Electromagnetic Radiation Influence on Nonlinear Charge and Energy Transport in Biosystems

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Abstract. The influence of electromagnetic radiation (EMR) on charge and energy transport processes in biological systems is studied in the light of the soliton model. It is shown that in the spectrum of biological effects of EMR there are two frequency resonances corresponding to qualitatively different frequency dependent effects of EMR on solitons. One of them is connected with the quasiresonance dynamic response of solitons to the EMR. At EMR frequencies close to the dynamic resonance frequency the solitons absorb energy from the field and generate intensive vibrational modes in the macromolecule. The second EMR resonance is connected with soliton decay due to the quantum mechanical transition of the system from the bound soliton state into the excited unbound states.

Key words: Charge and energy transport, davydov's soliton, nonthermal microwave resonant effect

1. Introduction

During the last decades the experimental and theoretical investigations of the biological effects of external high frequency electromagnetic radiations (EMR) have attracted a great deal of attention. On the one hand, with the increase of the usage and types of electrical appliances in everyday life and modern technologies, the problem of their influence on health and, respectively, the problem of scientifically justified safety standards are getting more important. On the other hand, applications of microwave therapy methods are ever increasing in modern medicine for the diagnosis and treatment of a wide range of diseases. In the meantime, these methods are based only on the empirically discovered ultra high frequency EMR bioeffects. Moreover, such effects can be both beneficial and detrimental and their degree depends not only on the exposition dose, but also on the EMR wavelength.

Although there exist few hypothesis on the possible resonant influence of EMR on biosystems [1, 2, 3, 4], the mechanisms of the nonthermal biological effects of EMR are still unclear. To a great deal this is connected with the complex nature of biological processes and their variety in living systems. The whole hierarchy of these processes is based on electromagnetic interactions and, thus, is sensitive to

the external EMR. This includes the direct influence of EMR on ion transport in membranes, charge transport in macromolecules, free radicals, molecular dynamics, etc. Through these primary processes all basic biochemical and biophysical processes and the metabolism of whole cells and organisms are sensitive to EMRs.

Here we study the influence of an external electromagnetic field on the energy and charge transport processes in biosystems in the light of the soliton model [5].

2. Soliton Mechanism of Charge and Energy Transport

The main biological processes occur with the consumption of energy released in the processes of the hydrolysis of adenosine triphosphate (ATP) into adenosine diphosphate (ADP). This energy is about two quanta of the amid-I vibration of the C-O bond of the peptide group. According to the hypothesis of Davydov [5, 6], the energy of the ATP hydrolysis stored in the amide-I vibration, can be transferred along the polypeptide chain to the remote place of consumption in the form of a soliton. The latter one is the autolocalized state of the excitation which propagates with the constant velocity together with the local deformation of the relatively soft polypeptide chain formed by weak hydrogen bonds along the α -helical protein molecules.

Another class of metabolically important reactions is connected with electron transport phenomena during the oxidative phosphorylation processes when the ADP is converted into the ATP molecule. Such a charge transfer takes place along the α -helical regions of the enzyme-macromolecular complexes participating in the reaction. It was suggested in [7] that protein molecules can also facilitate electron transport: the periodic potential of the peptide dipole moments in the α -helix creates a conducting band for an extra electron. Due to the interaction with chain deformation the autolocalization of electrons takes place and electrons can be transferred along the macromolecule in the form of electrosolitons or bisolitons [5, 8].

Although the both types of solitons are the eigenstates of the Fröhlich Hamiltonian, they correspond to the ground electron state only in the zero order adiabatic approximation which assumes that the total wavefunction of the system can be represented in the form of the product of electron and phonon wavefunctions. As it follows from the variational investigations [9], this is valid within some limited interval of the parameters of the system, namely, at the intermediate values of the electron-phonon coupling constant:

$$\chi_{cr,1} < \chi < \chi_{cr,2}. \quad (2.1)$$

Here the critical values of coupling parameter depend on the particular model of the macromolecule (number and structure of the electron/exciton bands, phonon modes, etc.) and corresponding physical parameters.

