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A Kink-Soliton Model of Charge Transport Through Microtubular Cytoskeleton

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Abstract. Contemporary trends in science and technology are characterized by integration of biological and technical systems, like in nanotechnology, nanobiology, and quantum medicine. In our case, we were motivated by a necessity to understand charge transport through microtubular cytoskeleton as a constitutive part of acupuncture system. The high frequency component of acupuncture currents, widely exploited in microwave resonance stimulation of acupuncture system in the past decade, implies that explanation of the cytoplasmatic conductivity should be sought in the framework of Frohlich theory. Accordingly, in this paper we critically analyze the problem of the microwave coherent longitudinal electrical oscillations as a theoretical basis for understanding soliton phenomena in microtubules, showing that charged kink-soliton nonlinear microtubular excitations might be a good candidate for charge transport in microtubules.

Introduction

Ionic acupuncture currents, and accompanying electromagnetic fields, have both ultralow frequency (ULF) [1] and microwave (MW) [2] components, i.e. the MW component is modulated by the ULF one, this being in overall agreement with the frequency and power windowing in tissue interactions with weak electromagnetic fields [3].

The Ukrainian-Russian research and clinical practice in quantum-like microwave resonance therapy (MRT) at ~ 50-80 GHz, fundamentally quantum-informationally efficient even in very serious psychosomatic diseases [2,4], implies that acupuncture system is a macroscopic quantum dynamic structure differentiated at the locations of maximums of three-dimensional standing waves, formed as a result of the reflection of coherent microwave (~ 100 GHz [5]) Frohlich excitations of molecular subunits in the cell membranes, proteins, microtubules etc. - supported also by other investigations, which have demonstrated that differentiation of the gap-junction (GJ) channels (of higher density at acupuncture points and meridians [6]) is slightly sensitive to voltage [7]. The very mechanism of the ionic transport through GJ-channels of the acupuncture system is presumably classical, but it still remains the deep question how the continuity of the ionic acupuncture system is achieved through cytoskeleton structure between the two opposite cell GJ-channels.

In this paper the problem of microwave coherent longitudinal electrical oscillations is considered as a theoretical basis for understanding the charged kink-soliton phenomena in microtubules, implying simultaneously the very nature of nondisipative MW electrical signals alongside microtubular cytoskeleton of acupuncture channels in MRT therapy.

Microwave Coherent Longitudinal Electrical Oscillations and Kink-Soliton Model of Charge Transport through Microtubules

The encouraging results of MRT therapy in curing people have additionally stimulated researchers to address the problem of energy and charge transport in biological systems. However, the influence of microwave radiation on the human organism is not adequately explained, as well as the nature of acupuncture currents. The high frequency component of these currents in the MW range, as well as a strong response of human organism to EM radiation in this range, imply that Frohlich ideas might be a real theoretical framework to explain these phenomena. Frohlich phenomenologically considered the chain of dipoles coupled by Coulomb interactions and showed that the energy entering the system, at some critical value, is channeled into energy of longitudinal electrical oscillations; Frohlich named this process a condensation, and described it by coherent behavior of the system in the form of coherent longitudinal electrical oscillations, with part of the energy dissipated on thermalization of the system of dipoles [5].

Frohlich made his theoretical model by considering quasi-one-dimensional chains of the cell membranes. These biological structures are interesting from our point of view as well, for their structural similarity with the chains of dimers in microtubules. The appearance of coherent oscillations in this system is related to the mean polarizing field, resulted in the excitation of dimers at the point of entrance of the energy into the chain of dipoles. By virtue of Coulomb interactions, this field transfers the energy to other dipoles within the system, at the characteristic frequency determined by parameters of the physical system. The excited chain of dipoles represents a metastable state, supported by the energy of chemical reactions or external electrical field. As a consequence, an excitation of dipoles is transferred through the chain by some velocity, which can be interpreted as a movement of the polarizing field.

