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Forecasting of the influence of physical fields on the metabolic nanocurrent in proteins

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Abstract

It is known that in order to complete the process of ATP synthesis in mitochondria, it is necessary to transfer in it electrons from places where electrons arise as a result of oxidative processes. Therefore, the study of the mechanisms of such a transfer is important, in particular, from the point of view of the regulatory effect on it for therapeutic purposes. The question of the possibility of considering the primary structure of proteins as an active nanowire of a semiconductor nature is analyzed. It has been shown that a non-uniform amino acid composition forms a residual electrostatic field, which is the cause of directional electron transfer. In particular, studies have been conducted on the effect of temperature on electron transfer processes along cellular organelles, which are polypeptide fragments of protein molecules. The calculations show that the electron, which is transferred by the residual field, creates micro currents in the range from 23 to 205 pA depending on the length of the protein-like nanowire (respectively, from 300 to 100 amino acid residues) and temperature in the physiologically relevant range: 33-41^{o}C. The possibility of controlling electron transfers along a protein-like nanowire using a magnetic field is investigated. The found threshold value of the magnetic field at which ATP synthesis can be blocked is consistent with observations. For magnetic field strength it will be: H=8·104A/m.

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1. Introduction

It has long enough been established that the single-electron energy states of protein-like polymers can have the electronic nature of semiconductors [1][2]. But, as noted in [3], the fact of amino acid heterogeneity of protein systems was not taken into account. However, it was found that the reason for the existence of micro currents through the primary structure of the protein in the absence of external fields is the long-range residual electrostatic field associated with the heterogeneous nature of the system due to radicals in amino acids [4][5].

Also the question of the adequacy of the considered semiconductor model of electron transfer along polypeptide fragments of proteins at an arbitrary temperature was investigated. The main test feature of this model adequacy was the natural physical fact of the absence of current in the absence of external electrostatic fields at any temperature.

With account of the effective electrostatic field due to amino acid heterogeneity, a current arises and provides active electron transport along the polypeptide chain. The dependence of the conduction states on this field is analyzed.

It is shown that with an increase in the magnitude of the field, the conduction states shift toward a decrease in energy. The current generated by one electron that is transported by this field is estimated. The calculations show that with increasing temperature, the current always increases in the physiologically relevant range of 33-41^{0}C within 23 to 205 pA, depending on the length of the polypeptide nanowire.

The magnetic field is one of the factors significantly affecting bio-systems[6][7][8], and a protein-like nanowire with a current from an injected electron is one of such bio-systems. The influence of the magnetic field on electron transfer through a protein nanowire is considered.

The possibilities of the controlling action of the magnetic field on the nano current were established to ensure a positive effect on the synthesis of ATP, which is essential in therapy. In particular, a threshold value of the magnetic field was found at which ATP synthesis can be blocked ($B>10^{-1}$ T or $H>8\cdot10^4$ A/m).

2. Averaged Electron-Atom Configuration of the Primary Structure of Proteins

Finding out the electronic configuration of a protein molecule and type of its crystallinity requires a certain averaged analysis. Here real protein will be analyzed without prior simplifications.

Nitrogen Model of the Atomic Subsystem

The protein molecule consists mainly of carbon atoms C (charge number z=6), nitrogen N (z=7) and oxygen O (z=8). In addition, a significant number of hydrogen atoms H (z=1) and a small number of sulfur atoms S (z=16) are present in the protein. A detailed analysis of the amino acid composition of proteins leads to the conclusion that their average atomic composition is close to nitrogen towards charge number. This is significantly exacerbated by the presence in the proteins, in addition to nitrogen, of CO molecular groups, which in the average sense, can be considered as NN groups and CH groups, which, in the same sense, can be considered simply as N. That is, we can say about the nitrogen average atomic model in which the charge number z=7.

Oxygen model of the Electronic Subsystem

If everything is relatively simple with an averaged analysis of an atomic (nuclear) subsystem, then an averaged analysis of an electronic subsystem is more complicated. For a single radical, one can set the ratio:

$$N_e/N_a = 8 + \Delta(N_e/N_a)$$

Here $\Delta(N_e/N_a) = (n_e - 8n_a - 3)/(n_a + 4)$, n_e is the number of electrons in a single amino acid residue, and n_a is the number of heavy (z>1) atoms in it. If in some approximation to assume that amino acids are evenly present in all proteins, then an analysis of deviations $\Delta(N_e/N_a)$ may be carried out from the point of view of subsequent averaging over the amino acid composition. It can be shown that all these deviations except two, methionine and cysteine, have negative values. Herewith most of them are significantly less than 1 in absolute value. Methionine and cysteine have not only abnormal signs of deviations, but also their abnormally large values, close to 1. Cysteine is of particular importance in proteins. It is a “fixer” of the tertiary structure. Therefore, one can assume that all other amino acids with a negative deviation compensate the excess positive charge of cysteine. Methionine, obviously, plays an auxiliary role when it is necessary to compensate negative deviations, but it is not necessary to fix the tertiary structure. If now to find the average value of all negative and all positive corrections, then we can establish that a fragment of a protein molecule consisting of various (non-repeating) amino acids would have a medium electronic configuration close to oxygen in the sense of the ratio $\frac{N_e}{N_a} \sim 8$.