3. Solitons in the Presence of EMF

In the presence of external radiation both the amide-type soliton and the electro-soliton can change their properties or even become unstable and dissociate [4, 10, 11, 12]. Here we study the influence of an alternating electromagnetic field (EMF) on energy and charge transport processes. The α -helical molecule can be represented as a system of three parallel polypeptide chains and here, for simplicity, we consider a quasiparticle (amide-I exciton or electron) in an isolated chain at zero temperature. In the presence of the external field the total Hamiltonian of the system can be written in the form

$$H(t) = H_0 + V(t) \quad (3.1)$$

where H_0 is the Fröhlich-type Hamiltonian of polypeptide chain:

$$H_0 = \sum_k E(k) B_k^+ B_k + \frac{1}{\sqrt{N}} \sum_{k,q} \chi(q) B_k^+ B_{k-q} (b_q + b_{-q}^+) + \sum_q \hbar \Omega_q b_q^+ b_q, \quad (3.2)$$

and $V(t)$ is the operator of quasiparticle interaction with the EMF:

$$V(t) = \frac{1}{2} \sum_k e^{-i\omega t} \vec{\mathcal{E}} \vec{d}_k B_k^+ B_k + h.c. \quad (3.3)$$

Here $B_k^+ (B_k)$ is the creation (annihilation) operator for a quasiparticle with wavenumber k and dispersion $E(k)$, $b_q^+ (b_q)$ is the Bose creation (annihilation) operator for a phonon with wavenumber q and frequency Ω_q , $\chi(q)$ is the electron-phonon coupling function, $\vec{\mathcal{E}}$ is the amplitude of EMF and $\vec{d}_k$ is the effective dipole momentum of the quasiparticle: $\vec{d}_k = \vec{d} \sin(ka)$ with a being the lattice constant. In the case of electron the operators B_k satisfy the Fermi anticommutator rules and the vector $\vec{d}$ is determined by the overlap of electron Wannier functions on the neighboring sites, while for an exciton the operators B_k satisfy the Bose commutator rules and $\vec{d}$ is determined by electro-optical anharmonicity of amide-I vibration.

The wavefunction of the system, $|\Psi(t)\rangle$, satisfies the Schrödinger equation

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = [H_0 + V(t)] |\Psi(t)\rangle, \quad (3.4)$$

and can be expanded over the complete set of the stationary states $|\Psi_\lambda(t)\rangle$ of the Hamiltonian H_0 (3.2) which includes the soliton $\lambda = s$ and delocalized band $\lambda = j$ states:

$$|\Psi(t)\rangle = \sum_\lambda a_\lambda(t) |\Psi_\lambda(t)\rangle. \quad (3.5)$$

The operator (3.3) describes the intraband transitions of a quasiparticle and is written in the assumption that the EMF frequency is less than the frequencies of quasiparticle interband transitions and wavevector of the field is small as compared with the reciprocal lattice vector. We assume that the perturbation $V(t)$ is

adiabatically included at the initial time moment and that the initial state of the system $|\Psi_s\rangle$ corresponds to the ground soliton state of a quasiparticle in the chain $a_\lambda(t=0) = \delta_{\lambda,s}$. The account of diagonal and nondiagonal matrix elements of the perturbation results in the two qualitatively different effects of EMR on solitons and is done below.

4. Dynamic Resonant Effect

The diagonal elements can be taken into account by the renormalization of the wave-functions and, hence, they do not enter into the probability of the quantum mechanical transition of the quasiparticle from an autolocalized into delocalized states. However, the diagonal terms lead not only to shifting of the energy levels, as it is usual for the linear systems, but also to nontrivial effects on the dynamical properties of the soliton. With account of this renormalization we obtain the following system of equations in the site representation for the quasiparticle wavefunction Ψ_n and the displacements u_n of peptide groups from their equilibrium positions [11, 12]:

