

# On the problem of joint motion of interacting quantum and classical systems in the process of excitation transfer in a quantum subsystem

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In this paper, we discuss the problem of joint motion of interacting quantum and classical systems in the process of excitation transfer in a quantum subsystem.

## 1. Introduction

In many processes where biopolymers participate there appears a situation when the change in the state of the “light” system, i.e. quantum subsystem (electrons, protons) is accompanied by the motion of heavier particles (of atoms C, O, N or globules). This motion is generally described by laws of classic mechanics. Moreover, the problem of combination of probabilistic description of quantum subsystem with the Laplace deterministic description of classical system appears.

In biological systems the main energy source is ATP splitting. It is a pure quantum process, energy being supplied by discrete portions  $\Delta E \sim 0.4\text{--}0.5$  eV. Further, in a macroscopic system energy is converted into the energy of conformational changes.

In refs. [1–3] a model of muscle contraction based on the hypothesis on the fact that at the first stage the energy  $\Delta E$  produces excitation of hydrogen A–H · · B bonds between atoms A and B which are contained in the myosin head and actin filament (fig. 1), is considered. These bonds are weak when interatomic distances  $AB = R_1$  are comparatively great, but they become stronger and larger-range in character provided the proton has been excited  $\epsilon_0 \rightarrow \epsilon_1$  [4]. The resulting force  $f = -\partial\epsilon_1/\partial R$  makes, according to our hypothesis, atoms AB approach each other and actin and myosin filaments slide.

The work done when approaching from the distance  $R_1$  to  $R_2 < R_1$ , i.e.  $\Delta A = \epsilon_1(R_1) - \epsilon_1(R_2)$ , does not exceed 30% of the excitation energy  $\Delta E = \epsilon_1(R_1) - \epsilon_0(R_1)$  [4]. Therefore in order to explain high muscle contraction efficiency (up to 80% [5]) the energy residue  $\Delta_1 E = \Delta E - \Delta A$ , after the work  $\Delta A$  has already been done, is supposed to be transferred to a weaker neighboring hydrogen

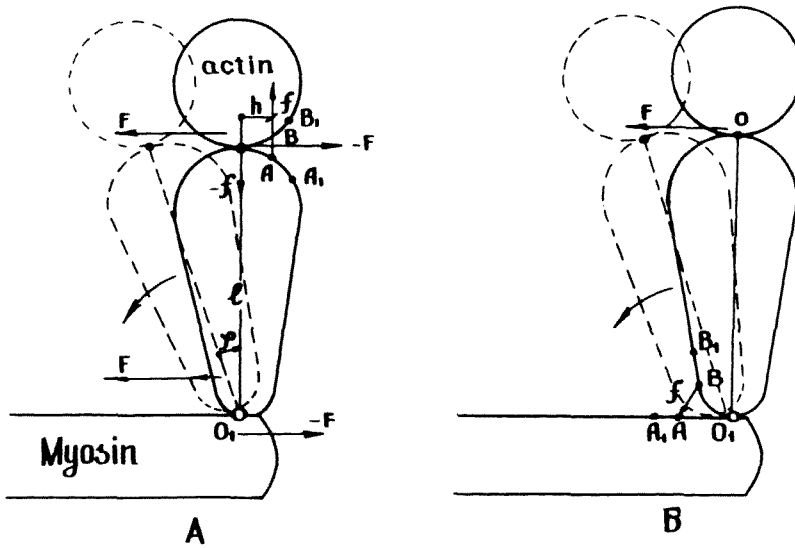


Fig. 1. The actin globule displacement due to the awing of amyosin head under the action of hydrogen bonds  $A-H \cdots B$ ,  $A_1-H_1 \cdots B_1$ , located near the actin-myosin attachment (A) or hinge (B).

bond. The process may continue until almost the whole of the initial energy  $\Delta E$  of ATP splitting is exhausted. When calculating [6,7] the probability of excitation energy residue transfer from the bond  $A-H \cdots B$  to the next bond  $A_1-H_1 \cdots B_1$  we come across the self-conforming problem: the energy transfer takes place in the process of classical sliding of polymers and at the same time this motion is caused by the force  $f$  which is essentially of quantum mechanical character. It is obvious that the force  $f$  is different before and after transition,  $f_1 = -\partial\epsilon_1/\partial R$  and  $f_2 = -\partial\epsilon_2/\partial R$ , respectively, where  $\epsilon_2$  is the excitation energy of the neighboring hydrogen bond  $A_1-H_1 \cdots B_1$ . The very moment of transition is a quantum mechanical variable. The quantum mechanical mean for the force cannot be used in this case, since we are not interested in the average character of a motion of an ensemble of solitary pairs of polymers, but in the motion of a single pair.

We further consider this problem from two different points of view. First, it can be interpreted as a pure quantum problem with subsequent passing to the classical limit with respect to a heavy subsystem. Second, as a quantum classical problem when a heavy subsystem is supposed to be classical and to be under the action of jumpwise changing force  $f_1 \rightarrow f_2$  but the moment of a jump is undefined.

## 2. Quantum mechanical approach to proton and actin globule motion

### 2.1. ADIABATIC APPROXIMATION

The estimates of probability of excitation transfer [6,7] from the bond  $A-H \cdots B$  to the bond  $A_1-H_1 \cdots B_1$  show that the average transfer time

$\tau \sim 10^{-12} - 10^{-11}$  s is shorter by 2-3 orders than the time  $t \sim 3 \times 10^{-9}$  s required to transfer the tractive force from the location of actin-myosin attachment to the z-plate of a sarcomere. Thus, only the last actin globule under the force  $f$  of a H-bond has the time to begin its motion in the period  $\tau$ . Hence we now consider only the system consisting of three quantum particles: protons of H-bonds with coordinates  $r_1$  and  $r_2$ , and actin globule, whose displacement denoted by  $\xi$  (see fig. 1).

The Hamiltonian of this system is

$$H = -\frac{\hbar^2}{2m}(\Delta_1 + \Delta_2) + V_1(r_1, \xi) + V_2(r_2, \xi) + V(r_{12}) - \frac{\hbar^2}{2M} \frac{\partial^2}{\partial \xi^2} + U(\xi), \quad (1)$$

where  $m$  and  $M$  are the masses of protons and of a globule,  $V_1$  and  $V_2$  are potential proton energies parametrically dependent on the globule displacement  $\xi$  (the H-bond lengths being dependent on it in their turn),  $V(r_{12}) = e^2/\epsilon_\infty r_{12}$  is the proton interaction energy,  $U(\xi)$  is the potential energy of the interaction of the given globule with neighboring ones, which are not considered to be in motion.