Nitrogen- Oxygen Model of Protein Molecule

Thus, we obtained a nitrogen-oxygen model of the primary structure of the protein, a feature of which is the charge imbalance between the average atomic subsystem (average nuclear charge z=7) and the average electronic subsystem (the number of electrons per heavy atom is 8). However, it is clear that only the protons of hydrogen atoms can play the role of “compensators” of the excess negative charge. By analogy with electrons, we can obtain the average ratio:

$$N_H/N_a = 1 + \Delta(N_H/N_a)$$

where $\Delta(N_H/N_a) = (n_H - n_a - 2)/(n_a + 4)$, and n_H is the number of hydrogen atoms in one amino acid residue. All deviations $\Delta(N_H/N_a)$ have no sign anomalies. Averaging this correction over all amino acids while preserving the signs of the corrections gives the average deviation of the ratio $\frac{N_H}{N_a}$ from 1 of only –4.3%. Consequently, equality $N_H = N_a$ can be considered fulfilled with such accuracy, and the protein molecule, respectively, can be considered electrically neutral. After this analysis, we can talk about the applicability of the nitrogen-oxygen model to the description of protein molecules, the main features of which are an approximate, but fairly accurate (error of only a few percent), the fulfillment of three equalities: z=7, $N_H = N_a$ and $N_e = 8N_a$ (or $N_e = (z + 1)N_a$).

These relations make it possible to bring the potential energy of the electron injected into the primary structure of the

protein to an effective form (due to the approximate compensation of identical summands with different signs). In it, in addition to the real external field, there is an effective residual field due to the remaining uncompensated terms. This supplement is due to protein heterogeneity and competes with the external field. Therefore, an external field can have a regulatory effect on the metabolic transfer of an electron.

This allows to fully defining the conversion to the representation of fill numbers. Namely: 1. Based on the averaged nitrogen model of the atomic structure of a protein, to accept the wave functions of the one-electron nitrogen ion as a basis for the transformation into a representation of the occupation numbers. 2. Based on the averaged oxygen model of the electronic structure of a protein, to accept a semiconductor-type nanowire with four completely filled valence bands and at least one conduction band.

3. Quantum Calculations of the Basic Conductivity States in a Protein Nanowire

The medium-oxygen-electronic structure makes it possible to apply a model in which a protein nanowire has 5 energy bands, one of which is a conduction band, and the other is a valence band. The presence of dissimilar radicals does not significantly affect the electronic configuration of the protein molecule, since radicals do not participate in the formation of the primary structure. But their presence, at the same time, significantly complicates the unit cell, which affects the structure of the spectrum of electronic states, in particular, on the energy structure of the conduction band. The structure of this conductivity band is the main subject of study in this section. In this section, to establish the basic energy structure of this band, we consider the zero approximation in which the protein molecule is in the absence of all external influences, including those associated with the amino acid heterogeneity of the protein molecule.

Injection of an Electron into the Conduction Band as Excited State of a Protein Molecule

To calculate the energy structure of the conduction band, taking into account the nitrogen-oxygen model and the structure of amino acid residues, we used the energy operator of the electronic subsystem in representation the occupation numbers and the state vector (wave function) constructed in accordance with the process of electron injection into the conduction band. The calculations showed that the conduction band splits into several sub bands [9][10]. The structural features of the amino acid residue, which is considered as a unit cell, lead to five well-separated sub bands that have different types of energy dependence on the wave vector: $\varepsilon(k)_i$, $i = 0, 1, 2, 3, 4$. The sub bands structure of the conduction state is shown in Figures 1 and 2.