In order to estimate the range of these electrical oscillations, we shall present a simple mathematical analysis assuming quasi-one-dimensionality (Q1D) of the system. We shall also take into consideration that some change in the concentration of dimers within the chain appears by entering of the external energy into the system of dipoles. The induced electrical field can be then evaluated from the Maxwell equation: $\mathrm{div}E = -\rho/\varepsilon_o = -nZe/\varepsilon_o$, where n is the concentration of dimers in microtubules and Ze is the charge of dimers ($Z = 18$). As the force acting on a dimer is $F = ZeE$, where $E = -nZex/\varepsilon_0$ follows from the above equation for an one-dimensional system, the equation of motion of the dimer reads: $d^2x/dt^2 + nZ^2e^2/\varepsilon_o m_d = 0$, where from the frequency of electrical oscillations immediately follows: $\omega \cong (nZ^2e^2/\varepsilon_o m_d)^{1/2}$. For typical values of parameters [8], $n_o = 10^{23}$ m^{-3}, $m_D = 5.5 \cdot 10^{-23}$ kg, the frequency of oscillation of the induced electrical field is $\omega_o = 1.5 \cdot 10^{10}$ Hz. If we then assume that concentration of the dimers, on the location of excitation of the chain of dipoles, can raise for two orders of magnitude, $n_1 = 100\ n_o$, the upper limiting value of the frequency of electrical oscillations might reach $\omega_l = 1.5 \cdot 10^{11}$ Hz. Accordingly, the frequency interval of electrical longitudinal oscillations of the system of dipoles is 10^{10} Hz $\leq \omega \leq 10^{11}$ Hz, which is in good agreement with previously obtained theoretical values.

The role of coherent longitudinal electrical oscillations in the charge transport is very important, as the existence of coherent longitudinal electrical oscillations in the system of dipoles is a necessary condition for the appearance of the kink-soliton nonlinear excitations. Properties of solitons in Q1D systems, as well as conditions for their appearance were explored by Ivić and collaborators in detail [9]. According to their results, the autolocalization of a quasiparticle (electron, exciton, vibron) in the presence of a weak interaction with phonons represents theoretical framework to describe solitons. If the energy of quasiparticle is fairly higher than the characteristic energy of the phonon subsystem (condition of adiabaticity), then under weak coupling with phonons the appearance of solitons in Q1D systems is possible. For instance, in our case the energy released in chemical reactions excites dimers, fulfilling the condition of adiabaticity. This energy, in the form of amid-I excitation (vibron), is coupled with longitudinal coherent electrical oscillations, creating nonlinear excitation of the Q1D chain - soliton. This robust stable spatio-temporal configuration continues to move through the chain, exciting dimers alternatively, corresponding in a real physical situation to the mobile polarizing field, which moves dimers from their equilibrium positions by Coulomb interactions. In order to describe these physical processes, it is necessary to consider all the relevant forces that act on the dipole.

The model Hamiltonian, originally formulated and explored by Satarić [10] to inquire into dynamics of the dimers in microtubules, has the following form:

$$H_s = \sum_{n=1}^{N} \left[\frac{M}{2}\left(\frac{du_n}{dt}\right)^2 + \frac{K}{4}(u_{n+1} - u_n)^2 - \left(\frac{A}{2}u_n^2 + \frac{B}{4}u_n^4\right) - Cu_n \right] \tag{1}$$

The first term above in brackets represents the kinetic energy associated with the longitudinal displacement u_n of n-th constituent dimers each of which has mass M; the second term arises from the restoring strain forces between adjacent dimers in microtubule; the third term corresponds to the double-well quartic potential, standardly used to describe critical phenomena (structural transitions in uniaxial ferroelectrics, ferromagnetics, etc.), where the model parameter A is typically a linear function of temperature and may change its sign at an instability temperature T_c and B is positive and temperature independent parameter; and the fourth term accounts for the influence of an intrinsic electric field E, generated by the giant dipole of the microtubular cylinder as a whole, on the n-th constituent dimer of the effective charge q. By solving the equation of motion which follows from the Hamiltonian Eq. 1, it can be shown [10] that the longitudinal displacement of the n-th dimer, in the presence of the damping force of the solvent liquid, $F = -\gamma\, du_n/dt$, is given by $u_n(t) = u_o \left[\mathrm{th}\sqrt{2\alpha}\xi - \frac{\sigma}{2} \right]$. In this expression $\xi = (x - vt)$ represents the moving coordinate of the kink-soliton, while the constant α is defined as $\alpha = \left[\frac{|A|}{M(v_0^2 - v^2)} \right]^{1/2}$, where $v_o = R_o\sqrt{K/M}$ is the sound velocity and v is the kink-soliton velocity, while R_0 is a linear dimension of the dimer. It should be noted that $\omega_0 = \sqrt{K/M}$ is the frequency of the longitudinal electrical oscillations, and $\sigma = qB^{1/2}A^{-3/2}E$. The expression for the velocity of soliton propagation through the microtubule has the following form [10]: $v = \frac{3v_0}{\gamma|A|}\left(\frac{MB}{2}\right)^{1/2} qE$, from which we see that the raise of intrinsic electric field gives rise to an increase of the kink-soliton velocity, thus contributing to its stabilization upon thermal fluctuations.