Due to the strong inequality  $m \ll M$  the eigenfunctions and Hamiltonian (1) energies can be defined by adiabatic approximation provided proton states are determined first:

$$\psi_{10}(r_1, r_2, \xi) = \varphi_1^{(1)}(r_1, \xi) \cdot \varphi_0^{(2)}(r_2, \xi), \quad (2)$$

$$\psi_{01}(r_1, r_2, \xi) = \varphi_0^{(1)}(r_1, \xi) \cdot \varphi_1^{(2)}(r_2, \xi), \quad (3)$$

where  $\psi_{10}$  corresponds to excitation of the first bond when the second bond is not excited,  $\psi_{01}$  corresponds to the excitation transfer to the second bond. Here the upper indices of  $\varphi$  denote the number of bond, and the lower ones, the level of excitation. The functions  $\varphi_j^{(i)}$  of zero approximation follow from the equation

$$\left( -\frac{\hbar^2}{2m} \Delta_i + V_i(r_i, \xi) \right) \cdot \varphi_j^{(i)}(r_i) = \epsilon_j^{(i)} \varphi_j^{(i)}(r_i), \quad j = 0, 1. \quad (4)$$

Taking account of proton interaction  $V(r_{12})$  their states can be found in the form of the superposition

$$\Psi = C_1(\xi) \cdot \psi_{10}(r_1, r_2, \xi) + C_2(\xi) \cdot \psi_{01}(r_1, r_2, \xi). \quad (5)$$

Then the energy of two protons in this approximation is

$$E_{\pm} = \frac{E_{10} + E_{01}}{2} \pm \sqrt{\frac{(E_{10} - E_{01})^2}{4} + |V_{12}(\xi)|^2}, \quad (6)$$

where

$$E_{10} = \epsilon_1^{(1)}(\xi) + \epsilon_0^{(2)}(\xi) + \int \psi_{10}^* V(r_{12}) \psi_{10} dr_1 dr_2, \quad (7)$$

$$E_{01} = \epsilon_0^{(1)}(\xi) + \epsilon_1^{(2)}(\xi) + \int \psi_{01}^* V(r_{12}) \psi_{01} dr_1 dr_2,$$

$$V_{12} = \int \psi_{10}^*(r_1, r_2, \xi) V(r_{12}) \psi_{01}(r_1, r_2, \xi) dr_1 dr_2. \quad (8)$$

Figure 2 shows the dependencies of  $E_{10}$  and  $E_{01}$  (thin lines) and of the energies of the first approximation  $E_+$  and  $E_-$  on  $\xi$ .  $E_+$  and  $E_-$  represent two branches of the adiabatic potential; two wave functions, denoted by  $\Psi_-(r_1, r_2, \xi)$  and  $\Psi_+(r_1, r_2, \xi)$ , respectively, correspond to them. They differ in coefficients  $C_1^\pm$  and  $C_2^\pm$ . When the motion takes place along the lower branch  $E_-(\xi)$  the function  $\Psi_-(r_1, r_2, \xi)$  describes the conversion of the state  $\psi_{10}(2)$  to  $\psi_{01}(3)$ , i.e. excitation transfer to the second bond. For the state  $\Psi_-$  the coefficient  $C_1(\xi)$  changes from 1 to 0, and the coefficient  $C_2(\xi)$  from 0 to 1 when  $\xi$  increases.

The quantum-mechanical force  $f_1 = -\partial E_- / \partial \xi$ , acting along the coordinate  $\xi$  corresponds to the potential  $E_-(\xi)$ .

On the second state of the adiabatic approximation we find the function of a heavy subsystem, i.e. coordinates  $\xi$  using Schrödinger equation

$$\left( -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial \xi^2} + U(\xi) + E_-(\xi) \right) \cdot \chi = E \cdot \chi, \quad (9)$$

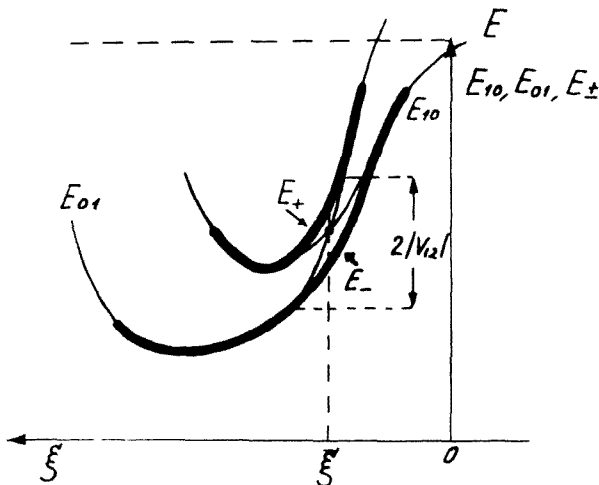


Fig. 2. Dependence of energies  $E_{10}$  and  $E_{01}$  on the coordinate  $\xi$  of the mutual displacement of polymers.

where the energy of a light subsystem  $E_-$  is a part of the potential energy for a heavy subsystem.

Then the wave function of the system is

$$\Psi = \chi(\xi) \cdot \Psi_-(r_1, r_2, \xi). \quad (10)$$

The solution of eq. (9) can be constructed in quasiclassical approximation,

$$\begin{aligned} \chi_-^0(\xi) = & \frac{b_1^-}{\sqrt{P_-(\xi)}} \exp \left[ \frac{i}{\hbar} \int_{\xi-\Delta}^{\xi} p_-(\xi') d\xi' \right] \\ & + \frac{b_2^-}{\sqrt{P_-(\xi)}} \exp \left[ -\frac{i}{\hbar} \int_{\xi-\Delta}^{\xi} p_-(\xi') d\xi' \right], \end{aligned} \quad (11)$$

where

$$P_-(\xi) = \sqrt{2m(E - E_-(\xi) - U(\xi))}. \quad (12)$$

The analogous solution  $\chi_+(\xi)$  has the form (11) but with substitution of  $P_+(\xi) = \sqrt{2m(E - E_+(\xi) - U(\xi))}$  for  $P_-(\xi)$  and other coefficients  $b_1^+$ ,  $b_2^+$  correspondingly.

