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THE THERMODYNAMICAL STABILITY OF A SYSTEM COMPOSED OF A GREAT NUMBER OF MOLECULAR CHAINS

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Stability conditions of the transmission of informations through nerve fibers by soliton mechanism are analysed. The fibers in mutual contact are characterized by a given temperature distribution.

1. *Introduction*

In biological processes transmitting informations through nerve fibers consisting of quasilinear structures such as α-peptide groups[1] one has usualy the case of crossed nerve pathes.

If the molecular chain model transmitting the information by local solitonic excitations[2] is chosen to describe the nerve pathes, it is important to assess the thermodynamical stability of the system when it is assumed that the transport takes place through many pathes simultaneously and that a given temperature distribution reigns over the molecular chain in a given moment i. e. using the relaxation theory we shall analyse the stability of the system transmitting informations (the momentum and energy) by determining the temperature of each subsystem (linear chain) as a function of time. The basic theory used here consists in the interpretation of the nonequilibrium statistics formalism in accordance with papers of Zubarev and Pokrovski[3,4]. The system is stable if the temperature depends very weakly on time, more weakly, let us say, than if the processes were refering to collective excitation of the system (the excitons). This can be shown explicitly by examining the analytical expressions of the solution.

2. Davydov's solitons on $T \neq 0$

Davydov[5] examined the dependence of the soliton state on temperature, in a molecular chain, applying the following model (that we used already in some preceding papers).

The linear molecular chain is described by the Hamiltonian

$$H = H_{ex} + H_{ph} + H_{int}. \tag{2.1}$$

In the simplified model the exciton Hamiltonian is

$$H_{ex} = \sum_n \left[\left(\mathscr{E}_0 + \frac{\hbar^2}{m R_0} \right) B_n^+ B_n - \frac{\hbar^2}{2 m R_0^2} B_n^+ (B_{n+1} + B_{n-1}) \right], \tag{2.2}$$

$\mathscr{E}_0$ is the energy of the exciton zone in the simplified two-level model, m is the effective mass of the free electron defining the excitation levels and R_0 is the constant of the crystal latice.

$$H_{ph} = \sum_q \hbar \Omega_q b_q^+ b_q, \tag{2.3}$$

is the longitudinal phonon Hamiltonian where b_q^+ and b_q are the creation and annihilation phonon operators having wave vectors $\vec{q}$, $\Omega_q = v_0 |\vec{q}|$ is the phonon frequency, while $v_0 = R_0 \sqrt{\frac{\varkappa}{M}}$ is the sound velocity. M is the molecular mass in the node, and $\varkappa$ is elasticity constant of the crystal.

The Hamiltonian of the exciton-phonon interaction is described by

$$H_{int} = \frac{1}{N^{1/2}} \sum_{qn} F(q) B_n^+ B_n (b_q + b_{-q}^+) e^{i n R_0 q}. \tag{2.4}$$

$F(q)$ is the intensity of the exciton-phonon interaction with constant coupling χ; while B_n and B_n^+ are the Bose operators of annihilation and creation electron on the n-node.

$$F(q) = i\sigma \left(\frac{\hbar |\vec{q}|}{2 M v_0} \right)^{1/2} \frac{q}{|\vec{q}|}; \ \sigma = 2 R_0 \chi \tag{2.5}$$

At $T \neq 0$ following the lines of Ref. 5 we ask for the state of the system in form of the Schrödinger amplitude

$$|\psi_\nu (t)\rangle = \sum_n \varphi_n (t) B_n^+ |O_{ex}\rangle U_n (t) | \nu\rangle, \tag{2.6}$$

where ν are phonon states given by the expression

$$|\nu\rangle = \prod_q |\nu_q\rangle = \prod_q \frac{(b_q^+)^{\nu_q}}{(\nu_q!)^{1/2}} \, | O_{ph}\rangle, \tag{2.7}$$

and where $|O_{ex}\rangle$ and $|O_{ph}\rangle$ are the exciton and phonon vacuum states, respectively. The unitary equilibrium mode displacement operator appearing in the result of exciton-phonon coupling has the form

$$U_n(t) = \exp\{\sum_q [\hat{\beta}^*_{qn}(t)\, b_q - \hat{\beta}_{qn}(t)\, b_q^+]\}, \tag{2.8}$$

$\hat{\beta}_{qn}$ are chosen as modulated waves,

$$\hat{\beta}_{qn}(t) = \beta_{qn}(t)\, e^{-i n R_0 q}, \tag{2.9}$$

where the $\varphi_n(t)$ is normalised by the condition

$$\langle \psi_\nu \mid \psi_\nu \rangle = \sum_n |\varphi_n(t)|^2 = 1. \tag{2.10}$$

In this formalism $\varphi_n(t)$ and $\beta_{qn}(t)$ play the role of dynamical variables and are determined from the Hamiltonian equation

$$i\hbar \frac{\partial \beta_{qn}(t)}{\partial t} = \frac{\partial \langle H \rangle}{\partial \beta^+_{qn}(t)}, \tag{2.11a}$$

$$i\hbar \frac{\partial \varphi_n(t)}{\partial t} = \frac{\partial \langle H \rangle}{\partial \varphi^*_n(t)}. \tag{2.11b}$$

$\langle H \rangle$ is the functional averaged over phonon states plaving the role of the Hamiltonian function, i. e.

$$\langle H \rangle = \sum_\nu \varrho_{\nu\nu} H_{\nu\nu}, \tag{2.12}$$

$$H_{\nu\nu} = \langle \psi_\nu \mid H_{ex} + H_{int} \mid \psi_\nu \rangle + \sum_n \langle \nu \mid U^+_n(t)\, H_{ph}\, U_n(t) \mid \nu \rangle, \tag{2.13}$$

$\varrho_{\nu\nu}$ is the diagonal element of the phonon density matrix operator

$$\varrho_{\nu\nu} = \frac{\langle \nu \mid e^{-\frac{H_{ph}}{\Theta}} \mid \nu \rangle}{\sum_n \langle \nu \mid e^{-\frac{H_{ph}}{\Theta}} \mid \nu \rangle}. \tag{2.14}$$