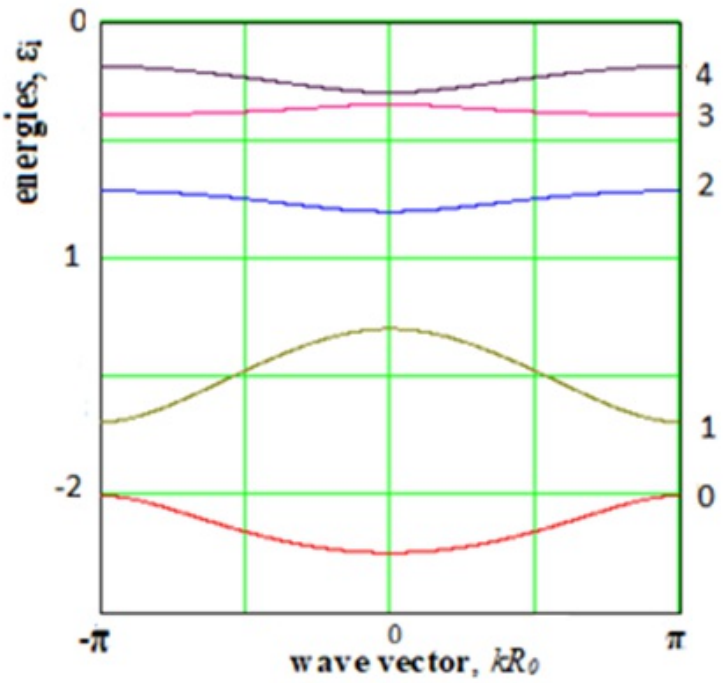

Figure 1. Dependences of the dimensionless energies ε_i on the dimensionless wave vector kR_0 (R_0 is the distance between amino acids).

It can be seen from figure 1 that three sub-zones (i = 0, 2, 4) have normal dispersion, with a minimum at the point k = 0, and two (i = 1, 3) have an abnormal (or reverse) dispersion, with a maximum at this point. The calculations of conduction states shown in Figures 1 and 2 are the result of a numerical solution of the eigenvalue problem for an electron injected into the conduction band [9][10].

On Figure 2 shows the dependences on the second factor in energies ε_i: on the dimensionless resonant exchange energy v . It can be seen that all sub bands are shifting by energy. However, this shift is not regular: sub bands 2, 3, 4 are unequivocally shifting towards energy increase, sub band number 0 is unambiguously shifted towards energy decrease, and sub band 1 is first shifted towards energy increase and then towards its decrease.

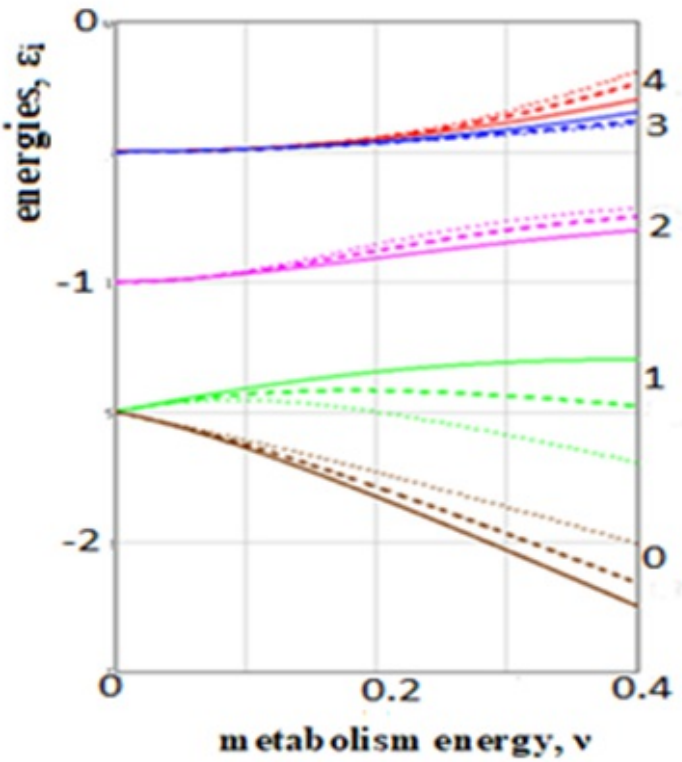

Figure 2. Dependences of the dimensionless energies ε_i on the dimensionless energy of resonance exchange v for the three key values of the wave vector (kR_0 ={0, π/2, π}). The energies are normalized by 1 eV.

Detailed graphical-numerical analysis of this two figures makes it possible to construct approximate analytical solutions for all five states of conductivity with high accuracy (the error does not exceed 1 percent):

$$\frac{\varepsilon(k)_i}{D} = -\begin{pmatrix}1.0\\3/2\\3/2\\1/2\\1/2\end{pmatrix} + \begin{pmatrix}v^2\\v\\-v\\v^2\\v^2\end{pmatrix} + \begin{pmatrix}3.15v^4\\-2.49v^2\\-1.42v^2\\-1.23v^4\\3.72v^4\end{pmatrix} - v^3\begin{pmatrix}0.68\\-3.10\\1.90\\-0.35\\0.87\end{pmatrix}\cos\left(kR_0\right)$$

Analytical representations of the solutions are necessary in order to calculate the current that is created by the electron injected into the conduction band and is proportional to the derivatives $\frac{\partial\varepsilon(k)_i}{\partial k}$.