## 2.2. DEVIATION OF THE SYSTEM FROM ADIABATICITY

The approximation considered above can be applied to an extent dependent on the fact how much the distance between adiabatic potentials  $E_+(\xi) - E_-(\xi)$  exceeds the matrix element of the operator of non-adiabaticity

$$\hat{H}_{NA} = -\frac{\hbar^2}{M} \frac{\partial}{\partial \xi} \Big|_{\Psi} \cdot \frac{\partial}{\partial \xi} \Big|_{\chi} - \frac{\hbar^2}{2M} \frac{\partial^2}{\partial \xi^2} \Big|_{\Psi}. \quad (13)$$

This operator is neglected when we pass from the exact Hamiltonian (1) to Hamiltonian (4). Here  $|\Psi$  and  $|\chi$  shows that the functions  $\Psi_{\pm}$  or  $\chi_{\pm}$  in (10) should be differentiable on  $\xi$ .

As it is shown in (6) the decomposition of potentials is of the order  $2|V_{12}|$ . According to the estimates in [1], it varies approximately close to 1 meV or a bit more. At the same time globule vibration frequencies are  $\approx 10^{12}$  rad/s. Thus they are comparable. So, we should take the deviation of the system from adiabaticity into account and define eigenfunctions of the Hamiltonian (1) in the form of the superposition

$$\Psi = \chi_-(\xi)\Psi_-(r_1, r_2, \xi) + \chi_+(\xi)\Psi_+(r_1, r_2, \xi), \quad (14)$$

where  $\Psi_-$  and  $\Psi_+$  are in the form of (5),  $\chi_+$  and  $\chi_-$  can be found from the system resulting after the operation  $H$  (1) with  $\Psi$  (14), multiplication  $\Psi_-^*$  and  $\Psi_+^*$  and integration on  $dr_1, dr_2$

$$\left\{ -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial \xi^2} + U(\xi) + E_-(\xi) - \frac{\hbar^2}{2M} \int \Psi_-^* \frac{\partial^2 \Psi_-}{\partial \xi^2} dr_1 dr_2 - E \right\} \chi_-(\xi) \\ = \frac{\hbar^2}{M} \int \Psi_-^* \frac{\partial \Psi_+}{\partial \xi} dr_1 dr_2 \frac{\partial \chi_+}{\partial \xi} + \frac{\hbar^2}{2M} \int \Psi_-^* \frac{\partial^2 \Psi_+}{\partial \xi^2} dr_1 dr_2 \chi_+(\xi) \quad (15)$$

$$\times \left\{ -\frac{\hbar^2}{2M} \frac{\partial^2}{\partial \xi^2} + U(\xi) + E_+(\xi) - \frac{\hbar^2}{2M} \int \Psi_+^* \frac{\partial^2 \Psi_+}{\partial \xi^2} dr_1 dr_2 - E \right\} \chi_+(\xi) \\ = \frac{\hbar^2}{M} \int \Psi_+^* \frac{\partial \Psi_-}{\partial \xi} dr_1 dr_2 \frac{\partial \chi_-}{\partial \xi} + \frac{\hbar^2}{2M} \int \Psi_+^* \frac{\partial^2 \Psi_-}{\partial \xi^2} dr_1 dr_2 \chi_-(\xi). \quad (16)$$

The right-hand sides of these equations correspond to the relations of the non-adiabaticity operator and the products  $\chi_- \Psi_-$  and  $\chi_+ \Psi_+$ . The integral parts on the left-hand sides can be considered as corrections with respect to adiabatic potentials  $E_{\pm}(\xi)$ . Since the dependence of  $\Psi_{\pm}$  on  $\xi$  is supposed to be weak, we neglect the second derivative with respect to  $\xi$  from  $\Psi_{\pm}(r_1, r_2, \xi)$ .

In the domain of small  $\xi$  when  $E_-$  is close to  $E$  the motion takes place under the action of the potential  $E_-(\xi)$  (the first bond is excited). We set that  $\chi_+^0(\xi)$  is equal to zero in a zero approximation,  $\chi_-^0(\xi)$  is in the form of (11), and  $b_-^2 = 0$  since the De-Broil wave moves towards increase. In order to define  $\chi_-^1$  in the first approximation, we use the solution  $\chi_-^0$  on the right-hand side of eq. (16). By the method of coefficients variation, we have

$$\chi_+^1 = \frac{B_1(\xi)}{\sqrt{p_+(\xi)}} \exp \left[ \frac{i}{\hbar} \int_{\bar{\xi}-\Delta}^{\xi} p_+(\xi') d\xi' \right] \\ + \frac{B_2(\xi)}{\sqrt{p_+(\xi)}} \exp \left[ -\frac{i}{\hbar} \int_{\bar{\xi}-\Delta}^{\xi} p_+(\xi') d\xi' \right]. \quad (17)$$

We choose the lower limit  $\bar{\xi} - \Delta$  in (11) and (17) in such a manner that the potential  $E_-(\xi)$  practically coincide with  $E_{10}(\xi)$ , and  $E_+(\xi)$  with  $E_{01}(\xi)$ . Applying the solution of eq. (17) to the left-hand side of eq. (16) we obtain  $B_1(\xi)$  and  $B_2(\xi)$  in the form of the quadratures

$$B_1 = i\hbar \int_{\bar{\xi}-\Delta}^{\xi} \frac{a(\xi')}{\sqrt{p_+(\xi')}} \frac{d\chi_-^0}{d\xi'} \exp \left[ -\frac{i}{\hbar} \int_{\bar{\xi}-\Delta}^{\xi'} p_+(\xi'') d\xi'' \right] d\xi' \quad (18)$$

$$B_2 = -i\hbar \int_{\bar{\xi}-\Delta}^{\xi} \frac{a(\xi')}{\sqrt{p_+(\xi')}} \frac{d\chi_-^0}{d\xi'} \exp \left[ -\frac{i}{\hbar} \int_{\bar{\xi}-\Delta}^{\xi'} p_+(\xi'') d\xi'' \right] d\xi', \quad (19)$$

where

$$a(\xi) = \int \Psi_+^* \frac{\partial \Psi_-}{\partial \xi} dr_1 dr_2. \quad (20)$$

$C_1^\pm$  and  $C_2^\pm$  are coefficients in the expression for  $\Psi_\pm$  (5), defined by the variational method for the solution of the problem for a light subsystem for arbitrary  $\xi$ .