$$i\hbar \frac{\partial \Psi_n}{\partial t} = -J(\Psi_{n-1} + \Psi_{n+1}) + \chi(u_{n+1} - u_{n-1})\Psi_n - ig(t)(\Psi_{n+1} - \Psi_{n-1}), \quad (4.1)$$

$$M \frac{d^2 u_n}{dt^2} = \chi(|\Psi_{n+1}|^2 - |\Psi_{n-1}|^2) + w(u_{n+1} + u_{n-1} - 2u_n) \quad (4.2)$$

where J is the transfer energy between the nearest sites determined by the dispersion law of the quasiparticle, M is the mass of a peptide group, w is the elasticity coefficient of the hydrogen bonds along the chain, and function $g(t)$ accounts for the influence of the periodic EMF with frequency ω :

$$g(t) = AJ \cos(\omega t), \quad A = \frac{1}{J} \vec{\epsilon} \vec{d}. \quad (4.3)$$

The system of nonlinear differential-difference equations (4.1)–(4.2) can be investigated by numerical calculations. For the analytical analysis it is convenient to use the continuum approximation, which transforms the system (4.1)–(4.2) to nonlinear partial differential equations. In the absence of the perturbation this system describes the autolocalized (soliton) state of a quasiparticle. The corresponding system of equations was solved in [11] analytically for the case of electromagnetic field of small amplitudes within the Mitropolsky-Bogolyubov-Krylov perturbation theory [13] and numerically in the general case in [12]. Here we briefly cite the corresponding results.

In the absence of the perturbation, when $g = 0$, Equations (4.1)–(4.2) admit the soliton-like solution which in the continuum form read as:

$$\rho_s(x, t) = -\frac{2\chi a}{w(1-s^2)} |\psi_s(x, t)|^2, \quad (4.4)$$

$$\psi_s(x, t) = \frac{\kappa \sqrt{1-s^2}}{\sqrt{G}} \frac{\exp\{i[k(x - \zeta(t)) + \vartheta(t)]\}}{\cosh \kappa[x - \zeta(t)]}, \quad (4.5)$$

$$\zeta(t) = \zeta_0 + \frac{\hbar k}{m^*} t, \quad \vartheta(t) = \frac{\hbar^2}{2m^*} (k^2 + \kappa^2) t, \quad (4.6)$$

$$G = \frac{4ma\chi^2}{\hbar^2 w}, \quad s = \frac{\hbar k}{m^* V_a}, \quad \kappa = \frac{G}{2(1-s^2)}. \quad (4.7)$$

This solution describes a stationary autolocalized state of a quasiparticle which moves along the chain with constant velocity $V = \hbar k/m^*$ and has the effective mass

$$M_s = m^* + \frac{8m^* \chi^4 a^2}{3\hbar^2 w V_a^2} \quad (4.8)$$

where V_a is the sound velocity in the chain and m^* is the effective mass of a quasiparticle in the conducting band.

In the presence of the weak periodic perturbation (4.3) in the zero adiabatic perturbation order the soliton wavefunction (4.5) is unchanged except for the slow time dependence of its center of mass coordinate, $\zeta(t)$, and phase $\vartheta(t)$. The corresponding master equation with account of the retardation effects in the deformation accompanying soliton, are obtained from the condition that the first order correction to the soliton wavefunction (4.5) does not contain the secular terms [14, 15]. For the steady-state motion of the driven soliton this gives

$$\ddot{\zeta}(t) = \frac{F_0}{m_d(\omega)} \cos[\omega t - \phi(\omega)]. \quad (4.9)$$

Here $m_d(\omega)$ is the dynamical mass of the soliton in the field and ϕ is the phase shift due the soliton acceleration under the external force:

$$m_d(\omega) = \sqrt{[m^* + \mu_1(\omega)]^2 + \mu_2^2(\omega)}, \quad \phi = \arcsin \frac{\mu_2(\omega)}{m_d(\omega)} \quad (4.10)$$

where the notations are used:

$$\mu_1(\omega) = \frac{\pi}{2\kappa V_a} \int_0^\infty \frac{x^4 dx}{\left[x^2 - \left(\frac{\omega}{\omega_0} \right)^2 \right] \sinh^2 x},$$

$$\mu_2(\omega) = \frac{4\chi^2 a \kappa}{\pi w V_a^2} \left(\frac{\omega}{\omega_0} \right)^2 \sinh^{-2} \frac{\omega}{\omega_0}. \quad (4.11)$$