Determination of Current Density

The current density has the following definition: $j = enV$, where e is the electron charge; n is the average bulk density of charges. For one injected electron, this density, up to a constant product for each protein molecule, en, is actually determined by the velocity V. Given this, the current is determined on the basis of the idea of the injected electron as a

free quasiparticle of the classical type in the conduction band of the primary structure of the protein molecule [3][11][12]. Therefore, now it's enough to consider the conventional velocity determination in solids for each of the conduction channels:

$$V(k)_i = \left(E_0/\hbar\right)\left[\frac{d\varepsilon(k)_i}{dk}\right] \qquad (1)$$

where E_0 is the width of the conduction band. Substituting the above explicit form of the analytical approximation for the energies $\varepsilon(k)_i$ into the definition for the velocity (1), one can find:

$$V(k)_i = \frac{E_0 R_0}{\hbar}\begin{pmatrix} 0.68 \\ -3.10 \\ 1.90 \\ -0.35 \\ 0.87 \end{pmatrix}\sin(kR_0)$$

where R_0 is the distance between neighboring amino acid residues. According to the general definition $j = enV$, for current densities we will have:

$$j_s = \frac{eE_0 R_0}{\hbar N_0 V_0}\begin{pmatrix} 0.68 \\ -3.10 \\ 1.90 \\ -0.35 \\ 0.87 \end{pmatrix}\sin(kR_0) \qquad (2)$$

Here, it is taken into account that for one injected electron $n = \frac{1}{N_0 V_0}$, where V_0 is the effective average volume of the amino acid residue, and N_0 is the number of amino acid residues.

According to any physical considerations – or classical, or quantum – it is obvious that the total current density j for the entire conduction band is determined by the sum $j = \sum_{s=0}^{s=4} j_s$ (in the classical language one speaks about parallel connection, and in quantum language – about the equal probability of the conduction channels). Substituting in this sum the values just obtained j_s, we get: $j = 0$. This, at first glance, unexpected result should in fact be regarded as a test with respect to the correctness of the considered model of conductivity of a protein nanowire. Indeed, in the absence of factors that violate the electrostatic equilibrium of the system and can be interpreted as external electrostatic fields, there should be no current.

4. Temperature Influence on the Basis Conductivity States

The calculation of the current density, in particular the test carried out in the previous section, was performed at zero

temperature. It is clear that such a consideration is far from the natural situation with a temperature close to 300K. In this section, we will consider practically the same question, but subject to the influence of a nonzero temperature on the electronic subsystem of fragments of polypeptide of protein molecules.

When considering the problem of electron injection into the conduction band of a polypeptide fragment of a protein molecule in the representation of occupation numbers, all energies naturally contains factor $\theta\left(\mu - E_f\right)$. In it, $\theta(x)$ is the Heaviside step function, which has the following properties: $\theta(x < 0) = 0$, $\theta(x = 0) = \frac{1}{2}$, $\theta(x > 0) = 1$ μ is the chemical potential, E_f is the energy that determines the position of energy bands (valence bands by the upper edge, and conduction bands by the lower one). These factors are actually Fermi-Dirac factors at zero temperature. To take into account the influence of a nonzero temperature on the physical characteristics of a protein nanowire discussed in the previous section, it is sufficient in the matrix elements that determine it to replace:

$$\theta\left(\mu - E_f\right) \Rightarrow \left[1 + exp\left\{\frac{E_f - \mu}{kT}\right\}\right]^{-1}.$$

Thanks to this replacement, it turned out that the energy E_0 is now temperature dependent, that is $E_0 = E_0(T)$ and for all the matrix elements that determine it, one way or another is connected with the factor $227.45^0/T$. The numerical value 227.45^0 comes from the structure $\left[\frac{\left(E_c - E_v\right)}{k}\right]/T$, where E_c and E_v the position of the lower edge of the conduction band E_c and the upper edge of the valence band E_v. In it, the difference $E_c - E_v$ for the mid-oxygen model of the electronic subsystem is 0.0196 eV, and the Boltzmann constant is $k = 8.6173 \cdot 10^{-5}$ eV/K. It is quite obvious that the expressions for current densities j_s now differ from (2) only in that the energy E_0 will now depend on temperature T. Given that the energy E_0 does not depend directly on the factors $227.45^0/T$, but on their certain algebraic combination, it is precisely for the dependence $E_0(T)$ that one can find $E_0(T) = E_c\left(1 - 114^0/T\right)$, where E_c is the width of the conduction band at T=300K. But, as can be seen from formula (2), this dependence is the identical for all conduction states and does not affect total current $j = \sum_{s=0}^{s=4} j_s$. That is, in the absence of external factors that can be interpreted as external electrostatic fields, the current in the system is absent at any temperature, which is a physically correct result.