From the Hamiltonian equation system (2.11a), (2.11b) the nonlinear Schrödinger equation (refering to $\varphi(x, t)$ and having a cubic nonlinearity) may be derived in continuum approximation

$$i \hbar \frac{\partial \varphi(x, t)}{\partial t} - [\mathscr{E}_0 + \frac{\hbar}{m R_0^2} (1 - e^{-\bar{w}})] \varphi(x, t) + \frac{\hbar}{2m R_0^2} e^{-\bar{w}} R_0^2 \frac{\partial^2 \varphi(x, t)}{\partial x^2} +$$

$$+ G |\varphi|^2 \varphi(x, t) = 0. \qquad (2.15)$$

The particular solution of (2.15) is the solution of a solitary wave depending on the variable $\xi = x - v t$, where x is the position along the molecular chain. The explicit soliton solution has the form[5]

$$\varphi(x, t) = \left[\frac{R_0 \, a(\Theta_T)}{2}\right]^{1/2} \frac{\exp\left\{k (x - x_0) + \frac{\hbar}{2m} (a^2 (\Theta_T) - k^2) - \frac{\mathscr{E}_0}{\hbar} t\right\} i}{\mathrm{ch}\, [a(\Theta_T)(x - x_0 - v t)]}, \qquad (2.16)$$

where

$$k = \frac{m v}{\hbar}; \quad a(\Theta_T) = \frac{R_0}{2 \hbar^2} m \, G(\Theta_T) \exp\left[\frac{R_0^2 a_0^2}{4} B f(\Theta_T)\right], \qquad (2.17)$$

$$G(\Theta_T) = \frac{\sigma^2}{M v_0^2 (1 - s^2)} \left(1 - \frac{B}{4} f(\Theta_T)\right),$$

$$a_0 = \frac{m R_0 \sigma^2}{2 M v_0^2 \hbar^2 (1 - s^2)},$$

$$B = \frac{\pi}{R_0} \frac{R_0^2 \sigma^2}{4 M v_0^3 (1 - s^2) \hbar},$$

$$f(\Theta_T) = \frac{R_0}{\pi} \frac{1}{N} \sum_q |q| (1 + 2 \bar{\nu}_q),$$

$$\bar{\nu} = \frac{1}{e^{\frac{\hbar \Omega_q}{\Theta_T}} - 1},$$

$$s = \frac{v}{v_0},$$

$$\Theta_T = K_B T. \qquad (2.18)$$

The expression $e^{-\overline{w}}$ is the Debye-Waller factor. The temperature effect in the case of solitons is such that the raising of temperature provokes a spreading of the soliton. The consequence of this fact is that the nonlinearity coefficient G tends to zero with the temperature, so that Eq. (2.9) becomes linear and describes in a certain interval of the temperature a plane wave.

3. *Kinetical coefficients of the system*

Let us take that we have n chains ordered by descending temperature and each of which is in contact with the preceding and the following one so that $\Theta_1 > \Theta_2 > \, > \ldots \Theta_{n-1} > \Theta_n$ (see Fig. 1)

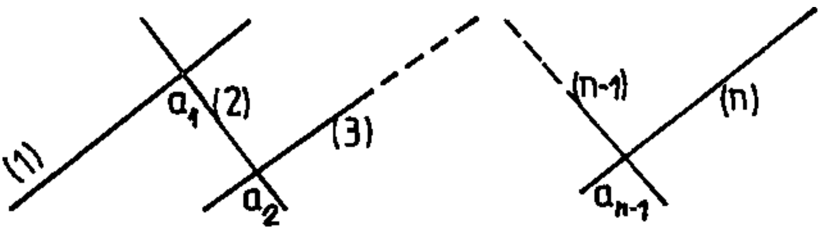

Fig. 1.

This system can be described by the Hamiltonian

$$H = \sum_{j=1}^{n} H_j + H_{int}^c, \tag{3.1}$$

H_j is the Hamiltonian belonging to the chain (j), H_{int}^c — is the phenomenological interaction corresponding to the contact

$$H_{int}^c = W \sum_{j=1}^{n-1} B_{j,a_j}^{+} B_{j+1,a_j} + \text{h. c.}, \tag{3.2}$$

a_j is the contact node belonging to chains j and $j+1$, W is phenomenological parameter of interaction.

The state in the chain j is obtained from the equation of motion

$$\mathrm{i}\,\hbar\,\dot{H}_j = [H_j, H] = [H_j, H_{int}^c]. \tag{3.3}$$

One has

$$[H_j, H_{int}^c] = [H_j^{ex}, H_{int}^c] + [H_{ph}^j, H_{int}^c] + [H_{int}^j, H_{int}^c],$$

where

$$[H_{ph}^j, H_{int}^c] = 0,$$

since there are no common variables and

$$[H_{int}^{l}, H_{int}^{c}] \approx 0,$$

since this is a small quantity of higher order, so that

$$[H_j, H_{int}^{c}] \approx [H_j^{ex}, H_{int}^{c}]. \qquad (3.4)$$

Taking into account that in all biophysical relevant cases $\mathscr{E}_0$ is of the order of magnitude of eV whille the resonant interaction $\frac{\hbar^2}{m R_0^2} \sim 10^{-3}$ to 10^{-2} eV the following approximation is valid $W \Delta > \frac{\hbar^2}{m R_0^2} W$ $\left(\text{where } \Delta = \mathscr{E}_0 + \frac{\hbar^2}{m R_0^2}\right)$ and

$$\dot{H}_j = \frac{1}{i \hbar} \{\Delta\, W [B_{j,aj}^{+} B_{j+1,aj} - B_{j-1,aj-1}^{+} B_{j,aj-1}] - \Delta\, W^* [B_{j+1,aj}^{+} B_{j,aj} - \\ - B_{j,a-j}^{+} B_{j-1,aj-1}]\}. \qquad (3.5)$$

The expression (3.5) is usefull in assessing the state through solitonic mechanisms and therefore in applied approximation it is not necessary to use analytical expression.

