A MODEL FOR SOLITON CHARGE TRANSPORT THROUGH MICROTUBULES

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Abstract. In this paper the theoretical model for charge transport through microtubules (MTs) by soliton mechanism is developed, and analyzed by methods of nonequilibrium statistical physics. Thus obtained electrical current through MT is estimated as ~ 0.1 nA.

Key-words: Microtubules, soliton, nonequilibrium statistical physics, electrical current.

1 INTRODUCTION

Microtubules (MTs) are the most fundamental filamentous structures that comprise the cytoskeleton, with energetic factors and information processing as intriguing aspects of their behavior [1]. As the charge transfer through MTs is an important prerequisite for their role in intra-cell information processing, in this paper we shall consider the theoretical model for charge transport through MTs by soliton mechanism, and analyze it by methods of nonequilibrium statistical physics.

2 MODEL

Our starting point in the analysis of the charge transport through MTs is the Hamiltonian [2,3]:

$$H = \sum_{n=1}^{N} [\frac{M}{2}(\frac{du_n}{dt})^2 + \frac{K}{4}(u_{n+1} - u_n)^2 - \frac{A}{2}u_n^2 + \frac{B}{4}u_n^4 - cu_n \tag{1}$$

In order to adapt the above Hamiltonian for further analysis, it is necessary to introduce the denotations for impulse and coordinate by virtue of boson operators:

$$\begin{aligned} p_n &= \left(\frac{\hbar}{2M\omega_0}\right)^{\frac{1}{2}}(b_n + b_n^{+}) \\ u_n &= i\left(\frac{M\omega_0\hbar}{2}\right)^{\frac{1}{2}}\left(b_n^{+} - b_n\right) \end{aligned} \tag{2}$$

so that Hamiltonian takes the form

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

where the following parameters were introduced:

$$
\begin{aligned}
E_0 &= -\frac{\hbar N}{2M\omega_0} + X_1 N + X_2 + \frac{\hbar\omega_0}{4} \\
\varepsilon &= -\frac{\hbar A}{2M\omega_0} + 12X_2 + 2X_1 + \frac{\hbar\omega_0}{4} \\
X_0 &= -\frac{\hbar A}{4M\omega_0} + 6X_2 + X_1 - \frac{\hbar\omega_0}{4} \\
X_1 &= \frac{k\hbar}{4M\omega_0},\ X_2 = \frac{B\hbar^2}{16M^2\omega_0^{\,2}} \\
X_3 &= c\left(\frac{\hbar}{2M\omega_0}\right)^{\frac{1}{2}}
\end{aligned}
\tag{4}
$$

The further analysis is a standard one, through elimination of the linear part X_3 of the Hamiltonian (3), which corresponds physically to the problem of nonlinear excitations of the system, i.e. solitons. So,

$$H_s = e^{-U} H e^{U} \tag{5}$$

where

$$U = Y\sum_m \left(b_m - b_m^{\,+}\right) \tag{6}$$

In the above equations 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:

$$
\begin{aligned}
H_s &= \sum_n \bar{\varepsilon} b_n^{\,+} b_n + X_0 \sum_n (b_n^{\,+2} + b_n^{\,2}) - \\
&- X_1 \sum_n \left(b_n b_{n+1} + b_n^{\,+} b_{n+1}^{\,+} + \right. \\
&\left. + b_n^{\,+} b_{n+1} + b_{n+1}^{\,+} b_n\right) + \\
&+ X_2 \sum_n \left(b_n^{\,+4} + b_n^{\,4} + 4b_n^{\,+3} b_n + \right. \\
&\left. + 6b_n^{\,+2} b_n^{\,2} + 4b_n^{\,+} b_n^{\,3}\right) - \\
&- 8YX_2 \sum_n \left(b_n^{\,+3} + b_n^{\,3}\right) - \\
&- 24YX_2 \sum_n \left(b_n^{\,+2} b_n + b_n^{\,+} b_n^{\,2}\right) + \\
&+ 12Y^2 X_2 \sum_n \left(b_n^{\,+2} + b_n^{\,2}\right)
\end{aligned}
\tag{7}
$$

where

$$
\begin{aligned}
Y &= \frac{X_3}{4X_1 - \varepsilon - 2X_0} \\
\tilde{\varepsilon} &= \varepsilon + 24Y^2 X_2
\end{aligned}
$$

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

$$H_e = \sum_k E_k a_k^{\,+} a_k \tag{8}$$

The electron charge injected in MT interacts with nonlinear excitations (solitons) via longitudinal acoustic phonons, and in order to simplify this interaction mathematically, we shall diagonalize Hamiltonian (7) by Bogolyubov transformations:

$$
\begin{aligned}
b_k &= u_k \tilde{b}_k + v_k{}^{*} \tilde{b}_{-k}^{\,+} \\
b_k^{\,+} &= u_k{}^{*} \tilde{b}_k^{\,+} + v_k \tilde{b}_{-k}
\end{aligned}
\tag{9}
$$

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:

$$H_s = \sum_k \tilde{\Delta}_k \tilde{b}_k^{\,+} \tilde{b}_k \tag{10}$$

where:

$$
\begin{aligned}
\tilde{\Delta}_k &= \Delta_k \left[1 + \frac{9}{2}\left(\frac{W_k}{\Delta_k}\right)^2\right] \\
\Delta_k &= \tilde{\varepsilon} - 2X_1 \cos kR_0 \\
W_k &= X_0 + 12Y^2 X_2 - X_1 \cos(kR_0)
\end{aligned}
\tag{11}
$$