5. Mechanisms of Electron Transfer Thru Protein Nanowires in Real Conditions

In the previous sections, the main attention was focused on the question of the adequacy of the nitrogen-oxygen model of a protein nanowire in the absence of any external physical fields. The main test feature of this adequacy was the requirement of no current under these conditions at any temperature. It was also shown that in a protein nanowire there always exists an effective external field due to amino acid heterogeneity of proteins. In test calculations, this field was artificially turned off. But in real conditions, it exists and causes active electron transfer even in the absence of a real external electrostatic field. In this section, the question of the appearance of current under the conditions of the presence

of this residual effective electrostatic field at any temperature is investigated. The question of the controlling effect of an external magnetic field on electron transfer through a protein nanowire is also considered.

Active Transport of an Electron Along a Protein Nanowire

Sequentially taking into account the effective electrostatic field when calculating the conduction states for an electron injected into the protein conduction band leads to the appearance of a dependence of the energy of all five sub-states of conduction on the dimensionless energy of the effective residual field w (it is obtained by normalizing, as before, its dimensional value to the width energy of conduction zones at zero temperature). If now we again use definitions (1), (2) then for the current density in each of the conduction states, provided that always $|w| > 0$ one can get:

$$j_s = \frac{eE_0R_0}{\hbar N_0 V_0}\left\{\begin{pmatrix}0.68\\-3.10\\1.90\\-0.35\\0.87\end{pmatrix} + \begin{pmatrix}0.006\\0.004\\-0.003\\0.004\\-0.009\end{pmatrix}(1+|w|)\sin(kR)\right\}$$

But current density is not a directly measurable characteristic. Therefore, we use the fact that the effective average volume of an amino acid residue is determined by the relation: $V_0 = R_0S$, where, as already noted, R_0 is the effective distance between amino acid residues, and S is the effective cross-sectional area of the primary structure of the polypeptide fragment of the protein-like molecule. Substituting this value V_0 into the expression for j_s, multiplying the obtained by the area S and taking into account the definition of currents $I_s = j_sS$, it may be obtained for such currents:

$$I_s = \frac{eE_0}{\hbar N_0}\left\{\begin{pmatrix}0.68\\-3.10\\1.90\\-0.35\\0.87\end{pmatrix} + \begin{pmatrix}0.006\\0.004\\-0.003\\0.004\\-0.009\end{pmatrix}(1+|w|)\sin(kR)\right\} \qquad (3)$$

To determine the total current I, you need, as before, to find the sum:

$$I = \sum_{s=0}^{s=4} I_s . \qquad (4)$$

Substituting the values (3) into the sum (4) and taking into account that the sum of the coefficients of the first term in the curly brackets of expression (3) is equal to zero, we will finally have $I = 0.002\frac{eE_0}{\hbar N_0}(1+|w|)\sin(kR)$ for the total current I. If we take into account that the wave vector k is small enough to approximately assume $\sin(kR) \approx 2\pi/N_0$, then the current I takes the form $I = 0.004\frac{\pi eE_0}{\hbar N_0^2}(1+|w|)$. Taking into account inequality $|w| \ll 1$, we can also obtain for estimates $I = \frac{\pi eE_0}{250\hbar N_0^2}$.

Now, using this definition, one can not only evaluate the current, but also analyze the effect of temperature on it. In Section IV, the dependence $E_0(T) = E_c\left(1 - 114^0/T\right)$ was given. That is, finally, the current at $w \Rightarrow 0$ is determined by the equality $I = \left(\frac{I_0}{N_0^2}\right)\left(1 - 114^0/T\right)$, where $I_0 \equiv \frac{\pi e E_c}{(250\hbar)}$. From this definition it follows that the current depends on two parameters - the number of amino acid residues N_0 and temperature T. Using the values of $E_c = 1.6 \cdot 10^{-19} J$, $e = 1.6 \cdot 10^{-19} C$, $\hbar = 10^{-34} J \cdot s$ in the amplitude factor I_0, one can obtain: $I_0 = 3.217 \mu A$.

The dependence of the current on temperature and the number of amino acid residues is presented in Table 1[12].

Table 1. **Dependence of current on temperature and number of amino acid residues**

N \ T	33°C (306°K)	35°C (308°K)	37°C (310°K)	39°C (312°K)	41°C (314°K)
100	201.85 pA	202.63 pA	203.40 pA	204.16 pA	204.90 pA
150	89.71 pA	90.06 pA	90.40 pA	90.74 pA	91.07 pA
200	50.46 pA	50.66 pA	50.85 pA	51.04 pA	51.23 pA
250	32.30 pA	32.42 pA	32.54 pA	32.66 pA	32.78 pA
300	22.43 pA	22.51 pA	22.60 pA	22.68 pA	22.77 pA

As can be seen from Table 1 in the physiologically relevant range $33 - 41^0 C$ (306-314K), the current always increases with increasing temperature. Moreover, for polypeptides (N_0 ~ 100), it grows from 201.85 pA to 204.90 pA, and for long protein-like chains (N_0 ~ 300) it grows from 22.43 pA to 22.77 pA.