According to the procedure applied by Pokrovski[4] and explicitly given in Ref. 3 (p. 261, 262) we can obtain the average value of the corresponding energy current

$$\langle \dot{H}_j \rangle = \sum_{s=1}^{n-1} \int_0^1 d\tau \int_{\substack{-\infty \\ \varepsilon \to 0}}^{0} e^{\varepsilon t}\, dt\, (\beta_s - \beta_n) \langle e^{M\tau} \dot{H}_j\, e^{-M\tau} \dot{H}_s(t) \rangle_q \quad (j = 1 \ldots n). \qquad (3.6)$$

The system of Eqs. (3.6) follows in consequence of the current conservation law in a system of interacting molecular chains

$$\sum_{j=1}^{n} \dot{H}_j = 0, \qquad (3.7)$$

where the averaging is made with respect to the local equilibrium density matrix ϱ_q given as

$$\varrho_q = \frac{\exp\{-M\}}{Sp\{\exp[-M]\}}. \qquad (3.8)$$

We used above the following notations $\beta_j^{-1} = K_B T$, ε is a small parameter including the time, and

$$M \cong \sum_{j=1}^{n} \gamma_j \sum_m B_{jm}^{+} B_{jm}, \qquad (3.9)$$

$$\gamma_j = (\Delta_j - \tilde{\mu}_j)\, \beta_j \approx (\Delta - \tilde{\mu})\, \beta_j, \tag{3.9a}$$

where $\tilde{\mu}$ denotes the corresponding chemical potential of the chain.

For a state near to the equilibrium, $(\beta_s - \beta_n)$ can be treated as nearly constant and taken in front of the integral sign denoting the time integration. So (3.6) becomes

$$\langle \dot{H}_j \rangle = \sum_{s=1}^{n-1} (\beta_s - \beta_n) \int_0^1 \mathrm{d}\,\tau \int_{-\infty}^0 \mathrm{e}^{\varepsilon t}\, \mathrm{d}t\, \langle \mathrm{e}^{M\tau}\, \dot{H}_j\, \mathrm{e}^{-M\tau}\, \dot{H}_s(t) \rangle_q, \tag{3.10}$$

where the kinetical coefficient is

$$L_{js} = \int_0^1 \mathrm{d}\,\tau \int_{-\infty}^0 \mathrm{e}^{\varepsilon t}\, \mathrm{d}t\, \langle \mathrm{e}^{M\tau}\, \dot{H}_j\, \mathrm{e}^{-M\tau}\, \dot{H}_s(t) \rangle_q, \tag{3.11}$$

and (3.10) becomes

$$\langle \dot{H}_j \rangle = \sum_{s=1}^{n-1} (\beta_s - \beta_n)\, L_{js}. \tag{3.12}$$

Since

$$\begin{aligned} \mathrm{e}^{M\tau}\, B^{+}_{j,a_j}\, \mathrm{e}^{-M\tau} &= \mathrm{e}^{\gamma_j \tau}\, B^{+}_{j,a_j}\,, \\ \mathrm{e}^{M\tau}\, B_{j,a_j}\, \mathrm{e}^{-M\tau} &= \mathrm{e}^{-\gamma_j \tau}\, B_{j,a_j}\,, \end{aligned} \tag{3.13}$$

it follows that it is possible to express the coefficient (3.11) through the retarded Green's function by integrating over τ

$$\begin{aligned} L_{js} = &- \frac{\Delta W}{(\gamma_j - \gamma_{j+1})} \int_{-\infty}^0 \mathrm{e}^{\varepsilon t}\, \mathrm{d}t\, \langle\langle B^{+}_{ja_j}\, B_{j+1a_j} \mid \dot{H}_s(t) \rangle\rangle - \\ &- \frac{\Delta W^*}{(\gamma_j - \gamma_{j+1})} \int_{-\infty}^0 \mathrm{e}^{\varepsilon t}\, \mathrm{d}t\, \langle\langle B^{+}_{j+1a_j}\, B_{ja_j} \mid \dot{H}_s(t) \rangle\rangle - \\ &- \frac{\Delta W}{(\gamma_j - \gamma_{j-1})} \int_{-\infty}^0 \mathrm{e}^{\varepsilon t}\, \mathrm{d}t\, \langle\langle B^{+}_{j-1a_{j-1}}\, B_{ja_{j-1}} \mid \dot{H}_s(t) \rangle\rangle - \\ &- \frac{\Delta W^*}{(\gamma_j - \gamma_{j-1})} \int_{-\infty}^0 \mathrm{e}^{\varepsilon t}\, \mathrm{d}t\, \langle\langle B^{+}_{ja_{j-1}}\, B_{j-1a_{j-1}} \mid \dot{H}_s(t) \rangle\rangle, \end{aligned} \tag{3.14}$$

where the Green's function is

$$\langle\langle A(t) \mid B(t') \rangle\rangle = \frac{\Theta(t - t')}{\mathrm{i}\,\hbar} < [A(t),\, B(t')] >. \tag{3.15}$$

Retaining only those Green's functions containing correlators, the kinetical coefficients may be written as

$$L_{js} = \frac{\Delta^2 |W|^2}{\mathrm{i}\hbar(\gamma_j - \gamma_{j+1})} \int_{-\infty}^{0} e^{\varepsilon t} \, dt \, [\langle\langle B^+_{ja_j} B_{j+1a_j} \,|\, B^+_{s+1a_s}(t) B_{sa_s}(t) \rangle\rangle -$$

$$- \langle\langle B^+_{ja_j} B_{j+1a_j} \,|\, B^+_{sa_{s-1}}(t) B_{s-1a_{s-1}}(t)\rangle\rangle] -$$

$$- \frac{\Delta^2 |W|^2}{\mathrm{i}\hbar(\gamma_j - \gamma_{j+1})} \int_{-\infty}^{0} e^{\varepsilon t} \, dt \, [\langle\langle B^+_{j+1a_j} B_{ja_j} \,|\, B^+_{sa_s}(t) B_{s+1a_s}(t)\rangle\rangle -$$