It follows from (4.10)–(4.11) that the phase shift ϕ tends to zero at low and high frequencies while the frequency dependence of the soliton dynamic mass is qualitatively different for low and high frequencies as compared with the fundamental constant ω_0 :

$$\omega_0 \equiv \frac{2\kappa V_a}{\pi}. \quad (4.12)$$

Namely, at low frequencies $\omega \ll \omega_0$ the soliton propagates as a classical Newtonian particle in a slowly oscillating external field with a dynamical mass equal to the effective mass of the soliton in the absence of the field (4.8), $m_d \approx M_s$. At high frequencies $\omega \gg \omega_0$, the deformation cannot follow the comparatively fast electron motion, and the dynamical mass approaches the mass of a free band quasiparticle, $m_d \approx m^*$.

During the oscillatory motion the soliton emits sound waves in the backward and forward directions. These sound waves are asymptotically described by the first-order corrections [11, 12]

$$\rho_1(x, t) = \begin{cases} A(\omega) \cos[\omega(t - (x - z)/V_a) - \phi], & x - z \rightarrow \infty, \\ -A(\omega) \cos[\omega(t + (x - z)q/V_a) - \phi], & x - z \rightarrow -\infty \end{cases} \quad (4.13)$$

where

$$A(\omega) = \frac{\chi m a^2 \omega^2}{\hbar m_d w V_a^2 \omega_0} \sinh^{-1} \left(\frac{\omega}{\omega_0} \right) \vec{\epsilon} \vec{d}. \quad (4.14)$$

The process of phonon emission is possible due to the absorption of energy by the soliton from the external field and is also frequency dependent. The energy absorption per field oscillation period, $T = 2\pi/\omega$,

$$E_T = \frac{\overline{dE}}{dt} \propto \{\omega, \omega \ll \omega_0, \omega^3 \exp(-\gamma\omega) \omega \gg \omega_0\} \quad (4.15)$$

is proportional to the electromagnetic field frequency at low frequencies, and decreases exponentially at high frequencies: with the maximum at the dynamic resonant frequency

$$\omega_{dyn} = 1.3\omega_0. \quad (4.16)$$

This analytical analysis of the frequency dependence of the dynamical mass of the soliton and emission of the sound waves was confirmed by numerical calculations of Equation (4.1)–(4.2) (see [12]). Moreover, the numerical calculations have proved the applicability of the perturbative analysis and the stability of solitons in rather strong EMFs aside from the resonant frequency. In the very strong EMFs when the adiabatic approximation breaks down, the amplitude of the soliton decreases significantly with the increase of the amplitude of oscillating tails and with the appearance of some stochasticity features in the system behavior.

5. EMR Induced Decay of Solitons

The nondiagonal matrix elements of the perturbation (3.3) determine the probability of a quantum transition from the initial soliton state $|\Psi_s\rangle$ into the delocalized band states $|\Psi_j\rangle$ with the probability amplitude $a_j(t)$

Figure 1. The dependence of the normalized probability of the soliton decay, $P = P_s(\omega)/|\vec{\mathcal{E}}\vec{D}_{s,k=0}|^2$, on the frequency of the external EMF ω measured in units $\omega_{k=0}$, $w = \omega/\omega_{k=0}$, and electron-phonon coupling, G at $\gamma = 1$.

$$a_j(t) = \frac{1}{i\hbar} \int_0^t \langle \Psi_j(t') | V(t') | \Psi_s(t') \rangle dt'. \quad (5.1)$$