During illness with an increasing of temperature in the range of 36 – 41°C, an increase in current has a positive effect on the body. With increasing current, the possibility of ATP synthesis in the mitochondria of cells increases. This, in turn, increases the synthesis of ATP and enhances the energy potential of the body in the fight against a painful condition. In conditions of lowering body temperature in the range 36 – 33^0C, decrease in current negative affects at the process of ATP synthesis. Slowing down the synthesis of ATP leads to a decrease in the protective energy resources of the body.

If we were not limited to very weak fields for estimates, then the expression for the current would have the following form:

$$I = \left(\frac{I_0}{N_0^2}\right)\left(1 - 114^0/T\right)(1 + |w|).$$

Controlling Influence of a Magnetic Field on Metabolic Current

Similarly to the residual electrostatic field w, the consistent consideration of the influence of the magnetic field on the state of conductivity leads to the appearance of a dependence of the energy of all five sub-states of conductivity on the

magnetic field as well. This dependence is determined by the dimensionless factor, which we denote as w_2. It is determined by normalizing, as before, the dimensional value of the magnetic field energy $\Lambda(\mathbf{L}\cdot\mathbf{H})$, on the energy of the width of the conduction band (E_0 if the influence of temperature is not taken into account, or E_c if it is taken into account). Here $\Lambda \equiv \frac{e}{(2m_e c)}$ is the electronic gyromagnetic ratio; $\mathbf{L} \equiv -i\hbar\left\langle \varphi_c(\mathbf{r})\left|[\mathbf{r}\times\nabla]\right|\varphi_c\left(\mathbf{r}+\mathbf{R_0}\right)\right\rangle$ is the vector matrix element of the operator of moment of impulse, where $\varphi_c(\mathbf{r})$ is the wave function of the conduction band; $\mathbf{H}$ is the magnetic field vector. If now we again use definitions (1), (2), (3), then for the current at zero temperature (T=0K) in each of the conduction states, provided that always $|w| > 0$ and $w_2 \neq 0$, one may obtained:

$$I_s = \frac{eE_0}{2\hbar N_0}\left\{\frac{\left(1+w_2\right)^3}{4}\begin{pmatrix}0.68\\-3.10\\1.90\\-0.35\\0.87\end{pmatrix}+\begin{pmatrix}0.0150\\0.0100\\-0.0075\\0.0100\\-0.0225\end{pmatrix}\left(1+w_2\right)(1+|w|)\right\}\sin(kR)$$

For a non-zero temperature in the physiologically relevant area: T~(310±10) K, parameter E_0 should be replaced by factor $E_c\left(1-114^0/T\right)$. Using condition (4) further, with taking into account $\sin(kR) \approx \frac{2\pi}{N_0}$, it is possible to obtain $I = \left(\frac{\pi e E_0}{\left(200\hbar N_0^2\right)}\right)\left(1+w_2\right)(1+|w|)$ for the total current, or for a nonzero temperature in the physiologically relevant region (T~(310±10) K):

$$I = \left(\frac{\pi e E_c}{\left(200\hbar N_0^2\right)}\right)\left(1-114^0/T\right)(1+|w|)\left(1+w_2\right).$$

Further, we focus only on the effect of the magnetic field. Then the current takes the form $I = I_0\left(1+\Lambda(\mathbf{L}\cdot\mathbf{H})/E_0\right)$, where $I_0 \equiv \left(\frac{\pi e E_0}{\left(200\hbar N_0^2\right)}\right)$. For convenience, we will analyze the dimensionless representation of this current: $i = 1 + h\cos\alpha$, where $i \equiv I/I_0$, $h = H/H_0$, $H_0 \equiv E_0/(\Lambda|\mathbf{L}|)$, α is the angle between the vectors $\mathbf{L}$ and $\mathbf{H}$ on some protein fragment under consideration (since the protein molecule has a complex spatial configuration, its fragments can have different orientations in relation to the magnetic field, that is, another angle α). The region $0 \le \alpha \le \pi/2$ is not necessary to analyze, since in this region the current is always greater than in the case $h = 0$. Therefore, Figure 3 shows an analysis of the dependence $i = 1 + h\cos\alpha$, only for the region $\pi/2 \le \alpha \le \pi$, where current smaller than in the case $h = 0$.