Further calculations of quantities  $B_1(\xi)$  and  $B_2(\xi)$  are shown in [8]. In the expression for  $P_\pm(\xi)$  the main term under the radical in the domain of intersection  $E_{10}(\xi)$  and  $E_{01}(\xi)$  is the full energy  $E$  and its order is that of the ATP splitting. (Here  $\bar{\xi} + \Delta$  is chosen in such a manner that when  $\xi \geq \bar{\xi} + \Delta$ ,  $E_-(\xi)$  practically coincide with  $E_{10}(\xi)$ , the intersection of  $E_{10}(\xi)$  and  $E_{01}(\xi)$  being supposed to take place when  $\bar{\xi} = \xi$ .) All the other terms in the formula (12) have the order of energy interaction  $V(r_{12})$ , which is small.

We are interested in the function  $\chi_+^1$  only in the domain  $\xi \geq \bar{\xi} + \Delta$ . Its square characterizes the probability of the fact that excitation remains with the first bond, since this function corresponds to the upper branch of the  $E_+(\xi)$ . Indeed, it is necessary to calculate the following expression:

$$D = |\chi_+^1(\bar{\xi} + \Delta)|^2 / |\chi_-^0(\bar{\xi} + \Delta)|^2. \quad (21)$$

On the contrary,  $1 - D$  is the fact that the system moves in accordance with the adiabatic potential  $E_-(\xi)$ .

### 2.3. RESULTS

Table 1 shows the values of the matrix element transfer  $V_{12}$ , calculated for different wave functions in [6, 7]. For each of them, the points are chosen in such a manner that the difference  $|E_{10}(\xi) - E_{01}(\xi)|$  is  $4|V_{12}|$  or  $8|V_{12}|$ . Moreover,  $E_{10}$  differs from  $E_-$  by  $|V_{12}|/4$  or  $|V_{12}|/8$ , respectively. The minimum divergence of  $E_+(\xi)$  and  $E_-(\xi)$  when  $\xi = \bar{\xi}$  is  $2|V_{12}|$ . Such an approximation is quite sufficient for the estimates to be reliable. In the last two columns the values of  $D$  when  $\xi = \bar{\xi} + \Delta$  and  $\xi = \bar{\xi} + 2\Delta$  are given. Their comparison shows that the increase in  $\bar{\xi} + \Delta$  does not influence much the probability of the system to "leave" the adiabatic potential  $E_-(\xi)$ . The probability is  $\leq 6\%$ . This explains the application of the potential  $E_-(\xi)$  for the classical consideration of globule motion under the action of the forces  $f = -\partial E_- / \partial \xi$ , since our solution  $\chi_-^0(\xi)$  corresponds to the classical approximation in quantum mechanics.

Table 1

The probability to define excitation of the first H-bond  $D$  when the parameters of the problem are different.

Matrix element of transfer $V_{12}$ [eV]	$\lambda$ [eV/Å]	$\bar{\xi} + \Delta = \bar{\xi} - \Delta$ [Å]	$D(\bar{\xi} + \Delta)$	$D(\bar{\xi} + 2\Delta)$
$1.35 \times 10^{-4}$	$1.35 \times 10^{-1}$	$3.985 \times 10^{-3}$	$6.04 \times 10^{-2}$	$9.627 \times 10^{-2}$
$7.77 \times 10^{-}$	$1.276 \times 10^{-1}$	$2.438 \times 10^{-2}$	$4.81 \times 10^{-4}$	$1.321 \times 10^{-3}$
0.02	$1.224 \times 10^{-1}$	$6.738 \times 10^{-1}$	$2.246 \times 10^{-1}$	$1.311 \times 10^{-2}$

### 3. Quantum and classical approach to the studies of actin globule and H-bond proton motion

In the methods described above for the determination of stationary states of the pure quantum system proton-globules, no time dependencies are included. Excitation transfer described by the state  $\Psi_-(r_1, r_2, \xi)$  takes place, so to say, "regardless of time". On the other hand, a classical experiment allows to define (by the value of globule acceleration) the force really acting on it at the particular moment. A somewhat different approach to the same problem corresponds to this mental experiment.

#### 3.1. NONSTATIONARY STATES OF H-BONDS

At the initial moment  $t = t_1$  the state of protons is described by  $\psi_{10}(r_1, r_2, \xi)$ . It depends parametrically on the globule displacement  $\xi$  (contained in the potentials  $V_1(r_1, \xi)$ ,  $V_2(r_2, \xi)$ ) and consequently on the time  $\xi = \xi(t)$ .

The following energy corresponds to it:

$$\epsilon_{10}(\xi(t)) = \epsilon_1^{(1)}(\xi(t)) + \epsilon_0^{(2)}(\xi(t)). \quad (22)$$

According to [3,4], we can obtain the time dependence of the initial state from the nonstationary Schrödinger equation:

$$\psi_{10}(r_1, r_2, \xi(t)) \exp\left\{-\frac{i}{\hbar} \int \epsilon_{10} dt\right\}. \quad (23)$$

Analogously, after energy transfer we have

$$\psi_{01}(r_1, r_2, \xi(t)) \exp\left\{-\frac{i}{\hbar} \int \epsilon_{01} dt\right\}, \quad (24)$$

$$\epsilon_{01}(\xi(t)) = \epsilon_0^{(1)}(\xi(t)) + \epsilon_1^{(2)}(\xi(t)). \quad (25)$$

Due to the presence of proton interactions  $V(r)$  the process of energy transfer can be described by the wave function

$$\begin{aligned} \Psi(r_1, r_2, \xi) = & C_1(t) \psi_{10}(r_1, r_2, \xi(t)) \exp\left\{-\frac{i}{\hbar} \int \epsilon_{10} dt\right\} \\ & + C_2(t) \psi_{01}(r_1, r_2, \xi(t)) \exp\left\{-\frac{i}{\hbar} \int \epsilon_{01} dt\right\}. \end{aligned} \quad (26)$$