The total probability per unit time of the EMR induced transition of the system which, according to (3.5) and (5.1), is given by the following expression

$$P_s = \frac{2}{\hbar^2} \Re \int_{-\infty}^t dt' \langle \Psi_s(t) | V^+(t) e^{-i\frac{H}{\hbar}(t-t')} V(t') | \Psi_s(t') \rangle, \quad (5.2)$$

was calculated in [10]:

$$P_s(\omega) = \frac{\sqrt{2\pi}}{\hbar B} \sum_k |\vec{\mathcal{E}}\vec{D}_{sk}|^2 \exp \left\{ -\frac{(\omega - \omega_k)^2}{2B^2} \right\}. \quad (5.3)$$

Here the notations are used:

$$\hbar\omega_k = \frac{\chi^4}{Jw^2} + \frac{\hbar^2 k^2}{2m^*}, \quad B^2 = \frac{\chi^2 V_a G^2}{\pi^4 \hbar w a}, \quad (5.4)$$

$$\vec{D}_{sk} = i \frac{\vec{d}}{2\sqrt{N}} \frac{\pi(ka + iG/2)}{\sqrt{G} \cosh \frac{\pi ak}{G}}. \quad (5.5)$$

The dependence of the probability on the EMF frequency and soliton half-width G is shown in Figure 1 at fixed value of the nonadiabaticity parameter [9] $\gamma = \hbar\omega_{ac}/2J$ where ω_{ac} is the Debye frequency of acoustic phonons. This dependence shows that the soliton dissociation probability has a frequency resonant

Figure 2. The dependence of the normalized probability of soliton decay $P = P_s(\omega)/|\vec{\epsilon} \vec{D}_{s,k=0}|^2$ on the EMF frequency $w = \omega/\omega_{k=0}$ at $G = 1.25$ and $\gamma = 1$.

behavior with the resonance frequency ω_{diss} depending on the value of the electron-phonon coupling. With the increase of G the resonance frequency tends to the value corresponding to the most probable soliton transitions into the delocalized band state with zero wavenumber $k = 0$: $\omega_{diss} \approx \omega_{k=0}$, where

$$\omega_{k=0} = \frac{\chi^4}{\hbar J w^2}. \quad (5.6)$$

At small values of G , ω_{diss} is displaced to the higher frequency value due to the input of the soliton transitions into the band states with $k \neq 0$. These transitions determine also the asymmetrical shape of the probability line, like it is shown in Figure 2.

For the numerical values of the parameters characteristic for amide-I vibration in the α -helix [16], the resonant photodissociation frequency equals 34–65 GHz [14, 10]. This qualitatively corresponds to the experimentally observed nonthermal millimeter electromagnetic wave bioeffects [2].

6. Discussion

Thus, it is shown that the electromagnetic radiation has a specific influence on the amide-I solitons and electrosolitons which can be relevant to the experimentally observed nonthermal effects of microwave EMFs on biosystems. According to the soliton theory, both types of solitons can exist only in the metabolically active states of systems, hence, the EMR induced effects on solitons can only be generated and sustained in biologically active states. And indeed, it has been shown that EMFs have a weak stimulatory effect on resting cells but a profound effect on partially activated cells [17].

In the spectra of the electromagnetic influence on solitons there are two characteristic frequencies, ω_{dyn} and ω_{diss} , determined by Equations (4.16) and (5.6), respectively. The corresponding bioeffects at these frequencies are qualitatively different. The dynamic resonant frequency of the field, ω_{dyn} , is connected with the resonant absorption of energy by a soliton from the field and the generation of acoustic waves. The corresponding frequency ω_{dyn} is determined by the characteristic time scale of the retardation effects which, in turn, is determined as the ratio of the soliton width to the sound velocity. On the one hand, the generated sound waves dissipate in the polypeptide chain which can result in the local heating of the system. On the other hand, such sound waves propagating along the α -helix as in a channel can carry some additional information and/or change the conformational states of the macromolecules, excite some other local modes, vibrations of the side groups, etc. This can change qualitatively some functional processes connected with conformational states of macromolecules or their fragments, since electromagnetic radiation of the corresponding frequencies causes the oscillations of solitons including oscillations of the chain distortion. For instance, it is well known that the opening and closing of calcium channels depend on channel conformations, and the experiments show strong effects of EMFs on calcium balance [18, 19].