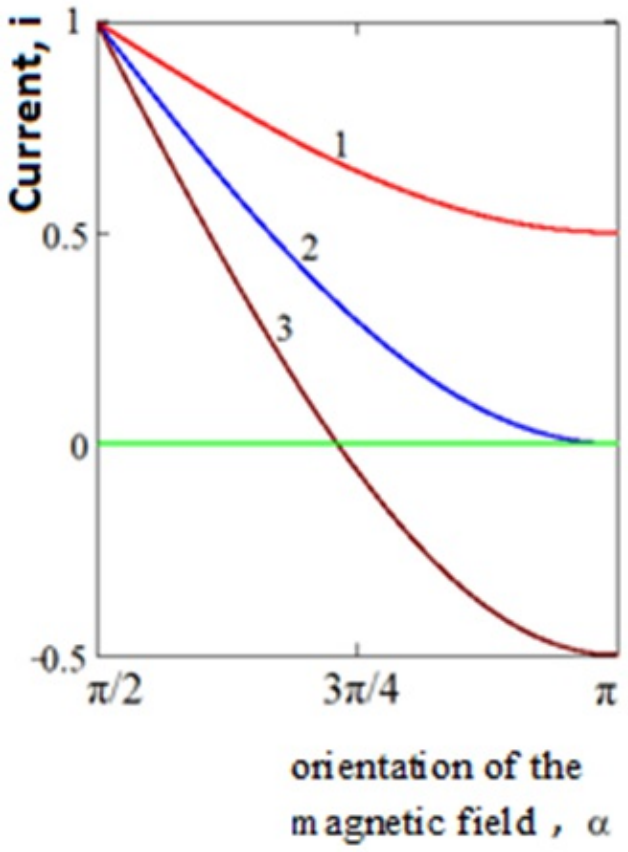

Figure 3. The dependence of current on the orientation of the magnetic field in region $\pi/2 \le \alpha \le \pi$. Curve 1 corresponds to the value $h = 0.5$ ($H = \frac{H_0}{2}$). Curve 2 corresponds to the value $h = 0.5$ ($H = \frac{H_0}{2}$). (here, the current in the sections of the nanowire, for which $\alpha = \pi$, can rotate to zero). Curve 3 corresponds to the value of $h = 1.5 (H = 1.5H_0)$ (here, the current in the sections of the nanowire, for which $\alpha \ge 3\pi/4$, becomes negative).

Figure 3 shows that 2 cases can be distinguished. The case of weak fields $H < H_0$ (or $h < 1$). In this case, always $i > 0$. For the case of strong fields $H > H_0$ (or $h > 1$), the current can reverse (become negative) in the sections of the nanowire, where $arccos(-1/h) \le \alpha \le \pi$. That is, in strong fields, metabolic electron transfer is blocked in such areas. This will block the directed electron transfer and, accordingly, will have a negative effect on the synthesis of ATP molecules, as an energy means of the functioning of the organism. So, a magnetic field will definitely give a positive effect only for weak fields. At such fields, the current can vary in magnitude in different sections of the nanowire, but cannot be reverse. This means that only fields lower than the value $H_0 \equiv E_0/(\Lambda|\mathbf{L}|) \equiv 2m_e cE_0/(e|\mathbf{L}|)$ can provide a positive effect on the metabolic electron transfer along protein-like nanowires. If to estimate the value of this field, we take: the effective electron mass $m_e^* \sim \left(10^{-1} \div 10^{-2}\right) m_e$, where $m_e = 9 \cdot 10^{-31} kg$, the minimum width of the conduction band $E_0 = 1.6 \cdot 10^{-19} J$ ($E_0 \sim 1 eV$

), and moment of impulse will put $|\mathbf{L}| \sim \hbar(\hbar = 10^{-34} J \cdot s)$, then one can obtain: $H_0 \sim 8 \cdot 10^4\ A/m(B_0 \sim 10^{-1} T)$. In practice, field intensities in the range from $1.5 \cdot 10^{-3} T$ to $0.5 \cdot 10^{-1} T$ are really used [6][8].

6. Conclusions

The article considers a relevant problem for understanding metabolic mechanisms: electron transfer through the primary structure of a protein molecule into mitochondria to complete the process of ATP synthesis. It is important to study the mechanisms of such a transfer. In the future, this will be the basis for solving the question of the possibility of regulating the metabolic transfer of electrons, which is important in clinical practice. Protein molecules have a heterogeneous structure due to the presence of radicals. Therefore, the question of averaged consideration of a protein molecule was studing.in detail. It was shown that the protein has a medium atomic structure of the nitrogen type and a medium oxygen electronic configuration. It confirms that the primary structure of the protein has the nature of a semiconductor nanowire. The structure of energy band for the conduction states of such a nanowire is calculated. It is shown that it consists of five conduction sub bands, two of which are anomalistic (reverse). An analytical approximation of the corresponding dispersion dependences of the obtained sub bands is found. This made it possible to calculate the metabolic electron velocities and currents, taking into account the influence of temperature. The article shows that, depending on the length of the protein-like nanowire (from 300 to 100 amino acid residues), in the physiological temperature range of 33-41^{o}C (306-314^{o}K), an electron that is transferred by the residual field creates micro currents in the range, respectively, from 23 to 205 pA. The possibility of the influence of a magnetic field on metabolic transfer processes is theoretically considered. The threshold value of the magnetic field is found at which ATP synthesis can be blocked. This is consistent with observations. For induction or magnetic field strength, this threshold is respectively: $B = 0.1\ T$ or $H \sim 80\ 000\ A/m$ Exceeding of these values may cause blocking conditions for the synthesis of ATP. The model developed and presented in the article can serve as an advisory basis for determining the magnitude of the magnetic field in order to achieve the optimal therapeutic effect.

