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Influence of electromagnetic radiation on molecular solitons

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Abstract. The soliton model of charge and energy transport in biological macromolecules is used to suggest one of the possible mechanisms for electromagnetic radiation influence on biological systems. The influence of the electromagnetic field (EMF) on molecular solitons is studied both analytically and numerically. Numerical simulations prove the stability of solitons for fields of large amplitude, and allow the study of emission of phonons. It is shown that in the spectra of biological effects of radiation there are two characteristic frequencies of EMFs, one of which is connected with the most intensive energy absorption and emission of sound waves by the soliton, and the other of which is connected with the soliton photodissociation into a delocalized state.

1. Introduction

The problem of the influence of electromagnetic radiation on biological systems is not only one of the most important but also one of the most complex problems for several branches of science, including medicine, biology, physics, radiobiology, environmental sciences, etc., both from an experimental and from a theoretical point of view [1, 2]. There are several reasons for this. The ever increasing use of electricity in everyday life, in technical appliances and technologies, the conventional electrical methods of medical diagnosis and treatment and the search for new, alternative methods to traditional medicine, constitute only a few examples. Experimental knowledge in this area has grown rapidly over the last two decades and in some respects it has stimulated theoretical models [3] and practical applications [4, 5]. However, despite that much research has already been done in this area, there are still many open questions about the mechanisms by which electromagnetic fields (EMFs) affect biological systems, either from the point of view of biological organisms or their populations as a whole, or at the cellular or molecular level. There is evidence that the biological effects of EMFs can be both beneficial [5] and detrimental (see, e.g., [6, 7] and references cited therein). Furthermore, the degree of such effects depends not only on the exposure dose and on the wavelength of the electromagnetic radiation, which can be approximately controlled by

physical means, but also, to a great extent, on the particular individual, involving psycho-physiological factors, electromagnetic sensitivity and hypersensitivity [7].

The range of effects of EMFs spans the whole hierarchy of biological processes, from the direct influence on ion transport and molecular dynamics (in response to electrical stimulation or as a means of signal or energy transfer along a molecular chain), to the basic biochemical and biophysical processes, and finally, to the metabolism of whole cells and organisms. The complexity of this problem is the result of the corresponding complexity of biological systems and of the fundamental role played by electromagnetic interactions in the structure-function relations in biological organisms [8].

In the present paper we consider only one aspect of the problem, namely, the influence of an external electromagnetic field on the energy and charge transport processes within the frame of the Davydov/Scott model [9]. This mechanism for the biological effects of radiation was first suggested in [10] and studied in more detail in [11, 12]. In Section 2 a brief presentation of the model is given, in Sections 3 and 4, respectively, the results of analytical and numerical investigations are presented, and in Section 5 we discuss the results obtained.

2. Davydov's soliton in the presence of external EMF

From the physical point of view all biological organisms are open dissipative systems and their metabolism is connected with the exchange of energy and matter with the environment. Many biological processes are connected with the storage and spatial transfer of energy and charge in cells. The primary mechanism for the production of the energy needed in biological processes is the hydrolysis of adenosine triphosphate (ATP) into adenosine diphosphate (ADP) which takes place with the release of free energy. The standard value of this energy quantum is only approximately 16 times larger than the energy of thermal vibrations at normal physiological conditions. The exceptional effectiveness and reliability of energy and charge transport over long distances cannot be explained in the frame of conventional linear approaches and in the 70's a nonlinear soliton mechanism was suggested [14, 9]. According to it, the free energy released in the hydrolysis of ATP is stored in the so-called amide I vibration, essentially a stretching of the C–O bond of the peptide group. This vibrational excited state becomes autolocalized due to its interaction with the local deformation of the relatively soft polypeptide chain formed by weak hydrogen bonds along α-helical protein molecules. A similar mechanism can be relevant for electron transport, for instance, during oxidative phosphorylation processes when the ADP is converted into the ATP. Such charge transfer takes place along the α-helical regions of the enzyme-macromolecular complexes participating in the reaction, and in [15, 16] the bisoliton model of charge transport in biological systems was proposed which is based on the following ideas. The peptide group possesses constant dipole momentum, $d = 3.5$ Debye [17], which can keep an extra electron in the bound state with the binding energy

0.9 eV [18]. In such a state the electron wavefunction is extended over the two nearest peptide groups and the periodic potential of the peptide dipole momenta in the polypeptide chain of the α-helix splits the electron on-site energy level into a conducting band of width $4J$, J being the overlap electron integral [19]. As was mentioned above, the polypeptide chain is formed by soft hydrogen bonds and the electron-phonon coupling in it is rather strong, hence, the interaction of band electrons with the local distortions of the chain is important. This interaction leads to the self-trapping or autolocalization of electrons in the electrosoliton states [20, 9] and to the binding of two isolated electrosolitons into a bisoliton [15, 16].