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

$$H_{\text{int}} = \frac{1}{\sqrt{N}} \sum_{kq} F(q)\left(\tilde{b}_q + \tilde{b}_{-q}^{\,+}\right) a_{k+q}^{\,+} a_k \tag{12}$$

where $F(q)$ is the structure factor which characterises 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 nonequilibrium distribution of the physical parameters in the system, which can be treated conveniently by the methods of nonequilibrium statistical physics, developed by Zubarev [4]. Therefore we shall solve the kinetic equation describing decrease of the number of charges due to interaction with MT [4]:

$$\frac{d\langle n_k\rangle}{dt} = \frac{1}{i\hbar}\left\langle\left[n_k\ ,H\right]\right\rangle_q + I_n \tag{13}$$

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:

$$I_n = -\frac{1}{\hbar^2}\int_{-\infty}^{0} e^{\varepsilon t}\left\langle\left[H_1(t),\left[n_k, H\right]\right]\right\rangle dt \tag{14}$$

In the Eq.(14), the operator $H_1(t) = e^{\frac{-iH_0 t}{\hbar}} H_{\mathrm{int}} e^{\frac{iH_0 t}{\hbar}}$, where $H_0 = H_s + H_e$ can be determined by Weyl identity [5], as well as the known commutation relations for fermion and boson operators. For instance,

$$e^{\frac{-iH_0 t}{\hbar}} a_k{}^{+} e^{\frac{iH_0 t}{\hbar}} = a_k{}^{+} - \frac{it}{\hbar}\left[H_0, a_k{}^{+}\right] + \\ + \frac{1}{2!}\left(\frac{it}{\hbar}\right)^2\left[H_0,\left[H_0, a_k{}^{+}\right]\right] + \ldots\ldots\ldots\ldots \tag{15}$$

As $\left[a_k{}^{+}a_{k'}, a_{k'}{}^{+}\right] = \delta_{kk'}a_{k'}{}^{+}$, it follows directly:

$$e^{\frac{-iH_0 t}{\hbar}} a_k^{+} e^{\frac{iH_0 t}{\hbar}} = e^{\frac{-iE_k t}{\hbar}} a_k^{+} \tag{16}$$

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 upon boson operators. By not entering deeper in the calculation of the integral of the nonequilibrium correction, let us state that appliction of the equation $\left\langle\left[n_k, H\right]\right\rangle_q = 0$ (an averaging over equilibrium boson ensamble), Vick theorem, and integration over small parameter $\varepsilon \to 0$, give rise to the following equation for the average number of electrons:

$$\frac{d\langle n_k\rangle}{dt} = \frac{1}{N}\sum_{kq}\left\{\frac{|F(q)|^2\left[(N_q+1)n_{k+q}(1-n_k) - N_q n_k(1-n_{k+q})\right]}{\hbar\widetilde{\Delta}_q}\right\} - \\ -\frac{1}{N}\sum_{kq}\left\{\frac{|F(q)|^2\left[(N_q+1)n_{k-q}(1-n_k) - N_q n_k(1-n_{k-q})\right]}{\hbar\widetilde{\Delta}_q}\right\} \tag{17}$$

where N_q is the equlibrium number of the bosons with the wavenumber q, and n_{k+q}, n_{k-q} i n_k are corresponding numbers of the fermions (electrons), while $\widetilde{\Delta}_q > E_{k,} E_{k+q,} E_{k-q}$ was assumed for the velocities of chaotic movements of electrons. The rather complicated Eq.(17) can be simplified for practical purposes, under the assumption that majority of electrons is concentrated around most probable wavenumber k and that longitudinal coherent excitations have the same wavenumber q, giving rise

$$\frac{d\langle n_k\rangle}{dt} \cong \frac{1}{N}\frac{|\ F(\ q\ )|^2}{\hbar\widetilde{\Delta}_q}\left(N_q+1\right)\left(n_{k+q} - n_{k-q}\right) \tag{18}$$

Now, it is possible to obtain electrical current through MT:

$$I = \frac{d\langle n_k\rangle}{dt}e \tag{19}$$

It is interesting to note that application of the typical values of the parameters: $|F(q)|^2 \cong 2.1\cdot 10^{-48} J[6], \widetilde{\Delta}_q \cong 2.91\cdot 10^{-24} J[3], e = 1.6\cdot 10^{-19} C$, $N_q \cong 1.5$ (for $T = 300\,K$, $\hbar\omega_q = 4.1\cdot 10^{-4} eV[7]$), $n_{k+q} - n_{k-q} \cong 1$ (roughly one charge per MT), $N = 13[2]$, gives estimation for electrical current through MT, $I \sim 0.1$ nA.

3 CONCLUSION

Microtubules (MTs) are the most fundamental filamentous structures that comprise the cytoskeleton, with energetic factors and information processing as intriguing aspects of their behavior. In this paper the theoretical model for charge transport through MTs by soliton mechanism is developed, and analyzed by methods of nonequilibrium statistical physics. Thus obtained electrical current through MT is estimated as ~ 0.1 nA.

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