Coefficients  $C_1$  and  $C_2$  are defined by the equations

$$i\hbar \dot{C}_1 = V_{12}(\xi) C_2(t) \exp\left\{\frac{i}{\hbar} \int (\epsilon_{10} - \epsilon_{01}) dt\right\},$$



$$i\hbar\dot{C}_2 = V_{21}(\xi)C_1(t) \exp\left\{-\frac{i}{\hbar} \int (\epsilon_{10} - \epsilon_{01}) dt\right\}. \quad (27)$$

Approximating  $\epsilon_{10}$  and  $\epsilon_{01}$  by parabolas having identical curvature  $\alpha'$ , we have

$$\begin{aligned} \epsilon_{10} &= \epsilon_{10}^0 + \frac{\alpha'}{2} (R_1 - \bar{R}_1)^2, \\ \epsilon_{01} &= \epsilon_{01}^0 + \frac{\alpha'}{2} (R_2 - \bar{R}_2)^2, \end{aligned} \quad (28)$$

where  $R_1, R_2$  – H-bond lengths,  $\bar{R}_1$  and  $\bar{R}_2$ , correspond to the minima of energies  $\epsilon_{10}^0$  and  $\epsilon_{01}^0$ . As it is shown in fig. 1 H-bond lengths can be expressed by the globule displacement  $\xi(t)$  or by the angle of myosin head swing  $\varphi = \xi/l$ , where  $l$  is the length of the head.

At the initial moment the head is in a vertical position, the lengths of bonds being  $R_1^0$  and  $R_2^0$ , then

$$\varphi = \frac{R_1 - R_1^0}{h_1} = \frac{R_2 - R_2^0}{h_2},$$

where  $h_1$  and  $h_2$  are the arms of tractive forces  $f_1$  and  $f_2$  of H-bonds. Therefore,

$$\begin{aligned} \epsilon_{10} &= \epsilon_{10}^0 + \frac{\alpha'}{2} \left( R_1^0 - \bar{R}_1 - h_1 \frac{\xi}{l} \right)^2, \\ \epsilon_{01} &= \epsilon_{01}^0 + \frac{\alpha'}{2} \left( R_2 - \bar{R}_2 - h_2 \frac{\xi}{l} \right)^2. \end{aligned} \quad (29)$$

Assuming that the difference  $h_2 - h_1$  is small in comparison with the values of  $h_1$  and  $h_2$ , we rewrite (29) in the form

$$\begin{aligned} \epsilon_{10} &= \epsilon_{10}^0 + \frac{\bar{\alpha}}{2} (l_1 - \xi)^2, \\ \epsilon_{01} &= \epsilon_{01}^0 + \frac{\bar{\alpha}}{2} (l_2 - \xi)^2, \end{aligned} \quad (30)$$

where

$$\bar{\alpha} = \alpha' \left( \frac{h}{l} \right)^2, \quad l_i = (R_i^0 - \bar{R}_i) \frac{l}{h}, \quad i = 1, 2.$$

In this approximation, the subintegral function in eq. (27) is nonlinear with respect to  $\xi$ . Since the average time of energy excitation is small, the change  $\xi(t)$  on this interval does not differ much from the linear case. We neglect this difference in a zero approximation.

It is convenient to choose the moment of the first H-bond excitation as the start-

ing time  $t$ , and to denote by  $\bar{t}$  the moment of intersection of potentials  $\epsilon_{10}$  and  $\epsilon_{01}$ . The corresponding globule displacement  $\xi(\bar{t})$  is denoted by  $\bar{\xi}$ . From (30), it is equal to

$$\bar{\xi} = \frac{1}{\bar{\alpha}(l_2 - l_1)} \left[ \frac{\bar{\alpha}}{2} (l_2^2 - l_1^2) + (\epsilon_{01}^0 - \epsilon_{10}^0) \right]. \quad (31)$$

Assuming that the time interval required, according to eq. (27), for the excitation transfer to take place, is sufficiently small and that the change in the velocity of globule motion is also small during this time, we can write

$$\xi(t) = \bar{\xi} + \dot{\xi}(\bar{t})(t - \bar{t}), \quad (32)$$

where  $t - \bar{t} \leq \Delta t$ . Then,

$$\begin{aligned} \frac{1}{\hbar} \int (\epsilon_{10} - \epsilon_{01}) dt &= \bar{\alpha}(l_2 - l_1) \int_{\bar{t}}^t \dot{\xi}(\bar{t})(t - t') dt \\ &= \frac{\bar{\alpha}}{\hbar} (l_2 - l_1) \dot{\xi}(\bar{t})(t - \bar{t})^2 / 2. \end{aligned}$$

To simplify our calculations we suppose the lower limits of integration in eqs. (27) and (33) to be equal to  $\bar{t}$ .

Applying (33) to the exponents of eq. (27), we obtain

$$i \frac{dC_1}{dT} = g C_2(T) e^{iT^2}, \quad (33)$$

$$i \frac{dC_2}{dT} = g^* C_1(T) e^{-iT^2}, \quad (34)$$

where, according to (33), dimensionless time  $T$  is introduced:

$$T = (t - \bar{t}) \sqrt{\frac{\bar{\alpha}(l_2 - l_1)}{2\hbar} \dot{\xi}(\bar{t})} = B(t - \bar{t}), \quad (35)$$

and dimensionless parameter  $g$  is introduced too:

$$g = \frac{\sqrt{2} V_{12}}{\sqrt{\hbar \bar{\alpha} (l_2 - l_1) \dot{\xi}(\bar{t})}} = \frac{V_{12}}{B\hbar}, \quad (36)$$

$$B = \sqrt{\frac{\bar{\alpha}(l_1 - l_2)}{2\hbar} \dot{\xi}(\bar{t})}.$$

Excluding  $C_1$  from eq. (34), we have

$$\frac{d^2 C_2}{dT^2} + 2iT \frac{dC_2}{dT} + |g|^2 C_2 = 0. \quad (37)$$

This equation is even with respect to the substitution of  $-T$  for  $T$ . Thus there must exist two solutions  $C_2(T)$ , even and odd with respect to  $T$ . We set

$$C_2(T) = (A_+ U_+(x) + A_- U_-(x)) e^{-ix}, \quad (38)$$

where  $x = T^2/2$ . For  $U_+(x)$ , the equation will be

$$\frac{d^2 U_+}{dx^2} + \frac{1}{2x} \frac{dU_+}{dx} + \left(1 + \frac{g^2 - i}{2x}\right) U_+ = 0. \quad (39)$$