In order to explain the charge transport mechanism in microtubules, it is necessary to start from the fact that the injected ion can be accelerated by the cell membrane potential [11] up to the velocities ~ 10^4 m/s, enough to excite kink-solitons after collisions of the ion with the polar molecule (tubuline dimer). By exciting kink-solitons, the dimer charges and microtubular periodic potential are perturbed, which is transferred through the long-range coulomb forces on the injected ionic charge. For the sake of mathematical simplification, this interaction is "replaced" by an interaction of the ion with phonons, out of which we shall take into account only longitudinal (acoustic) phonons.

An adequate mathematical approach to the physical interaction of the coherent condensed modes and an ionic charge can be sought in the framework of quantum mechanics, which can be approved by the fact that dynamic time of the system (time for excitation of the kink-soliton) might be considered much shorter than decoherence time [12]. Our starting point in the analysis of the charge transport through MTs is the Hamiltonian Eq. 1. In order to adapt this Hamiltonian for further analysis, it is necessary to introduce the denotations for coordinate and momentum by virtue of boson operators:

$$u_n = \left(\frac{\hbar}{2M\omega_0}\right)^{\frac{1}{2}}(b_n + b_n^+); \qquad p_n = i\left(\frac{M\omega_0\hbar}{2}\right)^{\frac{1}{2}}\left(b_n^+ - b_n\right)$$

so that Hamiltonian takes the form

$$\begin{aligned} H &= E_0 + \sum_n \varepsilon b_n^+ b_n + X_0 \sum_n (b_n^{+2} + b_n^2) - X_1 \sum_n \left(b_n b_{n+1} + b_{n+1}^+ b_n^+ - b_n^+ b_{n+1} - b_{n+1}^+ b_n \right) \\ &+ X_2 \sum_n \left(b_n^{+4} + b_n^4 + 4 b_n^{+3} b_n + 6 b_n^{+2} b_n^2 + 4 b_n^+ b_n^3 \right) - X_3 \sum_n \left(b_n^+ + b_n \right) \end{aligned} \tag{2}$$

where the following parameters were introduced:

$$E_0 = -\frac{\hbar N}{2M\omega_0} + X_1 N + X_2 + \frac{\hbar\omega_0}{4}; \quad \varepsilon = -\frac{\hbar A}{2M\omega_0} + 12X_2 + 2X_1 + \frac{\hbar\omega_0}{4}$$

$$X_0 = -\frac{\hbar A}{4M\omega_0} + 6X_2 + X_1 - \frac{\hbar\omega_0}{4}; \quad X_1 = \frac{k\hbar}{4M\omega_0}; \quad X_2 = \frac{B\hbar^2}{16M^2\omega_0^2}; \quad X_3 = c\left(\frac{\hbar}{2M\omega_0}\right)^{\frac{1}{2}}$$

Further analysis is a standard one, through elimination of the linear part X_3 of the Hamiltonian Eq. 2, which corresponds physically to the problem of nonlinear excitations of the system, i.e. solitons [13]. So, we apply the transformation $H_s = e^{-U} H e^{U}$, where $U = Y\sum_m \left(b_m - b_m^+\right)$. The constant Y of the unitary operator can be found from the request for elimination of the linear term, while index n enumerates all monomers of the microtubular chain, so that:

$$\begin{aligned} H_s &= \sum_n \bar{\varepsilon} b_n^+ b_n + X_0 \sum_n (b_n^{+2} + b_n^2) - X_1 \sum_n \left(b_n b_{n+1} + b_n^+ b_{n+1}^+ + b_n^+ b_{n+1} + b_{n+1}^+ b_n \right) \\ &+ X_2 \sum_n \left(b_n^{+4} + b_n^4 + 4 b_n^{+3} b_n + 6 b_n^{+2} b_n^2 + 4 b_n^+ b_n^3 \right) - 8X_2 Y \sum_n \left(b_n^{+3} + b_n^3 \right) - \\ &- 24 X_2 Y \sum_n \left(b_n^{+2} b_n + b_n^+ b_n^2 \right) + 12 X_2 Y \sum_n \left(b_n^{+2} + b_n^2 \right) \end{aligned} \tag{3}$$

where

$$Y = \frac{X_3}{4X_1 - \varepsilon - 2X_0}; \quad \tilde{\varepsilon} = \varepsilon + 24Y^2 X_2$$