In the presence of radiation, both the amide-type soliton and the electrosoliton can change their properties or even become unstable and dissociate. Here we study the influence of an external alternating electromagnetic field on the energy and charge transport processes within the simplest model of an isolated polypeptide chain at zero temperature. We assume that at the initial time the chain is in the ground soliton state formed by a quasiparticle (an amide I vibration or an electron) interacting with longitudinal displacements of peptide groups from their equilibrium positions. Such a system is described by the Fröhlich-type Hamiltonian:

$$H = \sum_k E(k) B_k^+ B_k + \frac{1}{\sqrt{N}} \sum_{k,q} \chi(q) B_k^+ B_{k-q} (b_q + b_{-q}^+) + \sum_q \hbar \Omega_q b_q^+ b_q. \tag{2.1}$$

Here $B_k^+ (B_k)$ are the creation (annihilation) operators for a quasiparticle with wavenumber k. For the case of an amide I vibration these operators satisfy commutator rules, while for an electron they satisfy anticommutator rules. Since in the present paper we consider only one quasiparticle in the chain (electron or exciton), the master equations are the same in the both cases, as will be shown below. The operators $b_q^+ (b_q)$ are the creation (annihilation) Bose-operators for a phonon with wavenumber q and

$$E(k) = E_0 + 4J \sin^2 \frac{ka}{2} \tag{2.2}$$

is the dispersion law of a quasiparticle in the band with the bottom energy E_0 and width $4J$, J being the resonance exchange energy for the quasiparticle between the nearest neighbors, Ω_q is the frequency of acoustic phonons, and $\chi(q)$ is the electron-phonon coupling function:

$$\Omega_q = 2\sqrt{\frac{w}{M}} \left| \sin \frac{qa}{2} \right|, \quad \chi(q) = 2i\chi \sqrt{\frac{\hbar}{2M\Omega_q}} \sin(qa), \tag{2.3}$$

where M is a unit cell mass, i.e. the average mass of a peptide group, w is the elasticity coefficient of the chain, and a is the lattice constant. According to the Born-Karman periodic boundary conditions, which we will use, the wave numbers in (2.1) are $k = 2\pi n/Na$, $n = 0, \pm 1, \ldots \pm (N-2)/2, N/2$, with N being the number of sites in the chain.

The operator, $V(t)$, of quasiparticle interaction with an external alternating EMF, $\vec{\mathcal{E}}(t)$,

$$\vec{\mathcal{E}}(t) = \frac{1}{2}[\vec{\mathcal{E}} e^{-i\omega t + i\vec{Q}\vec{R}} + c.c.] \tag{2.4}$$

can be written in the general form

$$V(t) = \frac{1}{2}\sum_k e^{-i\omega t}\vec{\mathcal{E}}\vec{d}_k B_k^+ B_k + h.c. \tag{2.5}$$

where $\vec{d}_k$ is the effective dipole moment and determined below. It is taken into account in (2.5) that the EMF wavevector $|\vec{Q}|$ is small as compared with the reciprocal lattice vector π/a.

In particular, in the coordinate representation, the operator of electron interaction with the EMF is proportional to the product of the vector-potential of EMF and electron momentum operator

$$V(t) = -\frac{ie\hbar}{mc}\vec{A}(t)\vec{\nabla}, \quad \vec{A}(t) = -\frac{ic}{\omega}\vec{E}e^{-i\omega t + i\vec{Q}\vec{r}} + c.c. \tag{2.6}$$

In the quantized field representation

$$\Psi^+(\vec{r}) = \sum_k \phi_k^*(\vec{r}) B_k^+, \quad \Psi(\vec{r}) = \sum_k \phi_k(\vec{r}) B_k \tag{2.7}$$

$$\phi_k(\vec{r}) = \frac{1}{\sqrt{N}}\sum_n \chi(x - na, y, z)e^{ikna}$$

with $\chi(x - na, y, z)$ being the Wannier wavefunction of an electron localized on the n-th peptide group, the operator (2.6) takes the form (2.5) in which

$$\vec{d}_k = i\vec{d}\sin(ka). \tag{2.8}$$

Here vector $\vec{d}$ is parallel to the chain axis x and is determined by the electron mass, m and charge, e by the expression

$$\vec{d} = \vec{j}\frac{e\hbar\lambda}{m\omega a} \tag{2.9}$$

where $\vec{j}$ is a unit vector along the chain, and λ is determined by the overlap of electron Wannier functions on neighbouring peptide groups.

In the case of amide I vibrations the interaction operator can be written in the dipole approximation

$$V(t) = -\vec{\mathcal{E}}(t)\vec{D} \tag{2.10}$$

where the dipole moment of the system $\vec{D}$ can be expanded in the Taylor series with respect to the normal vibrational coordinates $Q_k = (B_k + B_{-k}^+)/\sqrt{2}$ of the amide I vibrations. The zero term in this expansion is the static dipole moment of peptide groups. In the interaction operator this term can be neglected since it can be taken into account by a phase transformation of the wave function, and, hence, it does not affect optical transitions. The first term, linear with respect to the operators $B_k^+(B_k)$, describes the absorption (emission) of the light quantum with creation (annihilation) of one vibrational quantum, and is responsible for the finite radiation lifetime of the vibrational state (delocalized or self-trapped) [21]. The next term in the expansion of the dipole moment, $\vec{D}$, quadratic with respect to the operators B_k, B_k^+, is responsible for the electrooptical anharmonicity of the system and leads to the appearance of the overtones, i.e., the lines at double frequencies, in the absorption spectra. And indeed, such overtones are present in the IR spectra of peptide molecules [22]. Here we consider the EMF of frequencies ω less than the frequency of amide I vibrations, and therefore, can keep only the term proportional to $B_k^+ B_k$ and neglect the linear terms and terms which are proportional to $B_k B_{-k}$ and $B_k^+ B_{-k}^+$ in this quadratic part of the dipole momentum. This leads to the expression (2.5) in which $\vec{d}(k)$ is the expansion coefficient:

$$\vec{d}(k) = \frac{\partial^2 \vec{D}}{\partial Q_k \partial Q_{-k}^*}$$

which has the dimension of a dipole moment. As was mentioned above, this effective dipole moment is a characteristic of the optical anharmonicity of the vibration and is determined by the integral intensity of amide I overtones in the emission and absorption spectra of biological macromolecules.

Thus, we have shown that for both types of quasiparticles, electron and amide I vibrations, the operator of the quasiparticle interaction with the external EMF which is responsible for the intraband transitions, has the form (2.5) with the assumption that the EMF frequency is less than the frequencies of quasiparticle interband transitions.

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

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = [H + V(t)]|\Psi(t)\rangle, \tag{2.11}$$

and can be expanded over the complete set of stationary states of the Hamiltonian (2.1)

$$|\Psi(t)\rangle = \sum_j a_j(t)\, |\Psi_j(t)\rangle. \tag{2.12}$$

The perturbation $V(t)$ is assumed to be adiabatically included at the initial time moment and $a_j(0) = \delta_{j,s}$. We assume that the initial state $|\Psi_s\rangle$ corresponds to the ground state of an extra quasiparticle in the chain described by the Hamiltonian (2.1) and at strong enough quasiparticle-phonon coupling can be described [9, 21] by the wavefunction:

$$|\Psi_s(t)\rangle = |\Psi_e(t)\rangle\,|\Psi_{ph}(t)\rangle, \quad \langle\Psi_s(t)|\Psi_s(t)\rangle = 1, \tag{2.13}$$

where

$$|\Psi_e(t)\rangle = \sum_k \Psi_k(t) B_k^+ |0\rangle_e, \quad \sum_k |\Psi_k(t)|^2 = 1, \tag{2.14}$$

$$|\Psi_{ph}(t)\rangle = U(t)\,|0\rangle_{ph}, \tag{2.15}$$

and the unitary operator

$$U(t) = \exp\left\{\frac{1}{\sqrt{N}}\sum_q [\beta_q(t) b_q^+ - \beta_q^* b_q]\right\} \tag{2.16}$$

describes the rearrangement of the lattice due to its interaction with the quasiparticle. The coefficients $\Psi_k(t)$ and $\beta_q(t)$ satisfy the selfconsistent set of nonlinear equations and describe the autolocalized soliton-like state of the quasiparticle [9, 21, 23, 24].

The coefficients $a_j(t)$ in Equation (2.12) determine the probability of a quantum transition from the initial ground state $|\Psi_s\rangle$ into the state $|\Psi_j\rangle$, $j \neq s$ and are expressed via the nondiagonal matrix elements of the perturbation,

$$a_j(t) = \frac{1}{i\hbar}\int_0^t \langle\Psi_j(t')|V(t')|\Psi_s(t')\rangle dt'. \tag{2.17}$$

The total probability (per unit time) of a quantum transition of the system due to the influence of the EMF is given by the following expression

$$P_s = \frac{2}{\hbar^2}\Re\int_{-\infty}^t dt' \langle\Psi_s(t)|V^+(t) e^{-i\frac{H}{\hbar}(t-t')} V(t')|\Psi_s(t')\rangle. \tag{2.18}$$

The corresponding calculations are similar to the case of soliton photodissociation [10, 11] and one can show that the probability of soliton photodissociation is described by a sum of Gaussian functions:

$$P_s = \frac{\sqrt{2\pi}}{\hbar B}\sum_k |\vec{\mathcal{E}}\vec{D}_{sk}|^2 \exp\left\{-\frac{(\omega-\omega_k)^2}{2B^2}\right\}, \tag{2.19}$$

where the photodissociation resonance frequency, ω_k, and the width of Gaussian, B, are determined below:

$$\hbar\omega_k = \frac{\chi^4}{Jw^2} + \frac{\hbar^2 k^2}{2m^*}, \quad B^2 = \frac{12.6\chi^2 V_a \kappa^2}{\pi^3 \hbar w a}, \tag{2.20}$$

and the dipole momentum for the electrosoliton transition into the free band electron state with the wavenumber k, $\vec{D}_{sk}$, is:

$$\vec{D}_{sk} = i\frac{\vec{d}}{2\sqrt{N}}\frac{\pi(ka + i\kappa)}{\sqrt{2\kappa}\cosh\frac{\pi a k}{2\kappa}}. \tag{2.21}$$