The odd solution is written as follows:

$$U_- = \sqrt{x} v(x) = \frac{T}{\sqrt{2}} v(x), \quad (40)$$

then

$$\frac{d^2 v}{dx^2} + \frac{3}{2x} \frac{dv}{dx} + \left(1 + \frac{g^2 - i}{2x}\right) v = 0. \quad (41)$$

The series for  $U_+(x)$ , as well for  $V(x)$ , begins with 1. These solutions are

$$U_+(x) \sum_{n=0}^{\infty} U_n x^n, \quad U_-(x) = \sqrt{x} \sum_{n=0}^{\infty} v_n x^n, \quad (42)$$

where

$$U_0 = 1, \quad U_1 = i - g^2, \quad U_n = -\frac{1}{n(n-1/2)} \left[ U_{n-2} + \frac{g^2 - i}{2} U_{n-1} \right], \quad (43)$$

$$V_0 = 1, \quad V_1 = \frac{i - g^2}{3},$$

$$V_n = -\frac{1}{n(n+1/2)} \left[ v_{n-2} + \frac{g^2 - i}{2} v_{n-1} \right], \quad n \geq 2. \quad (44)$$

The constants  $A_+$ ,  $A_-$  are defined from initial conditions. Suppose when  $t = 0$  we have the first bond excited a fortiori, and  $C_1(t = 0) = 1$ ,  $C_2(t = 0) = 0$ , respectively.

### 3.2. CLASSICAL DESCRIPTION OF GLOBULE MOTION

The classical motion when  $t > 0$  is described by the system of equations [2,3] for  $N$  globules

$$M \frac{\partial^2 \xi_n}{\partial t^2} = \alpha (\xi_{n+1} + \xi_{n-1} - 2\xi_n), \quad 0 < n < N - 1, \quad (45)$$

where  $\xi_n$  is the displacement of the  $n$ th globule and  $\alpha$  is the coefficient of quasielastic

forces acting among globules. In this equation the displacements  $\xi_n$  are counted off from the globule equilibrium positions when the H-bond is not excited. For the last  $N$ th globule the displacement  $\xi_N$  must be used in the preceding formulas instead of  $\xi(t)$ . The  $N$ th globule displacement takes place due to the myosin head swing by hydrogen bonds (fig. 1). It is under the action of the horizontal component  $F$  of the H-bond force  $f$  and, according to [2,3], the equation of this globule motion is

$$M\ddot{\xi} = \alpha(\xi_{N-1} - \xi_N) + F. \quad (46)$$

If we add the equation which describes the rotation of the head around the hinge, the unknown force  $F$  can be excluded [2,3]. This results in the equation

$$\left(\frac{J}{l^2} + M\right)\ddot{\xi}_N = \alpha(\xi_{N-1} - \xi_N) + \frac{h}{l}f_1 - \frac{K}{l}\xi_N, \quad (47)$$

where  $f_1$ , according to (30), is given by

$$f_1 = -\frac{\partial \epsilon_{10}}{\partial R_1} = \bar{\alpha} \frac{l}{h} (l_1 - \xi_N), \quad (48)$$

$J$  is the moment of myosin head inertia and  $K$  is the coefficient of quasielastic force that returns the head back to its natural vertical position.

We now introduce a coordinate  $x = na$ , where  $a$  is a globule size into the approximation of continuous elastic filament. Then we fix the linear density  $\rho = M/a$ , the velocity of stretching wave  $c = \sqrt{\alpha a / \rho}$ , and the length of actin filament  $L = Na$ , and pass to the limit  $a \rightarrow 0$ ,  $M \rightarrow 0$ ,  $N \rightarrow \infty$ . Hence  $\xi_n = \xi(t)$  and eq. (45) becomes a partial equation, and owing to the approximation

$$\begin{aligned} \xi_n - \xi_{n-1} &\cong a \frac{\partial \xi}{\partial x}, & \xi_{n+1} + \xi_{n-1} - 2\xi_n &\cong a^2 \frac{\partial^2 \xi}{\partial x^2}, \\ \frac{\partial^2 \xi}{\partial t^2} &= c^2 \frac{\partial^2 \xi}{\partial x^2}, \end{aligned} \quad (49)$$

eq. (47) will be expressed in the form of a boundary condition,

$$\frac{1}{\alpha} \left( \frac{J}{al^2} + \rho \right) \frac{\partial^2 \xi}{\partial t^2} + \frac{\partial \xi}{\partial x} + \frac{1}{\rho c^2} \left( \bar{\alpha} + \frac{K}{l} \right) \xi = \frac{\bar{\alpha}}{\rho c^2} l_1 \quad (50)$$

when  $x = L$ . In this case,  $\rho$  and  $c$  are finite and therefore  $\alpha \rightarrow \infty$  as  $1/a$ . The term proportional to the acceleration can be neglected. Thus eq. (49) is reduced the boundary condition

$$\frac{\partial \xi}{\partial x} + \frac{1}{\rho c^2} \left( \bar{\alpha} + \frac{K}{l} \right) \xi = \frac{\bar{\alpha}}{\rho c^2} l_1, \quad \text{when } x = L. \quad (51)$$

The solution of eq. (49) satisfies the condition (51) (as well as conditions  $\xi = 0$ ,  $\dot{\xi} = 0$ , when  $x = 0$ ) and is as follows:

$$\xi(x, t) = Bx + \sum_{s=1}^N A_s \sin k_s x \cos(\omega_s t + \alpha_s), \tag{52}$$

where  $\omega_s = ck_s$ ; the wave number  $k_s$  and the constant  $B$  follow from (51), which yields the equation

$$\frac{tgk_s L}{k_s L} = -\frac{\rho c^2}{(\bar{\alpha} + K/l)L} = -\epsilon, \tag{53}$$

$$B = \frac{\bar{\alpha} l_1 \epsilon}{\rho c^2 (1 + \epsilon)}. \tag{54}$$

Moreover, the functions  $\sin k_s x$  and  $\sin k'_s x$  when  $k_s \neq k'_s$  are orthogonal in the interval  $0 \leq x \leq L$  and

$$\int_0^L \sin k_s x \sin k'_s x dx = \delta_{ss'} \frac{L}{2} \left[ 1 + \frac{\epsilon}{1 + (\epsilon k_s L)^2} \right].$$