Another type of EMF resonant bioeffects takes place at $\omega \approx \omega_{diss}$. This frequency corresponds to the splitting energy of the soliton level from the band bottom. As a result, the soliton can absorb the energy from the electromagnetic field and decay. This changes qualitatively the character of charge and energy transport which become far less effective, if possible at all.

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References

1. Fröhlich, H. (ed.): *Biological Coherence and Response to External Stimuli*, Springer-Verlag, N.Y., 1988.
2. Devyatkov, N.D., Golant, M.B. and Betskii, O.V.: *Millimeter Waves and their Role in Vital Activity*, Moscow, Radio i Svyaz', 1991.
3. Grundler, W., Kaiser, F., Keilmann, F. and Walleszhek, J.: Mechanisms of electromagnetic interaction with cellular systems, *Naturwissenschaften*. **79** (1992), 551–559.
4. Eremko, A.A.: Dissociation of Davydov's solitons in the field of electromagnetic wave, *Dokl. Ac. Nauk UkrSSR* **3** (1984), 52–55.
5. Davydov, A.S.: *Solitons in Molecular Systems*, Dordrecht, Reidel, 1985.

6. Davydov, A.S.: Solitons and energy transfer along protein molecules, *J. Theor. Biol.* **66** (1977), 379–387.
7. Ukrainskii, I.I. and Mironov, S.L.: The origination of the conducting band in polypeptide chains, *Teor. Eksper. Chem.* **15** (1979), 144–151.
8. Brizhik, L.S. and Davydov, A.S.: Electrosoliton pairing in soft molecular chains, *Fiz. Nizk. Temp.* **10** (1984), 748–753.
9. Brizhik, L.S., Eremko, A.A., La Magna, A. and Pucci, R.: The ground state of an extra electron interacting with acoustic phonons in a molecular chain, *Phys. Lett. A* **205** (1995), 90–96.
10. Eremko, A.A.: Dissociation of Davydov solitons by electromagnetic wave, in: P.L. Christiansen and A.C. Scott (eds), *Davydov's Soliton Revisited*, Plenum, New York, 1990, pp. 429–438.
11. Brizhik, L.S. and Eremko, A.A.: Possible mechanism of electromagnetic radiation influence on charge transport in biosystems, *Physics of the Alive* **5** (1997), 9–17.
12. Brizhik, L., Cruzeiro-Hansson, L. and Eremko, A.: Influence of electromagnetic radiation on molecular solitons. Submitted to *J. Biol. Physics*.
13. Bogolyubov, N.N., Mitropolsky, Yu.A.: *Asymptotical Methods in the Theory of Nonlinear Vibrations* (in Russian), Moscow, Nauka, 1974.
14. Keener, J.P. and McLaughlin, D.W.: Solitons under perturbation, *Phys. Rev. A* **16** (1977), 777–790.
15. Davydov, A.S. and Eremko, A.A.: Soliton deceleration in molecular chains, *Teor. Mat. Fiz.* **43** (1980), 367–377.
16. Scott, A.C.: Davydov's soliton, *Phys. Rep.* **217** (1992), 1–67.
17. Walleczek, J.: Electromagnetic field effects on cells of the immune system: the role of calcium signalling, *FASEB J.* **6** (1992), 3177–3185.
18. Karabakhtsian, R., Broude, N., Shalts, N., Kochlaty, S., Goodman, R. and Henderson, A.S.: Calcium is necessary in the cell response to EM fields, *FEBS Letters* **349** (1994), 1–6.
19. Hanson, M.: What's the fuss about calcium? Interaction between calcium free radicals and heavy metals and relevance to health, in: J. Katajainen and B. Knave (eds), *Electromagnetic Hypersensitivity*, Soborg, Power-Print Shop (1995), pp. 27–31.