It follows from (2.21) that the most probable transition is that of the electrosoliton into the delocalized band state with zero wavenumber $k = 0$. Therefore, the soliton photodissociation probability (2.19) has a resonance, ω_{diss}, dependent on the field frequency:

$$\omega_{diss} = \omega_{k=0} = \frac{\chi^4}{\hbar J w^2}. \tag{2.22}$$

The diagonal elements of the perturbation can be taken into account by the renormalization of the wavefunctions, hence, they do not affect the transition probability. However, the diagonal terms lead not only to shifts in the energy levels, as is usual for linear systems, but also to nontrivial effects in the dynamical properties of the soliton. After the renormalization of the wavefunction we obtain the following system of equations for the quasiparticle and phonon variables [12, 13]:

$$i\hbar\frac{\partial\Psi_k}{\partial t} - [\Lambda_1 + E(k) + V_k(t)]\Psi_k - \frac{1}{N}\sum_q \chi(q)(\beta_q + \beta^*_{-q})\Psi_{k-q} = 0, \tag{2.23}$$

$$-i\hbar\frac{\partial\beta_q}{\partial t} + \hbar\Omega_q\beta_q = -\chi^*(q)\sum_k \Psi^*_k\Psi_{s-q}, \tag{2.24}$$

where

$$\Lambda_1 = \frac{1}{N}\sum_q\left[\hbar\Omega_q|\beta_q|^2 - \frac{1}{2}\left(i\hbar\frac{\partial\beta_q}{\partial t}\beta^*_q + c.c.\right)\right], \tag{2.25}$$

$$V_k(t) = \frac{1}{2}[(\vec{\mathcal{E}}\vec{d}_k)e^{-i\omega t} + c.c.]. \tag{2.26}$$

In the absence of perturbation the system of nonlinear equations (2.23)–(2.24) describes the autolocalized (self-trapped) states and has been widely investigated both analytically and numerically (see, e.g. [21, 23, 24, 28, 29] and references therein). Usually these equations are written in site representation, in terms of variables with a clear physical meaning, namely, the probability amplitudes of a quasiparticle on the n-th site, Ψ_n, and for the displacements of chain sites from their equilibrium positions, u_n. In this case the integro-differential equations (2.23)–(2.24) can be transformed either to the system of nonlinear differential-difference equations which are suitable for numerical calculations, or, in the continuum approximation, to partial differential equations which allow for an analytical analysis. In the next section we study the corresponding system of equations in the presence of electromagnetic field analytically, following the Mitropolsky-Bogolyubov-Krylov perturbation theory [25]. The results of numerical calculations are given in Section 4.

3. Analytical Analysis of Soliton Dynamics

For the analytical investigation of the Equations (2.23)–(2.24) let us introduce the functions

$$\psi(x,t)=\frac{1}{\sqrt{L}}\sum_k \Psi_k(t)e^{ikx},\quad u(x,t)=\frac{1}{N}\sum_q\left(\frac{\hbar}{2M\Omega_q}\right)^{1/2}(\beta_q+\beta^*_{-q})e^{iqx} \tag{3.1}$$

of continuous variable x. One can see that the latter functions are periodical, i.e. $\psi(x+L,t)=\psi(x,t)$ and $u(x+L,t)=u(x,t)$. From the first equation in (3.1) we have:

$$\Psi_k(t)=\tfrac{1}{\sqrt{L}}\textstyle\int_{-L/2}^{L/2}\psi(x)e^{-ikx}dx, \tag{3.2}$$

where $L=aN$ is the length of the chain.

If Ψ_k and β_q are assumed to be essentially nonzero only for small wave numbers, we can use the long-wave approximation:

$$E(k)\simeq E_0+\tfrac{\hbar^2k^2}{2m^*},\quad \Omega_q\simeq V_a|q|,\quad \chi(q)\simeq 2i\chi\sqrt{\tfrac{\hbar}{2M\Omega_q}}qa\quad \vec{d}_k\simeq i\vec{d}\,ak, \tag{3.3}$$

where $m^*=\hbar^2/2Ja^2$ is the quasiparticle effective mass and $V_a=a\sqrt{w/M}$ is the sound velocity in the chain.

Then, taking into account (3.1)–(3.3), we can rewrite the Equations (2.23)–(2.24) in the following form:

$$i\hbar\frac{\partial\psi}{\partial t}+\frac{\hbar^2}{2m^*}\frac{\partial^2\psi}{\partial x^2}-[\Lambda+2\chi\rho]\psi=-ig(t)a\frac{\partial\psi}{\partial x}, \tag{3.4}$$

$$\frac{\partial^2\rho}{\partial t^2}-V_a^2\frac{\partial^2\rho}{\partial x^2}=\frac{2\chi aV_a^2}{w}\frac{\partial^2|\psi(x,t)|^2}{\partial x^2}, \tag{3.5}$$

where $\rho(x,t)$ is the chain deformation,

$$\rho(x,t)=\frac{\partial u(x,t)}{\partial x} \tag{3.6}$$

and the function $g(t)$ accounts for influence of the EMF:

$$g(t)=AJ\cos(\omega t),\quad A=\frac{1}{J}\vec{\mathcal{E}}\vec{d}. \tag{3.7}$$

In the absence of perturbation, when $g=0$, Equations (3.4)–(3.5) admit the soliton-like solution:

$$\rho_s(x,t)=-\frac{2\chi a}{w(1-s^2)}|\psi_s(x,t)|^2, \tag{3.8}$$

$$\psi_s(x,t)=\frac{\kappa\sqrt{1-s^2}}{\sqrt{G}}\frac{\exp\{i[k(x-\zeta(t))+\vartheta(t)]\}}{\cosh\kappa[x-\zeta(t)]}, \tag{3.9}$$

where

$$\zeta(t)=\zeta_0+\frac{\hbar k}{m^*}t,\quad \vartheta(t)=\frac{\hbar^2}{2m^*}(k^2+\kappa^2)t, \tag{3.10}$$

$$G = \frac{4ma\chi^2}{\hbar^2 w}, \quad s = \frac{\hbar k}{m^* V_a}, \quad \kappa = \frac{G}{2(1-s^2)}. \tag{3.11}$$

This solution describes a stationary autolocalized state of a quasiparticle which moves along the chain with constant velocity $V = \hbar k/m^*$. More generally, the substitution of the solution of Equation (3.5), in the form given by Equation (3.8), into (3.4) transforms the latter into the nonlinear Schrödinger equation whose periodic solution is expressed via elliptic functions. But at $-L/2 < x - Vt \leq L/2$, for long enough chain, the periodic solution can be reduced to the expression (3.9).

The weak influence of the electromagnetic field on the soliton can be accounted for within the adiabatic perturbation theory [25, 26, 27], according to which the solution of Equations (3.4)–(3.5) reads as

$$\rho(x,t) = -\frac{2\chi a}{w(1-s^2)}|\psi(x,t)|^2 + \varepsilon r_1(x,t), \tag{3.12}$$

$$\psi(x,t) = \psi_s(x,t) + \varepsilon f_1(x,t). \tag{3.13}$$

Here ε is a small parameter and $\psi_s(x,t)$ is the soliton wavefunction (3.9) and its time dependent parameters, κ, ζ, k, and ϑ obey the following equations:

$$\dot{\kappa} = 0, \quad \dot{\zeta} = \frac{\hbar k}{m^*} + \varepsilon \frac{a}{\hbar} g(t),$$

$$\dot{k} = -\varepsilon \frac{2\chi G}{\hbar} \int_{-\infty}^{\infty} r_1(x,t) \tanh[\kappa(x-\zeta)]|\psi_s|^2 dx,$$

$$\dot{\vartheta} = \frac{\hbar^2}{2m^*}(k^2+\kappa^2) - \varepsilon \frac{2\chi G}{\hbar\kappa} \int_{-\infty}^{\infty} r_1\{1 - \kappa(x-\zeta)\tanh[\kappa(x-\zeta)]\}|\psi_s|^2 dx. \tag{3.14}$$

The first order correction of the deformation in the adiabatic approximation is governed by the equation:

$$\frac{\partial^2 r_1}{\partial t^2} - V_a^2 \frac{\partial^2 r_1}{\partial x^2} = -\frac{2\chi a}{w} \ddot{\zeta} \frac{\partial |\psi_s|^2}{\partial x} \tag{3.15}$$

with the initial condition $r_1(t \to -\infty) = 0$, and its expression is

$$r_1 = -\frac{\chi a}{\pi w V_a} \int_{-\infty}^{t} dt' \, \ddot{\zeta}(t') \int_{-\infty}^{\infty} dq \frac{\sin[V_a q(t-t')]}{q}$$

$$\int_{-\infty}^{\infty} dx' \, e^{iq(x-x')} \frac{\partial |\psi_s(x',t')|^2}{dx'}. \tag{3.16}$$

From (3.14) we find that the soliton width is not changed by the weak field:

$$\kappa = \frac{1}{2}G \tag{3.17}$$

and obtain an equation for the soliton center of mass motion,

$$m^*\ddot{\zeta}(t) + \int_0^\infty \ddot{\zeta}(t-\tau)K(\tau)d\tau = F_0\cos(\omega t), \tag{3.18}$$

where

$$F_0 = \frac{m^*\omega a}{\hbar}\vec{\mathcal{E}}\vec{d}, \tag{3.19}$$

$$K(\tau) = -\frac{4\chi^2 a\kappa}{\mu V_a^2}\frac{d}{d\tau}\frac{\kappa V_a\tau\cosh(\kappa V_a\tau) - \sinh(\kappa V_a\tau)}{\sinh^3(\kappa V_a\tau)}. \tag{3.20}$$