$$- \langle\langle B^+_{j+1a_j} B_{ja_j} \,|\, B^+_{s-1a_{s-1}}(t) B_{sa_{s-1}}(t)\rangle\rangle] +$$

$$+ \frac{\Delta^2 |W|^2}{\mathrm{i}\hbar(\gamma_j - \gamma_{j-1})} \int_{-\infty}^{0} e^{\varepsilon t} \, dt \, [\langle\langle B^+_{j-1a_{j-1}} B_{ja_{j-1}} B^+_{s+1a_s}(t) B_{sa_s}(t)\rangle\rangle -$$

$$- \langle\langle B^+_{j-1a_{j-1}} B_{ja_{j-1}} B^+_{sa_{s-1}}(t) B_{s-1a_{s-1}}(t)\rangle\rangle] -$$

$$- \frac{\Delta^2 |W|^2}{\mathrm{i}\hbar(\gamma_j - \gamma_{j-1})} \int_{-\infty}^{0} e^{\varepsilon t} \, dt \, [\langle\langle B^+_{ja_{j-1}} B_{j-1a_{j-1}} \,|\, B^+_{sa_s}(t) B_{s+1a_s}(t)\rangle\rangle -$$

$$- \langle\langle B^+_{ja_{s-1}} B_{j-1a_{j-1}} \,|\, B^+_{s-1a_{s-1}}(t) \; B_{sa_{s-1}}(t)\rangle\rangle]. \qquad (3.16)$$

Approximating the Green's function an substituting it by correlators averaged over the solitonic states $|\psi\rangle$, from (2.7) one can find the contributions that Davydov's solitons give to kinetical coefficients (3.16)

$$L_{jj} = \frac{\Delta^2 |W|^2}{\mathrm{i}\hbar(\gamma_j - \gamma_{j+1})} \int_{-\infty}^{0} e^{\varepsilon t} \, dt \, [\langle\langle B^+_{ja_j} B_{j+1a_j} \,|\, B^+_{j+1a_j}(t) B_{ja_j}(t)\rangle\rangle] -$$

$$- \frac{\Delta^2 |W|^2}{\mathrm{i}\hbar(\gamma_j - \gamma_{j+1})} \int_{-\infty}^{0} e^{\varepsilon t} \, dt \, [\langle\langle B^+_{j+1a_j} B_{ja_j} \,|\, B^+_{ja_j}(t) B_{j+1a_j}(t)\rangle\rangle] -$$

$$- \frac{\Delta^2 |W|^2}{\mathrm{i}\hbar(\gamma_j - \gamma_{j-1})} \int_{-\infty}^{0} e^{\varepsilon t} \, dt \, [\langle\langle B^+_{j-1a_{j-1}} B_{ja_{j-1}} \,|\, B^+_{ja_{j-1}}(t) B_{j-1a_{j-1}}(\mathrm{t})\rangle\rangle] +$$

$$+ \frac{\Delta^2 |W|^2}{\mathrm{i}\hbar(\gamma_j - \gamma_{j-1})} \int_{-\infty}^{0} e^{\varepsilon t} \, dt \, \langle\langle B^+_{ja_{j-1}} B_{j-1a_{j-1}} \,|\, B^+_{j-1a_{j-1}}(t) B_{ja_{j-1}}(t)\rangle\rangle, \qquad (3.17)$$

so that the Green's function is

$$\langle\langle B^+_{ja_j} B_{j+1a_j} \,|\, B^+_{j+1a_j}(\mathrm{t}) B_{ja_j}(t)\rangle\rangle =$$

$$= \frac{\Theta(-t)}{\mathrm{i}\hbar} \langle [B^+_{ja_j} B_{j+1a_j}, B^+_{j+1a_j}(t) B_{ja_j}(t)]\rangle. \qquad (3.18)$$

Since

$$\left.\begin{aligned} B_{ja_j}(t) &= e^{-i\frac{\Delta}{\hbar}} B_{ja_j} \\ B^+_{ja_j}(t) &= e^{i\frac{\Delta}{\hbar}} B^+_{ja_j} \end{aligned}\right\}, \tag{3.19}$$

it follows

$$\langle\langle B^+_{ja_j} B_{j+1a_j} \mid B^+_{j+1a_j}(t) B_{ja_j}(t)\rangle\rangle =$$

$$= \frac{\Theta(-t)}{i\hbar}\left[\langle B^+_{ja_j} B_{ja_j}\rangle - \langle B^+_{j+1a_j} B_{j+1a_j}\rangle\right], \tag{3.20}$$

where

$$\langle B^+_{ja_j} B_{ja_j}\rangle = Sp^{(\psi_\nu)}(B^+_{ja_j} B_{ja_j}\varrho) = \sum_\nu \langle\psi_\nu \mid B^+_{ja_j} B_{ja_j}\varrho \mid \psi_\nu\rangle =$$

$$= \frac{1}{Q}\,|\varphi_{a_j}(t)|^2 \sum_\nu \langle\psi_\nu \mid U^+_a\, e^{-\Sigma\frac{\hbar\Omega_q}{\Theta} b^+_q b_q} U_a \mid \psi_\nu\rangle = |\varphi_{a_j}(t)|^2, \tag{3.21}$$

since

$$Q = \sum_\nu \langle\psi_\nu \mid U^+_a\, e^{-\Sigma\frac{\hbar\Omega_q}{\Theta} b^+_q b_q} U_a \mid \psi_\nu\rangle = \frac{e^{-\frac{\Delta}{\Theta_j}}}{\prod\limits_q (1 - e^{-\lambda_{jq}})}. \tag{3.22}$$

So that

$$\langle\langle B^+_{ja_j} B_{j+1a_j} \mid B^+_{j+1a_j}(t) B_{ja_j}(t)\rangle\rangle =$$

$$= \frac{\Theta(-t)}{i\hbar}\left[|\varphi_{a_j}(t)|^2 - |\varphi_{j+1a_j}(t)|^2\right], \tag{3.23}$$

where

$$|\varphi_{a_j}(t)|^2 = \frac{a_j(\Theta_j) R_0}{2}\,\frac{1}{\mathrm{ch}^2\, a_j(\Theta_j)(x_{a_j} - x_j^{(0)} - v_j t)}. \tag{3.24}$$

