partial x^2} - AU + BU^3 + \gamma \frac{\partial U}{\partial t} - q_{eff} E = 0 \quad (2)$$

The solution of the equation (2) is a traveling kink-like wave

$$U(\alpha(x-vt)) = U_0[1 - \frac{\sigma}{2} - \frac{2}{e^{2^{1/2}\alpha(x-vt)}}], \tag{3}$$

where α, σ, U_0 depend on the parameters of the hamiltonian (1). Provided $v << v_0 = KR_0 = 1700\ m/s$, where R_0 is the distance between two neighbouring dimers, the expression for the velocity is

$$v = \frac{3v_0}{\gamma A}(\frac{MB}{2})^{1/2} q_{eff} E. \tag{4}$$

Kink in the Presence of an Impurity

The behaviour of the kink waves in the presence of an impurity was studied numerically with the initial condition (3) at $t = 0$. The impurity was chosen as a derivative of the gaussian potential $V(x)$ that assumed the form

$$V(x) = V_0 \sum_{k=0}^{m} \exp\{-\beta[x - (x_0 + na)]^2\}. \tag{5}$$

In (5) x_0 is the origin, m is the number of potential "bumps", a is the distance between two neighbouring bumps, β is a constant.

4. Coupled Displacement and Polarization

When the displacement and the polarization of a dimer in a MT protofilament are coupled the hamiltonian of the system is

$$H = \frac{c\dot{u}^2}{2} + \frac{c\dot{P}^2}{2} - \frac{u^2}{2} + \frac{u^4}{2} - \frac{P^2}{2} + \frac{P^4}{2} \pm \gamma u P. \tag{6}$$

In (6) c is a constant, γ is coupling between u and P. $\dot{u}$, $\dot{P}$ are the derivatives of u and P respectively with respect to a variable y. The equations of motion corresponding to (6) are

$$c\ddot{u} = u - u^3 \mp \gamma P, \tag{7}$$

$$c\ddot{P} = P - P^3 \mp \gamma u. \tag{8}$$

For the specific case $u = -P$ and the initial conditions $u(0) = -1.5$, $P(0) = 1.5$, $\dot{u} = 0$, $\dot{P} = 0$ which implies $V(-1.5, 1.5) = 0$, the solution of the equations (7), (8) is the bump-like soliton

$$u(y) = \frac{\pm 1.5}{\cosh[(\frac{(1+\gamma)}{c})^{1/2} y]}, \tag{9}$$

$$P(y) = \frac{\mp 1.5}{\cosh[(\frac{(1+\gamma)}{c})^{1/2} y]}. \tag{10}$$

Setting $c = v^2 - v_0^2$, $y = x - vt$, the set of equations (7), (8) can be written as a set of two coupled partial differential equations

$$\frac{\partial^2 u}{\partial t^2} = v_0^2 \frac{\partial^2 u}{\partial x^2} + u - u^3 - \gamma P, \tag{11}$$

$$\frac{\partial^2 P}{\partial t^2} = v_0^2 \frac{\partial^2 u}{\partial x^2} + P - P^3 - \gamma u. \tag{12}$$

The equations (11), (12) describe two coupled bump-like solitons traveling in time at the velocity v, provided $u(x - vt) = -P(x - vt)$.