Equation (3.18) describes the motion of a particle in the presence of an external periodical force with amplitude F_0 and the kernel (3.20) describes the retardation effects in the deformation which accompanies the soliton. The solution which describes the stationary motion of the driven soliton has the form:

$$\ddot{\zeta}(t) = \tfrac{F_0}{m_d(\omega)}\cos[\omega t - \phi(\omega)], \tag{3.21}$$

where the dynamical mass of the soliton, $m_d(\omega)$ and the phase shift due the soliton acceleration under the external force, ϕ, are:

$$m_d(\omega) = \sqrt{[m^* + \mu_1(\omega)]^2 + \mu_2^2(\omega)}, \quad \phi = \arcsin\frac{\mu_2(\omega)}{m_d(\omega)}. \tag{3.22}$$

where,

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

$$\mu_2(\omega) = \frac{4\chi^2 a\kappa}{\pi w V_a^2}\left(\frac{\omega}{\omega_0}\right)^2\sinh^{-2}\frac{\omega}{\omega_0}, \tag{3.23}$$

$$\omega_0 \equiv \frac{2\kappa V_a}{\pi}. \tag{3.24}$$

The analysis of expressions (3.22)–(3.23) shows that the dynamical mass, $m_d(\omega)$, depends on the parameter, δ,

$$\delta = \frac{JG^2}{m^* V_a^2} \tag{3.25}$$

which is the ratio of the soliton binding energy to the kinetic energy of the free band quasiparticle moving with sound velocity.

It follows from (3.22)–(3.23) that, in the low frequency limit, when the inequality $\omega \ll \omega_0$ is fulfilled, the phase shift ϕ tends to zero, and the soliton behaves as a classical Newtonian particle in a slowly oscillating external field with a dynamical mass, m_d, equal to the effective mass of the soliton in the absence of the field,

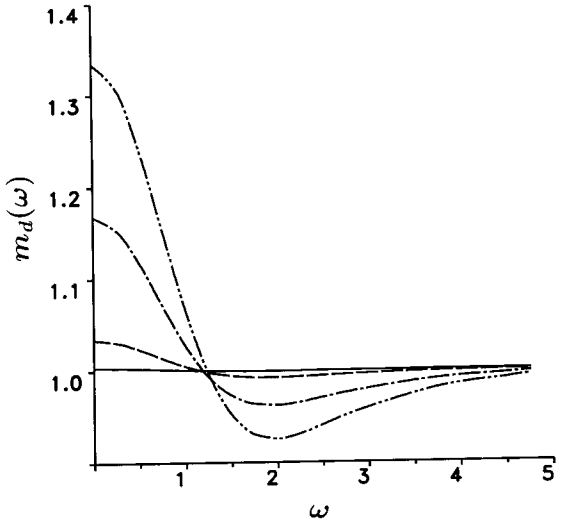

Figure 1. Frequency dependence of the dynamic mass, m_d (3.22), at small values of the parameter δ determined in Equation (3.25). The solid line is for $\delta = 0.01$, the dashed line is for $\delta = 0.1$, the dot-dash line for $\delta = 0.5$ and the double dot-dash line for $\delta = 1.0$.

$$m_d \approx m^* + \frac{8m^*\chi^4 a^2}{3\hbar^2 w V_a^2}. \tag{3.26}$$

At high frequencies of the external field, when $\omega \gg \omega_0$, the phase shift also tends to zero. However, in this case, the deformation cannot follow the comparatively fast electron motion, and the dynamical mass approaches the mass of a free band quasiparticle,

$$m_d \approx m^*. \tag{3.27}$$

This analysis of the frequency dependence of the dynamical mass is confirmed by numerical calculations of Equations (3.22)–(3.23) for various values of δ as shown in Figures 1–2.

The deformational system is described by the first-order correction (3.16) which can be rewritten as the sum of two terms:

$$r_1 = -\frac{\chi a}{w V_a}\int_0^\infty \ddot{\zeta}(t-\tau)\{|\psi_s(\zeta_+)|^2 - |\psi_s(\zeta_-)|^2\}d\tau, \tag{3.28}$$

where

$$\xi_\pm = x - \zeta(t) \pm V_a\tau\left(1 \pm \frac{\bar{v}(\tau)}{V_a}\right) \approx x - \zeta(t) \pm V_a\tau,$$

$$\bar{v}(\tau) = \frac{\zeta(t) - \zeta(t-\tau)}{\tau}, \quad \frac{\bar{v}(\tau)}{V_a} \ll 1. \tag{3.29}$$

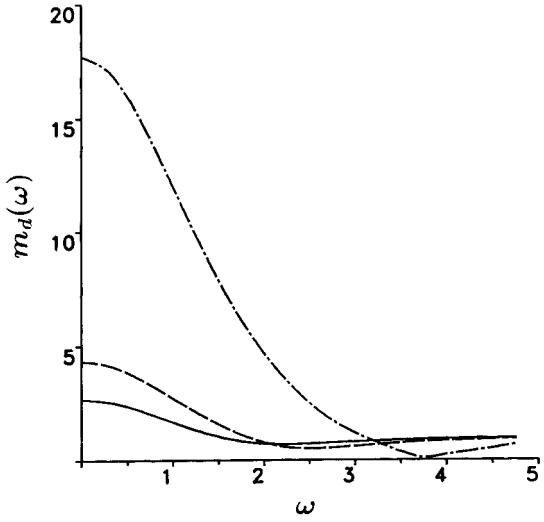

Figure 2. The frequency dependence of the dynamic mass at large values of δ. The solid line is for $\delta = 5$, the dashed line is for $\delta = 10$ and the dot-dash line for $\delta = 50$.