References

1. ^*M. G. Evans, J. Gergrly, "A discussion of the possibility of bands of energy levels in proteins electronic interaction in non bonded systems", Biochimica et Biophysica Acta, vol. 3, p. 188, 1949. https://doi.org/10.1016/0006-3002(49)90091-8*
2. ^*B. Rosenberg, "Electrical Conductivity of Proteins. II. Semiconduction in Crystalline Bovine Hemoglobin", The Journal of Chemical Physics, vol. 36, p. 816, 1962. http://dx.doi.org/10.1063/1.1732615*
3. a, b*A. Ishizaki, T. R. Calhoun, G. S. Schlau-Cohen, G. R. Fleming, "Quantum Coherence and its Interplay with Protein Environments in Photosynthetic Electronic Energy Transfer", Physical Chemistry Chemical Physics, vol. 12, pp. 7317–7318, 2010. https://pubs.rsc.org/en/content/articlelanding/2010/cp/c003389h/unauth#!divAbstract*
4. ^*A. D. Suprun, L. V. Shmeleva, "Alpha-helical regions of the protein molecule as organic nanotubes", Nanoscale Research Letters, vol. 9, p. 200, 2014. https://doi.org/10.1186/1556-276X-9-200*

5. ^*A. D. Suprun, L. V. Shmeleva, "Primary structure of proteins as a nanowire for metabolic electronic transport", Nanoscale Research Letters, vol. 10, p. 121, 2015. https://doi.org/10.1186/s11671-015-0763-0*
6. a, b*Ocal I., Yilmaz M. B., Kocaturk-Sel S., Tufan T., Erkoc M. A., Comertpay G., Oksuz H., Barc, E. D., "ATP sensitive K+ channel subunits (Kir6. 1, Kir6. 2) are the candidate mediators regulating ameliorating effects of pulsed magnetic field on aortic contractility in diabetic rats", Bioelectromagnetics, vol. 39, pp. 299-311, 2018. https://onlinelibrary.wiley.com/doi/abs/10.1002/bem.22111*
7. ^*Novitskaya G. V., Feofilaktova T. V., Molokanov D. R., Dobrovolskii M. V., Novitskii Y. I., "Influence of a Permanent Magnetic Field on the Composition and Content of Sugars in Leaves and Storage Roots of Radish Plants of Major Types of Magnetic Orientation", Russian Journal of Plant Physiology, vol. 65, pp. 57-62, 2018. https://link.springer.com/article/10.1134/S1021443718010089*
8. a, b*Kim E. C., Leesungbok R., Lee S. W., Lee H. W., Park S. H., Mah S. J., Ahn S. J., "Effects of moderate intensity static magnetic fields on human bone marrow-derived mesenchymal stem cells", Bioelectromagnetics, vol. 36, pp. 267-276, 2015. https://onlinelibrary.wiley.com/doi/abs/10.1002/bem.21903*
9. a, b*Khmelinskii I., Makarov V. I., "Energy propagation along polypeptide α-helix: Experimental data and ab initio zone structure", Biosystems, vol. 185, p. 104016, 2019. https://doi.org/10.1016/j.biosystems.2019.104016*
10. a, b*A. D. Suprun, L. V. Shmeleva. Temperature Effect on the Basis States for Charge Transfer Through a Polypeptide Fragments of Proteins and on the Nanocurrent in It. Chapter 13 in "Nanophysics, Nanomaterials, Surface Studies, and Applications". Part of the Springer Proceedings in Physics book series 2017, Vol. 195, P. 175–186. https://link.springer.com/chapter/10.1007/978%2D3%2D319%2D56422%2D7_13*
11. ^*Natanzon Yu. E., Brizhik L. S., Eremko A. A., "Self-trapping and dynamics of a quasi-particle in a one-dimensional molecular chain under interaction with optical phonons", Ukrainian Journal of Physics, vol. 51, No 4, pp. 413–422, 2006. https://inis.iaea.org/search/search.aspx?orig_q=RN:38054298*
12. a, b*L. V. Shmeleva and A. D. Suprun. Mechanism of Active Electron Transfer in a Protein-Like Nanowire Under Real Conditions. Chapter 5 in "Nanophysics, Nanomaterials, Surface Studies, and Applications". Springer International Publishing AG, Part of Springer Nature 2018 (book series), Springer Proceedings in Physics 210, P. 59–71. https://doi.org/10.1007/978%2D3%2D319%2D91083%2D3_5*