In this way the diagonal matrix element is

$$L_{jj} = -\frac{2\Delta^2 |W|^2}{\hbar^2(\gamma_j - \gamma_{j+1})}\int_{-\infty}^{0} e^{\varepsilon t}\, dt\, \left[|\varphi_{ja_j}|^2 - |\varphi_{j+1a_j}|^2\right] -$$

$$- \frac{2\Delta^2 |W|^2}{\hbar^2(\gamma_j - \gamma_{j-1})}\int_{-\infty}^{0} e^{\varepsilon t}\, dt\, \left[|\varphi_{ja_{j-1}}|^2 - |\varphi_{j-1a_{j-1}}|^2\right], \tag{3.25}$$

that is for $s = j + 1$

$$L_{jj+1} = -\frac{\Delta^2 |W|^2}{i\hbar(\gamma_j - \gamma_{j+1})}\int_{-\infty}^{0} e^{\varepsilon t}\, dt\, \langle\langle B^+_{ja_j} B_{j+1a_j} \mid B^+_{j+1a_j}(t) B_{ja_j}(t)\rangle\rangle +$$

$$+ \frac{\Delta^2 |W|^2}{i\hbar(\gamma_j - \gamma_{j+1})}\int_{-\infty}^{0} e^{\varepsilon t}\, dt\, \langle\langle B^+_{j+1a_j} B_{ja_j} \mid B^+_{ja_j}(t) B_{j+1a_j}(t)\rangle\rangle, \tag{3.26}$$

and for $s = j - 1$

$$L_{jj-1} = \frac{\Delta^2 |W|^2}{i\hbar(\gamma_j - \gamma_{j-1})} \int_{-\infty}^{0} e^{\varepsilon t} dt \langle\langle B^+_{j-1a_{j-1}} B_{ja_{j-1}} | B^+_{ja_{j-1}}(t) B_{j-1a_{j-1}}(t) \rangle\rangle -$$

$$- \frac{\Delta^2 |W|^2}{i\hbar(\gamma_j - \gamma_{j-1})} \int_{-\infty}^{0} e^{\varepsilon t} dt \langle\langle B^+_{ja_{j-1}} B_{j-1a_{j-1}} | B^+_{j-1a_{j-1}}(t) B_{ja_{j-1}}(t) \rangle\rangle. \quad (3.27)$$

That is

$$L_{jj+1} = \frac{2\Delta^2 |W|^2}{\hbar^2(\gamma_j - \gamma_{j+1})} \int_{-\infty}^{0} e^{\varepsilon t} dt \, [|\varphi_{ja_j}|^2 - |\varphi_{j+1a_j}|^2] \quad (3.26a)$$

$$L_{jj-1} = - \frac{2\Delta^2 |W|^2}{\hbar^2(\gamma_j - \gamma_{j-1})} \int_{-\infty}^{0} e^{\varepsilon t} dt \, [\varphi_{j-1a_{j-1}}|^2 - |\varphi_{ja_{j-1}}|^2]. \quad (3.27a)$$

There is no other coefficients. Hence the average current is

$$\langle \dot{H}_j \rangle = L_{jj-1}(\beta_{j-1} - \beta_n) + L_{jj}(\beta_j - \beta_n) + L_{jj+1}(\beta_{j+1} - \beta_n) \quad (j = 1, 2 \dots n) \quad (3.28)$$

For $n = 2$

$$\langle \dot{H}_1 \rangle = L_{11}(\beta_1 - \beta_2),$$

$$\langle \dot{H}_2 \rangle = -\langle \dot{H}_1 \rangle. \quad (3.29a)$$

For $n = 3$

$$\langle \dot{H}_1 \rangle = L_{11}(\beta_1 - \beta_3) + L_{12}(\beta_2 - \beta_3),$$

$$\langle \dot{H}_2 \rangle = L_{21}(\beta_1 - \beta_3) + L_{22}(\beta_2 - \beta_3),$$

$$\langle \dot{H}_3 \rangle = L_{32}(\beta_2 - \beta)_3. \quad (3.29b)$$

According to the relaxation theory the average current in the *j-th* molecular chain can be transformed in the following way[3]

$$\langle \dot{H}_j \rangle = \frac{d}{dt} \langle H_j \rangle_q = \frac{d}{d\beta_j} \langle H_j \rangle_q \frac{d\beta_j}{dt} = -\langle H_j^2 \rangle \frac{d\beta_j}{dt}. \quad (3.30)$$

The expression for $\langle H_j \rangle_q$ can be derived and expressed through solitonic currents (it means by omiting the index j in the first approximation)

$$\langle H \rangle_q \simeq \Delta \sum_{\nu} \sum_{n} \langle \psi_\nu | B_n^+ B_n \frac{e^{-\beta\Delta \sum_s B_s^+ B_s}}{Q} \varrho_{ph} | \psi_\nu \rangle =$$

$$= \Delta \sum_n \sum_\nu \sum_{fg} \langle \nu \mid U_f^+ (t)\, \varrho_{ph} (\beta)\, U_g (t) \mid \nu \rangle\, \varphi_f^* (t)\, \varphi_g (t) \times$$

$$\times \langle 0 \mid B_f B_n^+ B_n\, e^{-\beta \Delta B_g^+ B_g} B_g^+ \mid 0 \rangle \frac{1}{Q}, \tag{3.31}$$

$$\frac{\partial}{\partial \beta} \langle H \rangle_q = -\Delta^2 \sum_n \sum_{fg\nu} \langle \nu \mid U_f^+ (t)\, \varrho_{ph} (\beta)\, U_g (t) \mid \nu \rangle \times$$

$$\times \langle 0 \mid B_f B_n^+ B_n B_g^+ B_j\, e^{-\beta \Delta B_g^+ B_g} B_g^+ \mid 0 \rangle \frac{\varphi_g \varphi_f^+}{Q}. \tag{3.32}$$