Coefficients  $A_s$  are defined from the initial conditions. When  $t = 0$ , the first bond becomes excited, globules are motionless, then  $\xi(0, x) = \dot{\xi}(0, x) = 0$  for all  $x$ , i.e.

$$Bx + \sum_{s=1}^N A_s \sin k_s x \cos \alpha_s = 0, \tag{55}$$

$$\sum_{s=1}^N A_s \omega_s \sin k_s x \sin \alpha_s = 0. \tag{56}$$

Hence from (56) it follows that  $\alpha_s = 0$ . Multiplying both parts of eq. (55) by  $\sin k'_s x$  and integrating with respect to  $x$  within the limits  $0, L$ , we obtain

$$A_s = \frac{2BL(-1)^s (1 + \epsilon) \sqrt{1 + (\epsilon k_s L)^2}}{k_s L [1 + \epsilon + (\epsilon k_s L)^2]}. \tag{57}$$

Then the solution of the system of equations (49) and (51), when  $x = L$ , is

$$\xi(L, t) = BL \left[ 1 - 2\epsilon(1 + \epsilon) \sum_{s=1}^N \frac{\cos \omega_s t}{1 + \epsilon + (\epsilon k_s L)^2} \right]. \tag{58}$$

When  $t = \bar{t}$  we have

$$\xi(L, \bar{t}) = \bar{\xi} = BL + \sum_{s=1}^N A_s \sin k_s L \cos(\omega_s \bar{t}).$$

Hence the equation for  $t$  determination is

$$\frac{\bar{\xi} - BL}{2BL\epsilon(1 + \epsilon)} = - \sum_{s=1}^N \frac{\cos \omega_s \bar{t}}{1 + \epsilon + (\epsilon k_s L)^2} . \tag{59}$$

This equation can be solved numerically when some parameters  $\bar{\alpha}$ ,  $l_1$ ,  $l_2$ ,  $\epsilon_{10}^0$ ,  $\epsilon_{01}^0$  are reasonably chosen. From (58) it follows that

$$\begin{aligned} \dot{\xi}(L, \bar{t}) &= - \sum_{s=1}^N A_s \sin k_s L \omega_s \sin \omega_s \bar{t} \\ &= 2Bc\epsilon(1 + \epsilon) \sum_{s=1}^N \frac{k_s L \sin \omega_s \bar{t}}{1 + \epsilon + (\epsilon k_s L)^2} . \end{aligned} \tag{60}$$

This variable defines the parameter  $g$  (36) and consequently the solution for  $C_1(T)$  and  $C_2(T)$  in the form of (38)–(44) or of the linear combination of degenerate hypergeometric functions [7] (asymptotic solutions). Figure 3 shows the results of tabulation of coefficients. It also shows dependencies of  $C_1(T)$  and  $C_2(T)$  when  $g = 1$ . It implies the probability of the fact that excitation transfer occurs in a small interval of time  $t' \sim t' + dt'$ ,

$$\begin{aligned} W(t')t' &= \frac{d}{dt} |C_2(t')|^2 dt' = B[C_2(T)\dot{C}_2^*(T) \\ &+ C_2^*(T)\dot{C}_2(T)]dt' = W(T)dT , \end{aligned} \tag{61}$$

where  $T = B(t - \bar{t})$ .  $\dot{C}_1$  and  $\dot{C}_2$  can be expressed using eqs. (34). Figure 4 shows the dependence  $W(T)$ .

### 3.3. GLOBULE MOTION DURING THE EXCITATION TRANSFER

Up to the moment  $t'$  the motion of globules correspond to the solution of (58),

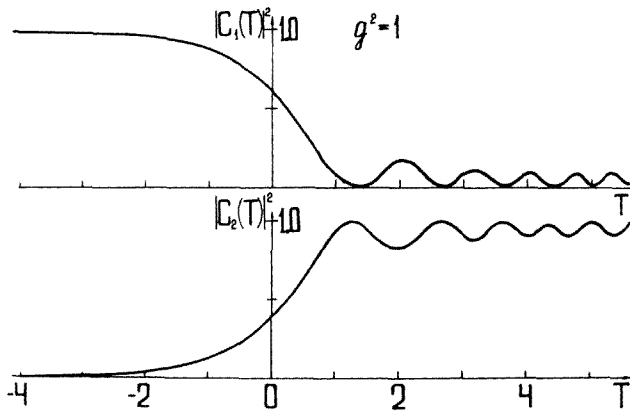


Fig. 3. Time dependences of  $|C_1(T)|^2$  and  $|C_2(T)|^2$  when  $g = 1$ .

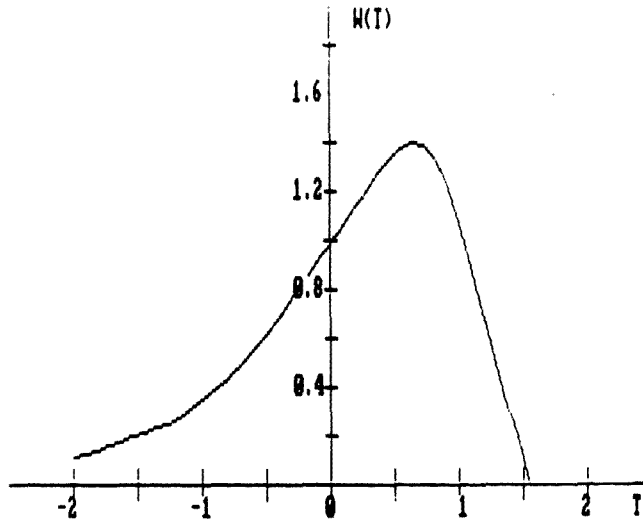


Fig. 4. Dependence of  $W(T)$ .

and after it, when  $t > t'$ , to the analogous solution for which the dependence (58) is the initial condition. It is of the form

$$\xi(x, t) = B'x + \sum_{s=1}^N A'_s \sin k_s x \cos(\omega_s t + \beta_s). \tag{62}$$

From the boundary condition (51) it follows that

$$B' = \frac{\bar{\alpha} l_2 \epsilon}{\rho c^2 (1 + \epsilon)}, \tag{63}$$

where  $\epsilon$  correspond to (53).