Equation (3.28) asymptotically describes two sound waves generated by the oscillating soliton motion which move in opposite directions:

$$r_1(x,t) = \begin{cases} A(\omega)\cos[\omega(t-(x-z)/V_a)-\phi], & x-z \to \infty, \\ -A(\omega)\cos[\omega(x-z)q/V_a)-\phi], & x-z \to -\infty \end{cases} \tag{3.30}$$

where

$$A(\omega) = \frac{\chi m a^2 \omega^2}{\hbar m_d w V_a^2 \omega_0} \sinh^{-1}\left(\frac{\omega}{\omega_0}\right) \vec{\mathcal{E}}\vec{d}. \tag{3.31}$$

The energy flow absorbed by an electrosoliton from the electromagnetic field per field oscillation period, $T = 2\pi/\omega$, is equal to the following value:

$$E_T = \overline{\frac{dE}{dt}} = -\frac{\omega}{2\pi V_a \omega_0^2}\left(\frac{e\mathcal{E}_l \lambda \chi a}{m_d(\omega)}\right)^2 \sinh^{-2}\frac{\omega}{\omega_0}, \tag{3.32}$$

where $\mathcal{E}_l$ is the EMF amplitude projection on the chain axis and the dynamical mass is determined in (3.22). Substituting its asymptotics at low and high frequencies (3.27), (3.28) in (3.32), we find that this flow is proportional to the electromagnetic field frequency at low frequencies, and decreases exponentially at high frequencies:

$$E_T \propto \begin{cases} \omega, & \omega \ll \omega_0, \\ \omega^3 \exp(-\gamma\omega), & \omega \gg \omega_0 \end{cases} \tag{3.33}$$

attaining the maximum absolute value at

$$\omega_{dyn} = 1.3\omega_0. \tag{3.34}$$

The energy absorbed from an EMF by an electrosoliton results in the emission of phonons, and, according to (3.32), this process is characterized by the dynamic resonance frequency (3.34).

4. Numerical Experiments

The analytical studies of Equations (2.23)–(2.24) performed in the previous section are based on several assumptions, including the long-wave (continuum) approximation. Although the continuum perturbative analysis developed in Section 3 has proved to be successful and nontrivial effects of the influence of EMS on the soliton dynamics were predicted, the range of applicability of this method to a nonlinear system remains an open question. The direct numerical investigation of the corresponding equations avoids the use of approximations and is thus very important. To integrate Equations (2.23)–(2.24) numerically let us rewrite them in the site representation using the unitary transformation

$$\Psi_n(t) = \frac{1}{\sqrt{N}} \sum_k \Psi_k(t) e^{ikan}, \quad u_n(t) = \frac{1}{N} \sum_q \left(\frac{\hbar}{2M\Omega_q} \right)^{1/2} (\beta_q + \beta^*_{-q}) e^{iqna}. \tag{4.1}$$

In this representation, taking into account (2.2), (2.3) and (2.8), one can rewrite equations (2.23)–(2.24) in the following form

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

$$-ig(t)(\Psi_{n+1} - \Psi_{n-1}), \tag{4.2}$$

$$M \frac{d^2 u_n}{dt^2} = \chi(|\Psi_{n+1}|^2 - |\Psi_{n-1}|^2) + w(u_{n+1} + u_{n-1} - 2u_n). \tag{4.3}$$

Here $\Lambda = \Lambda_1 + E_0$, u_n is the displacement of the n-th molecule, and $g(t)$ is given by Equation (3.7).

It is easy to see that the Equations (3.4)–(3.5) are the continuum approximations of the discrete equations (4.2)–(4.3) and that the connection between the corresponding variables is given by the relations $\Psi_n(t) = \sqrt{a}\psi(an, t)$ and $u_n(t) = u(an, t)$ which follow from comparison of (3.1) with (4.1).

Below, we present the results of the numerical calculations of Equations (4.2)–(4.3) for a chain with 50 sites with periodic boundary conditions. For the initial state we chose the exact minimum energy one-quantum state of the unperturbed Davydov model [24, 28, 29]. Although the problem of the numerical values of the parameters of the Hamiltonian (2.1) is still open at present, there are approximate estimates for the resonance energy and electron-phonon coupling constant for the charge transport processes in peptides. The values of parameters we use here are those applied to the amide I vibrations in an α-helix [23]; $J = 1.55 \cdot 10^{-22} J$,

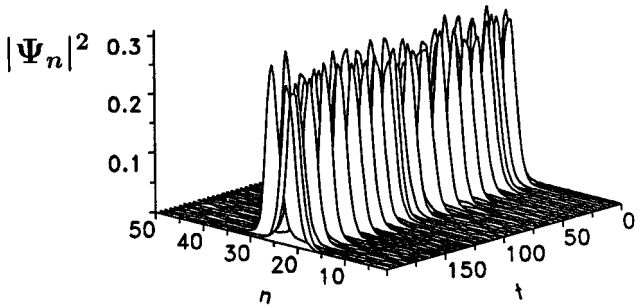

Figure 3. Variation with time of the probability of a quasiparticle excitation in site n, $|\Psi_n|^2$ in an external field of amplitude $A = 0.9$ and frequency $\omega = 0.5$. Here and in the figures below amplitude, A is dimensionless and given by Equation (3.7), and the frequency, ω, is in ps^{-1}.