We have neglected the term

$$\frac{\partial}{\partial \beta} \langle \nu \mid U_f^+ (t)\, \varrho_{ph} (\beta)\, U_g (t) \mid \nu \rangle,$$

as a smaller order term

$$\frac{\partial}{\partial \beta} \langle H \rangle_q = -\Delta^2 \sum_{g\nu} \langle \nu \mid U_g^+ (t)\, \varrho_{ph} (\beta)\, U_g (t) \mid \nu \rangle \mid \varphi_g \mid^2 \frac{e^{-\beta \Delta}}{Q}. \tag{3.32a}$$

Since

$$Q = \sum_{g\nu} \langle \nu \mid U_g^+ (t)\, \varrho_{ph} (\beta)\, U_g (t) \mid \nu \rangle\, e^{-\beta \Delta} \mid \varphi_g \mid^2, \tag{3.32b}$$

one has

$$\left. \begin{aligned} &\frac{\partial}{\partial \beta} \langle H \rangle_q = -\Delta^2, \\ &\langle \dot{H}_j \rangle_q \cong -\Delta^2 \frac{d\beta_j}{dt} \end{aligned} \right\}. \tag{3.33}$$

The system (3.28) gives us the possibility to find the temperature dependence as a function of time of individual molecular chains being in contact with each other. For $n = 2$ one has

$$\left. \begin{aligned} -\Delta^2 \frac{d\beta_1}{dt} &= L_{11} (\beta_1 - \beta_2), \\ -\Delta^2 \frac{d\beta_2}{dt} &= L_{21} (\beta_1 - \beta_2). \end{aligned} \right\} \tag{3.34}$$

Since $L_{11} = -L_{21}$ one has

$$\left. \begin{aligned} &\beta_1 + \beta_2 = \text{const} = A, \\ &\beta_1 = A - \beta_2. \end{aligned} \right\}$$

A is determined from initial conditions. In this way the first equation from the system (3.34) can be determined by substituting (3.35) in (3.34)

$$-\Delta^2 \frac{d\beta_1}{dt} = L_{11} (2 \beta_1 - A). \tag{3.35a}$$

According to (3.25) and (3.24) it follows that

$$L_{11} = - \frac{2 \Delta^2 |W|^2}{\hbar^2 (\gamma_1 - \gamma_2)} \int_{-\infty}^{0} e^{\varepsilon t} dt \left[|\varphi_{1a}(t)|^2 - |\varphi_{2a}(t)|^2 \right] =$$

$$= - \frac{\Delta^2 |W|^2 R_0}{\hbar^2 (\gamma_1 - \gamma_2)} \left[\frac{1}{v_1} (\text{th}\, \alpha_1 (x_a - x_0) - \frac{1}{v_2} (1 - \text{th} \alpha_2 (y_a - y_0)) \right]. \tag{3.36}$$

Since

$$\int_{-\infty}^{0} e^{\varepsilon t} dt \, | \varphi_a(t)|^2 = \int_{0}^{\infty} e^{-\varepsilon t} dt \frac{\alpha R_0}{2} \frac{1}{\text{ch}^2 \alpha (x_a - x_0 + vt)} =$$

$$= \frac{\alpha R_0}{2} \frac{1}{\alpha v} 1 (1 - \text{th}\, \alpha (x_a - x_0)). \tag{3.37}$$

We assume that the effect caused by the soliton is substantial when the argument is small i. e., when $\alpha (x_a - x_0) \ll 1$ that is $\text{th}\, \alpha (x_a - x_0) \cong \alpha (x_a - x_0)$.

If one takes into account that according to the Davydov's calculation[5], the dependence of the coefficient α on temperature is linear

$$\alpha (\Theta) \cong \alpha_0 (1 - D \Theta) \tag{3.38}$$

one can write the differential equation for the inverse temperature in the f oım: $(\gamma_J = \Delta \beta_J)$

$$\frac{d\beta_1}{dt} = \frac{|W|^2 R_0}{\Delta \hbar^2} \left[K + \frac{\alpha_0 D (x_1 - x_0)}{v_1 \beta_1} - \frac{\alpha_0 D (y_a - y_0)}{v_2 (A - \beta_1)} \right], \tag{3.39}$$

where

$$K = \frac{v_2 - v_1}{v_1 v_2} - \frac{\alpha_0 (x_a - x_0)}{v_1} + \frac{\alpha_0 (y_a - y_0)}{v_2}, \tag{3.40}$$

that can be solved separating the variables and introducing the following notations

$$M = \frac{|W|^2 R_0 K}{\hbar^2 \Delta},$$

$$L_1 = \frac{|W|^2 R_0}{\Delta \hbar^2} \frac{a_0 D}{v_1} (x_a - x_0),$$

$$L_2 = \frac{|W|^2 R_0}{\Delta \hbar^2} \frac{\alpha_0 D}{v_2} (y_a - y_0), \tag{3.41}$$

and

$$\frac{d\beta_1}{dt} = M \frac{\beta_1^2 - \eta \beta_1 - \xi}{\beta_1^2 - A \beta_1}, \tag{3.42}$$

that give

$$\beta_1(t) + U_1 \ln \left(\beta_1 - \frac{\eta}{2} + \sqrt{\frac{\eta^2}{4} + \xi}\right) + U_2 \ln \left(\beta_1 - \frac{\eta}{2} - \sqrt{\frac{\eta^2}{4} + \xi}\right) =$$

$$= M t + \text{const}, \tag{3.43}$$

$$U_1 = \frac{\left(\sqrt{\frac{\eta^2}{4} + \xi} - \frac{\eta}{2}\right)(\eta - A) - \xi}{2\sqrt{\frac{\eta^2}{4} + \xi}};$$

$$U_2 = \frac{\xi + \left(\frac{\eta}{2} + \sqrt{\frac{\eta^2}{4} + \xi}\right)(\eta - A)}{2\sqrt{\frac{\eta^2}{4} + \xi}}, \tag{3.44}$$

$$\left.\begin{aligned} \eta &= A - \frac{L_1 + L_2}{M}, \\ \xi &= \frac{A L_1}{M}. \end{aligned}\right\} \tag{3.45}$$