$A_s$  and  $\beta_s$  are determined from the initial conditions, when  $t = t'$ ,

$$Bx + \sum_{s=1}^N A_s \sin k_s x \cos \omega_s t' = B'x + \sum_{s=1}^N A'_s \sin k_s x \cos(\omega_s t' + \beta_s), \tag{64}$$

$$\sum_{s=1}^N A_s \omega_s \sin k_s x \sin \omega_s t' = \sum_{s=1}^N A'_s \omega_s \sin k_s x \sin(\omega_s t' + \beta_s). \tag{65}$$

Hence

$$A'_s = A_s \frac{\sin \omega_s t'}{\sin(\omega_s t' + \beta_s)}. \tag{66}$$

Then applying  $A'_s$  (66) to eq. (64), multiplying both of its parts by  $\sin k_s x$  and integrating on  $dx$  from 0 up to  $L$ , we find

$$\beta_s = -\omega_s t' + \operatorname{arctg} \left( \frac{\sin \omega_s t'}{b + \cos \omega_s t'} \right), \quad (67)$$

where  $b = B'/B - 1 = l_2/l_1 - 1$ .

Hence the solution, when  $t \geq t'$ , has the form

$$\xi(L, t) = BL \left[ \frac{l_2}{l_1} - 2\epsilon(1 + \epsilon) \sum_{s=1}^N \frac{\sin \omega_s t'}{[1 + \epsilon + (\epsilon k_s L)^2]} \times \frac{\cos(\omega_s(t - t') + \operatorname{arctg} a_s)}{\sin(\operatorname{arctg} a_s)} \right], \quad (68)$$

where

$$a_s = \frac{\sin \omega_s t'}{l_2/l_1 - 1 + \cos \omega_s t'}.$$

Figure 5 shows the dependence  $\xi(L, t)$ ; curve 1 corresponds to the globule motion under the force  $f_1 = -\partial\epsilon_{10}/\partial\xi_N$  of the first hydrogen bond, curves 2, 3 and 4 correspond to the motion, when excitation has transferred to the second bond under the force  $f_2 = -\partial\epsilon_{01}/\partial\xi_N$ . Depending on our choice with respect to  $t'$ , we obtain different trajectories: the moment  $t'$  is the beginning of the motion under  $f_2$ . Different experiments give different trajectories with probability  $W(t')$ , depending on the values of  $t'$  for excitation transfer (curves 2, 3, 4).

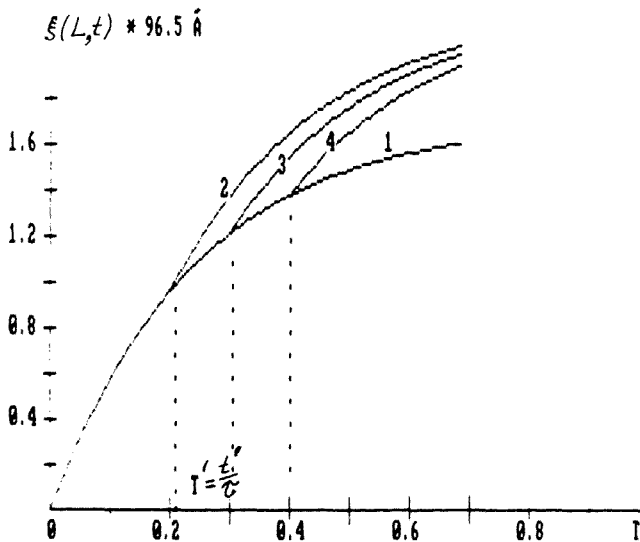


Fig. 5. Time dependences of the displacement of the polymer under the action of the force  $f_1$  when the first H-bond is excited (curve 1). Curves 2, 3 and 4 correspond to the motion when excitation has already been transferred to the second H-bond under the action of the force  $f_2$ , the values of  $t'$  being different ( $\tau = 2\pi/\omega_1$  is the period corresponding to the smallest of frequencies).



#### 4. Discussion

The comparison of two theories shows that they presuppose different characters of globule motion. In the first case, they move under the action of the average potential  $E_-(\xi)$ , so to say, and the force  $f = -\partial E_- / \partial \xi$ . In the second case, they move under the action of a jumpwise changing force from  $f_1$  to  $f_2$  and the moment of this jump  $t'$  is indefinite. Thus the questions arise: How do globules actually move? What is the truth? Such a paradox resembles the "Schrödinger cats" [9].

The solution is based on the assumption that the  $\psi$  function is the record of data on the state of the system. If the system with coordinates  $r_1, r_2, \xi$  is isolated, then the function  $\psi$  changes according to the Schrödinger equation.

This corresponds to the pure quantum version of the theory – the motion is along the trajectory of the potential  $E_-(\xi)$ , and finally we can observe the states  $\psi_2$  and  $\psi_1$  with probabilities 95% and 5%, respectively. The moment  $t'$  of quantum transition is excluded.

In the case of the mixed quantum and classical description, we observe acceleration of globules. Each time a cognitive operation takes place and each time it establishes that we have potentials  $\epsilon_1$  or  $\epsilon_2$ . This also gives the moment  $t'$  of excitation transfer, which is different in different experiments.

With probability 5%, calculated earlier, we observe trajectory 1 under the action of the force  $f_1$  up to the end, and with probability 95% transitions into the trajectories 2, 3, 4.

Both of our approaches correspond to different statements of an experiment. In the first case, we observe only the starting and finite moments of the motion (e.g. acceleration of globules). In the second case, the observation is supposed to be continuous and the experiment gives, each time, additional information on the state of the motion of the globule system. This allows to define the moment  $t'$  of excitation transfer by practice. The case is similar to that of observation of radioactive splitting (e.g. using a Geiger counter). The probability of splitting is given by the law  $e^{-t'/\tau}$ . At the same time each experiment allows to define the actual moment of splitting, which is different under different observations. Moreover, this actual moment  $t'$  of decay can vary from a fraction of a second up to milliards of years.

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