From the viewpoint of our problem, the above Hamiltonian is not sufficient to describe the charge transport, and it is therefore necessary to introduce a fermion (electronic) subsystem, defined as follows:

$$H_e = \sum_k E_k a_k^+ a_k \tag{4}$$

The ionic charge injected in MT interacts with nonlinear excitations (solitons) via longitudinal acoustic phonons, and in order to simplify this interaction mathematically, we shall diagonalize the Hamiltonian Eq. 3 by direct Fourier transform of the boson operators:

$$b_n = \frac{1}{\sqrt{N}} \sum_k b_k e^{-ikn}; \quad b_n^+ = \frac{1}{\sqrt{N}} \sum_k b_k^+ e^{ikn}$$

and by Bogolyubov transformations:

$$b_k = u_k \tilde{b}_k + v_k^* \tilde{b}_{-k}^+; \quad b_k^+ = u_k^* \tilde{b}_k^+ + v_k \tilde{b}_{-k}$$

where the operators b_k, b_k^+ are Fourier transforms of the boson operators. With so defined denotations, the Hamiltonian of the boson subsystem related to solitons has the following form:

$$H_s = \sum_k \tilde{\Delta}_k \tilde{b}_k^+ \tilde{b}_k \tag{5}$$

where:

$$\tilde{\Delta}_k = \Delta_k \left[1 + \frac{9}{2} \left(\frac{W_k}{\Delta_k} \right)^2 \right]; \quad \Delta_k = \tilde{\varepsilon} - 2X_1 \cos kR_0; \quad W_k = X_0 + 12Y^2 X_2 - X_1 \cos(kR_0)$$

Interaction of the two described subsystems is expressed mathematically by the Hamiltonian:

$$H_{\text{int}} = \frac{1}{\sqrt{N}} \sum_{kq} F(q)\left(\tilde{b}_q + \tilde{b}_{-q}^{+}\right) a_{k+q}^{+} a_k \tag{6}$$

where $F(q)$ is the structure factor which characterizes interaction of electrons with longitudinal acoustic phonons, and N is the number of tubuline dimers within MT.

The appearance of the charge within MT introduces short non-equilibrium distribution of the physical parameters in the system, which can be treated conveniently by the methods of nonequilibrium statistical physics, developed by Zubarev: therefore we shall solve the kinetic equation describing decrease in the number of charges due to interaction with MT [14],

$$\frac{d\langle n_k \rangle}{dt} = \frac{1}{i\hbar} \left\langle \left[n_k\ , H \right] \right\rangle_q + I_n \tag{7}$$

where n_k is the number of electrons with the wavenumber k, and H is the Hamiltonian of the system: $H = H_s + H_e + H_{int}$. The term I_n represents nonequilibrium correction determined as follows, $I_n = -\frac{1}{\hbar^2} \int_{-\infty}^{0} e^{\varepsilon t} \langle [H_1(t), [n_k, H]] \rangle dt$, where $H_1(t) = e^{\frac{-iH_0 t}{\hbar}} H_{\text{int}} e^{\frac{iH_0 t}{\hbar}}$ and $H_0 = H_s + H_e$ - and can be determined by Weyl identity [15] and the known commutation relations for fermion and boson operators. For instance, $e^{\frac{-iH_0 t}{\hbar}} a_k^{+} e^{\frac{iH_0 t}{\hbar}} = a_k^{+} - \frac{it}{\hbar}\left[H_0, a_k^{+}\right] + \frac{1}{2!}\left(\frac{it}{\hbar}\right)^2 \left[H_0, \left[H_0, a_k^{+}\right]\right] + \ldots$; as $\left[a_k^{+} a_{k'}, a_{k'}^{+}\right] = \delta_{kk'} a_{k'}^{+}$, it follows directly $e^{\frac{-iH_0 t}{\hbar}} a_k^{+} e^{\frac{iH_0 t}{\hbar}} = e^{\frac{-iE_k t}{\hbar}} a_k^{+}$. The similar commutation relations hold in the framework of the boson statistics: $\left[b_k^{+} b_k, b_{k'}\right] = -\delta_{kk'}\ b_k$, $\left[b_k^{+} b_k, b_{k'}^{+}\right] = \delta_{kk'} b_{k'}^{+}$, which enables the similar application of the Weyl identity to boson operators. By not entering deeper in the calculation of the integral of the nonequilibrium correction, let us state that application of the equation $\langle [n_k, H] \rangle_q = 0$ (an averaging over equilibrium boson ensemble), Vick theorem, and integration over small parameter $\varepsilon \to 0$, gives rise to the following equation for the average number of electrons:

$$\frac{d\langle n_k \rangle}{dt} = \frac{2\pi}{N} \sum_{kq} \left\{ \frac{|F(q)|^2 \left[(N_q + 1) n_{k+q} (1 - n_k) - N_q n_k (1 - n_{k+q}) \right]}{\hbar \tilde{\Delta}_q} \right\} - \\ - \frac{2\pi}{N} \sum_{kq} \left\{ \frac{|F(q)|^2 \left[(N_q + 1) n_{k-q} (1 - n_k) - N_q n_k (1 - n_{k-q}) \right]}{\hbar \tilde{\Delta}_q} \right\}$$

where N_q is the equilibrium number of the bosons with the wavenumber q, and n_{k+q}, n_{k-q} and n_k are the corresponding numbers of fermions (electrons), while $\tilde{\Delta}_q >> E_{k,} E_{k+q,} E_{k-q}$ was assumed for the velocities of chaotic movements of electrons. The above rather complicated expression can be simplified for practical purposes, on the assumption that majority of electrons are concentrated around most probable wavenumber k and that longitudinal coherent excitations have the same wavenumber q, giving rise

$$\frac{d\langle n_k \rangle}{dt} \cong \frac{2\pi}{N} \frac{|\ F(\ q\ )|^2}{\hbar \tilde{\Delta}_q} \left(N_q + 1\right)\left(n_{k+q} - n_{k-q}\right) \tag{8}$$

Now, by inserting Eq. 8, it is possible to obtain electrical current through MT:

$$I_{MT} = \frac{d\langle n_k \rangle}{dt} e \tag{9}$$

It is interesting to note that the application of typical values of the parameters - $|F(q)|^2 \cong 2.1 \cdot 10^{-48}$ J^2 [9], $\tilde{\Delta}_q \cong 2.91 \cdot 10^{-24}$ J [5], $e = 1.6 \cdot 10^{-19}$ C, $N_q \cong 1.5$ (for $T = 300$ K, $\hbar\omega_q = 4.1 \cdot 10^{-4}$ eV) [5], $n_{k+q} - n_{k-q} \cong 1$ (roughly one charge per MT), $N \cong 1300$ (number of constituent dimers in 13 protofilaments of the ~ 1 μm microtubular length) [16] - gives an estimation of the electrical current through MT, I_{MT} ~ 5 pA. Then the upper limit of the electrical current through an acupuncture channel, of estimated ~ 1 mm^2 cross-section [17] and estimated upper surface density of MTs less than 10^9 MT/mm^2 (for 25 nm MT´s outer diameter [16]), is $I_{acu} < 10^9 \cdot I_{MT} \sim 5$ mA, which is in good agreement with the experimental data [17].

Conclusion

The encouraging results on the microwave resonance stimulation of the acupuncture system in curing people have additionally stimulated researchers to address the problem of energy and charge transport in biological systems. However, the influence of microwave radiation on human organism is still not adequately explained, as well as the nature of acupuncture currents, although Frohlich ideas have set a good theoretical framework for explanation of these phenomena. In this paper we have critically analyzed the problem of longitudinal electrical oscillations as a theoretical basis for understanding the soliton phenomenon in microtubules, showing that nonlinear charged kink-solitons might be a good candidate for charge transport in microtubular cytoskeleton as a constitutive part of acupuncture system - of importance for quantum medicine, nanobiology and nanotechnology.

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