In the case when solitons are located just in the contact point $L_1 = 0$, $L_2 = 0$; that gives the solution for

$$\beta_1(t) = M_0 t + \text{const}, \tag{3.46}$$

$\beta_1(0) = \mathit{const}$ is the value of $\beta_1(t)$ for $t = 0$. Or if we are interested for the evolution of temperature in the chain 1 then in the basic (3.46) we have

$$\Theta_1 = \frac{1}{\beta_1^{(0)} + \frac{|W|^2 R_0 (v_2 - v_1) t}{\hbar^2 \Delta v_1 v_2}}, \tag{3.47}$$

which decreases or increases from initial value in dependence from difference of the velocity solitons in the chains which contact. While Θ_2 for the same case is

$$\Theta_2 = \frac{1}{\beta_2^{(0)} - \frac{|W|^2 R_0 (v_2 - v_1) t}{\hbar^2 \Delta v_1 v_2}}. \tag{3.48}$$

In the case $n = 3$ we have the following system of differential equations

$$-\Delta^2 \frac{d\beta_1}{dt} = L_{1,1} (\beta_1 - \beta_3) + L_{1,2} (\beta_2 - \beta_3),$$

$$-\Delta^2 \frac{d\beta_2}{dt} = L_{2,1} (\beta_1 - \beta_3) + L_{2,2} (\beta_2 - \beta_3),$$

$$-\Delta^2 \frac{d\beta_3}{dt} = L_{3,2} (\beta_2 - \beta_3). \tag{3.49}$$

Since

$$L_{2,1} = -L_{1,1}, \; L_{3,2} + L_{2,2} + L_{1,2} = 0, \tag{3.49a}$$

and having in view (3.49) it follows that

$$\beta_1 + \beta_2 + \beta_3 = const = A,$$

$$\beta_3 = A - \beta_1 - \beta_2. \tag{3.50}$$

On the other side considering the expressions (3.49a) we have

$$-\Delta^2 \frac{d\beta_1}{dt} = L_{1,1} (\beta_1 - \beta_2),$$

$$-\Delta^2 \frac{d\beta_2}{dt} = -L_{1,1} (2 \beta_1 + \beta_2 - A) + L_{2,2} (2 \beta_2 + \beta_1 - A). \tag{3.51}$$

If we denote

$$L_{1,1} = - \frac{2 \Delta |W|^2}{(\beta_1 - \beta_2) \hbar^2} \int_{-\infty}^{0} e^{\varepsilon t} dt \, [|\varphi_1 (a_1)|^2 - |\varphi_2 (a_1)|^2],$$

$$L_{2,2} = - \frac{2 \Delta |W|^2}{(\beta_2 - \beta_3) \hbar^2} \int_{-\infty}^{0} e^{\varepsilon t} dt \, [|\varphi_2 (a_2)|^2 - |\varphi_3 (a_2)|^2] -$$

$$- \frac{2 \Delta |W|^2}{(\beta_2 - \beta_1) \hbar^2} \int_{-\infty}^{0} e^{\varepsilon t} dt \, [|\varphi_2 (a_1)|^2 - |\varphi_1 (a_1)|^2], \tag{3.52}$$

than it follows

$$\left.\begin{aligned} L_{1,1} &= -\frac{A_{1,2}(a_1)}{\beta_1-\beta_2}, \\ L_{2,2} &= -\frac{A_{1,2}(a_1)}{\beta_1-\beta_2}-\frac{A_{2,3}(a_2)}{\beta_2-\beta_3}, \end{aligned}\right\} \tag{3.53}$$

where

$$A_j(a_j)=\frac{2\Delta|W|^2}{\hbar^2}\int_{-\infty}^{0}e^{\varepsilon t}\,dt\,(|\varphi_i(a)|^2-|\varphi_j(a)|^2). \tag{3.53a}$$

For that

$$\left.\begin{aligned} -\Delta^2\frac{d\beta_1}{dt} &= -A_{1,2}(a_1), \\ -\Delta^2\frac{d\beta_2}{dt} &= A_{1,2}(a_1)-A_{2,3}(a_2). \end{aligned}\right\} \tag{3.51b}$$

Respectively, after a short calculation from the same approximation as in the case $n = 2$ we obtain

$$\frac{d\beta_1}{dt}=M_{1,2}+\frac{L_1}{\beta_1}-\frac{L_2}{\beta_2}, \tag{3.54a}$$

$$\frac{d\beta_2}{dt}=M_{2,3}-M_{1,2}-\frac{L_1}{\beta_1}+\frac{2L_2}{\beta_2}-\frac{L_3}{A-\beta_1-\beta_2}, \tag{3.54b}$$

where

$$M_{1,2}=\frac{R_0|W|^2}{\Delta\hbar^2}\left[\frac{v_1-v_2}{v_1v_2}-\frac{a_0(x_{a_1}-x_0)}{v_1}+\frac{a_0(y_{a_1}-y_0)}{v_2}\right],$$

$$L_1=\frac{R_0|W|^2}{\Delta\hbar^2}\frac{a_0D}{v_1}(x_{a_1}-x_0),$$

$$L_2=\frac{R_0|W|^2}{\Delta\hbar^2}\frac{a_0D}{v_2}(y_{a_1}-y_0),$$

$$L_3=\frac{R_0|W|^2}{\Delta\hbar^2}\frac{a_0D}{v_3}(z_{a_2}-z_0),$$

$$M_{2,3}=\frac{R_0|W|^2}{\Delta\hbar^2}\left[\frac{v_3-v_2}{v_2v_3}-\frac{a_0(y_{a_2}-y_0)}{v_2}-\frac{a_0(z_{a_1}-z_0)}{v_3}\right]. \tag{3.55}$$

This is a system of nonlinear differential equations which can be solved only for some special physical hypothesis and conditions.

And, more generally, having in view the temperature dependence of solitonic parameters, one can see, that for any number n it is only possible to get nonlinear differential equations. But since the solitonic parameters are only weakly dependent on temperature (D is small) we can admit that terms such as L and M in (3.54) remain constant in kinetical processes. So from (3.9a) it follows that:

$$\gamma_j - \gamma_{j+1} = \Delta(\beta_j - \beta_{j+1}),$$

and

$$A_{j,j+1}(a_j) = \frac{2\Delta |W|^2}{\hbar^2} \int\limits_{-\infty}^{0} e^{\varepsilon t}\, dt\, [|\varphi_j(a_j)|^2 - |\varphi_{j+1}(a_j)|^2]. \tag{3.56}$$

So, the relevant kinetic coefficients may be written as:

$$L_{j,j-1} = -\frac{A_{j-1,j}(a_{j-1})}{\beta_j - \beta_{j-1}},$$

$$L_{jj} = -\frac{A_{j,j+1}(a_j)}{\beta_j - \beta_{j+1}} - \frac{A_{j,j-1}(a_{j-1})}{\beta_j - \beta_{j-1}},$$

$$L_{j,j+1} = -\frac{A_{j-1,j}(a_{j-1})}{\beta_j - \beta_{j-1}}, \tag{3.57}$$

so that the average current in the j-th chain, according to the formula (3.49), is

$$\langle \dot{H}_j \rangle = -A_{j,j+1}(a_j) - A_{j,j-1}(a_{j-1}). \tag{3.58}$$

From (3.33)

$$\langle \dot{H}_j \rangle_q = \Delta^2 \frac{d\beta_j}{dt},$$

it follows

$$\frac{d\beta_j}{dt} = \frac{1}{\Delta^2} [A_{j,j+1}(a_j) + A_{j,j-1}(a_{j-1})], \tag{3.59}$$

respectively. After integration over time ($a_j \equiv a$, $a_{j-1} \equiv b$)

$$\frac{d\beta_j}{dt} = \frac{R_0 |W|^2}{\hbar^2 \Delta} \left[\frac{1}{v_j}(1 - \mathrm{th}\, a_j(x_j^a - x_j^0)) - \frac{1}{v_{j+1}}(1 - \mathrm{th}\, a_{j+1}(y_{j+1}^a - y_{jj}^0)) + \right.$$

$$\left. + \frac{1}{v_j}(1 - \mathrm{th}\, a_j(x_j^b - x_j^0)) - \frac{1}{v_{j-1}}(1 - \mathrm{th}\, a_{j-1}(z_{j-1}^b - z_j^0))\right]. \tag{3.60}$$

From the last formula we can see that for the soliton mechanism of transmission, the participation of the solitons distant from contacts a and b is insignificant for the energy transport and which is therefore vanishing in this case.

If

$$\begin{aligned} \operatorname{th} a_j (x_j^a - x_j^0) &= 0, \\ \operatorname{th} a_{j+1} (y_{j+1}^a - y_j^0) &= 0, \\ \operatorname{th} a_{j-1} (z_{j-1}^b - z_j^0) &= 0, \end{aligned} \tag{3.61}$$

we hawe

$$\frac{\mathrm{d}\beta_j}{\mathrm{d}t} = \frac{W^2 R_0}{\hbar^2 \Delta}\left[\frac{1}{v_j} - \frac{1}{v_{j+1}} - \frac{1}{v_{j-1}} + \frac{1}{v_j}(1 - \operatorname{th} a_j (x_j^b - x_j^a))\right],$$

$$\frac{\mathrm{d}\beta_j}{\mathrm{d}t} = \frac{W^2 R_0}{\hbar^2 \Delta}\left\{\frac{1}{v_j}[2 - \operatorname{th} a_j (x_j^b - x_j^a)] - \frac{v_{j+1} + v_{j-1}}{v_{j+1} v_{j-1}}\right\},$$

$$\beta_j = \frac{W^2 R_0}{\hbar^2 \Delta}\left\{\frac{2 - \operatorname{th} a_j (x_j^b - x_j^a)}{v_j} - \frac{v_{j+1} + v_{j-1}}{v_{j+1} v_{j-1}}\right\} t + \beta_j(0). \tag{3.62}$$

4. *Conclussion*

In the absence of soliton mechanism in transport processes, when only collective (excitonic) excitations are present, from the structure of the kinetic coefficient (6.5) in the Ref. 6 one has

$$L_{\dot{H}\dot{H}} = \frac{2\pi\Delta |W|^2}{\hbar(\beta_1 - \beta_2) N^2} \sum_{kq} (\overline{N}_{1q} - \overline{N}_{2k} - 1)\, \delta(\varepsilon_{1q} - \varepsilon_{2k}), \tag{4.1}$$

where

$$\overline{N}_{1q} = (\mathrm{e}^{\beta_1 \varepsilon_{1q}} - 1)^{-1}.$$

Contrary to the case of the solitonic mechanism, from (4.1) it follows that in the case of the presence of collective excitations, special conditions of locality does not exsist and so the kinetical coefficient (4.1) can not be neglected. In other words, the system of chains in contact which would be on different temperatures would not be able to transmit the information, because it would be energeticaly instable.

In spite of the exsisting contacts, the solitonic transmission mechanism is able to secure the transmission of informations along the chain. The participation of collective excitations is fatal for this transmission since such excitations are able to transfer the energy from chain to chain and to average the temperature throught the system and to introduce the entropy. The locality secures that one has almost always

$$1 - \operatorname{th} a_j (x_j^a - x_j^0) = 0, \tag{4.2}$$

because it would be a rare occurrence to find a soliton very often near the contact. The expression (3.60) consists of two terms per soliton. Only one can give its contribution at a time owing to the soliton locality. This is the reason for the small value of the kinetical coefficient and for the possibility of the transmission of information along the molecular chain.

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TERMODINAMIČKA STABILNOST SISTEMA MNOŠTVA MOLEKULARNIH LANACA KOJI SE DODIRUJU U MALOM BROJU ČVOROVA

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Analizirani su uslovi stabilnosti u transportu informacija preko nervnih vlakana pomoću solitonskog mehanizma. Vlakna u međusobnom kontaktu se karakterizuju pomoću date temperaturske distribucije.