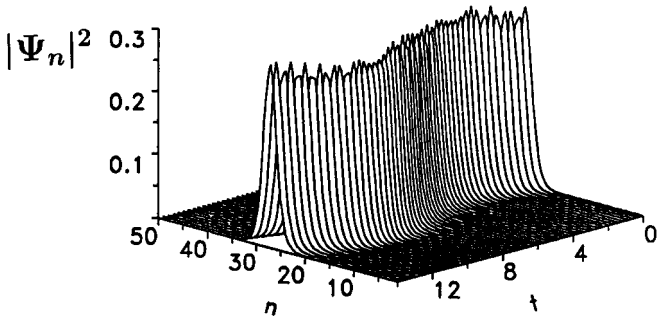

Figure 4. Variation with time of the probability of a quasiparticle excitation in site n, $|\Psi_n|^2$, in an external field of amplitude $A = 0.9$ and frequency $\omega = 0.5$ in a small time interval.

$\chi = 62pN$, $w = 39N/m$, $M = 5.7 \cdot 10^{-25}$ kg, $a = 4.5 \cdot 10^{-10}$ m which give the following values: $\delta = 50$, $\omega_{dyn} = 1.1$ THz, $\omega_{diss} = 38$ GHz.

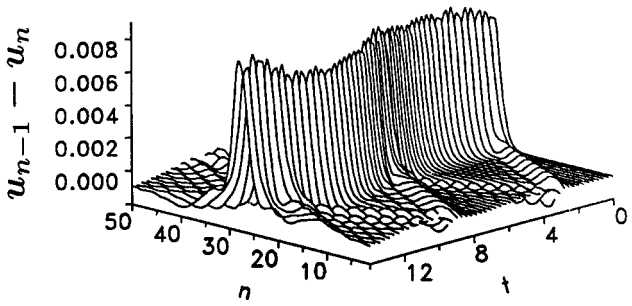

Figure 5. The time dependence of the difference of the neighboring molecule displacements $u_{n-1} - u_n$ at the same values of the field parameters as in Figures 3–4.

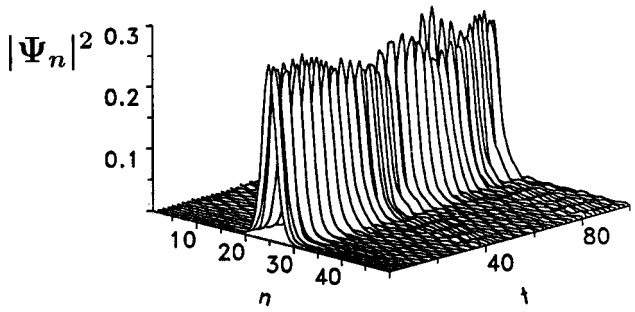

Figure 6. Variation with time of the probability of a quasiparticle excitation in site n, $|\Psi_n|^2$ in an external field of amplitude $A = 0.9$ and frequency $\omega = 1.5$.

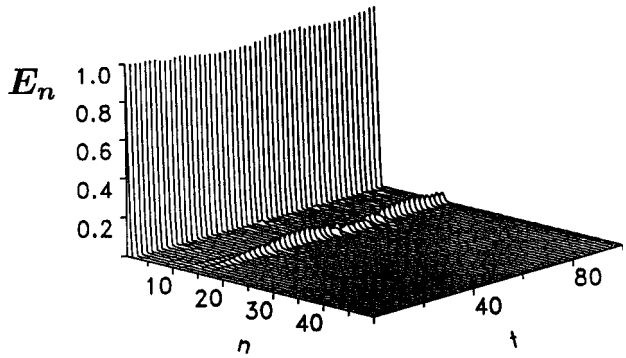

Figure 7. The time dependence of energy distribution E_n between the different states n for the same values of the field parameters as in Figure 6.

The results of numerical calculations of Equations (4.2)–(4.3) are represented in Figures 3–15. The amplitude of the external EMF, A is given in dimensionless units as it is determined by Equation (3.7), and frequency ω is in ps^{-1}.

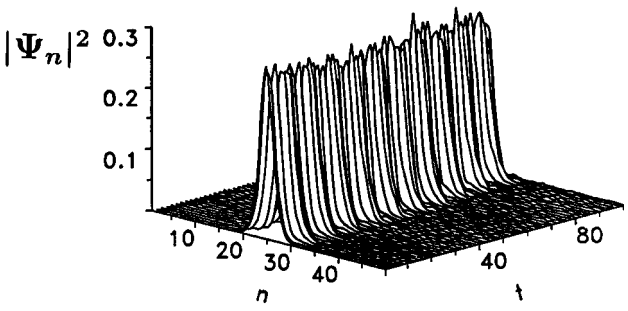

Figure 8. Variation with time of the probability of a quasiparticle excitation in site n, $|\Psi_n|^2$, in an external field of amplitude $A = 0.9$ and frequency $\omega = 2.5$.

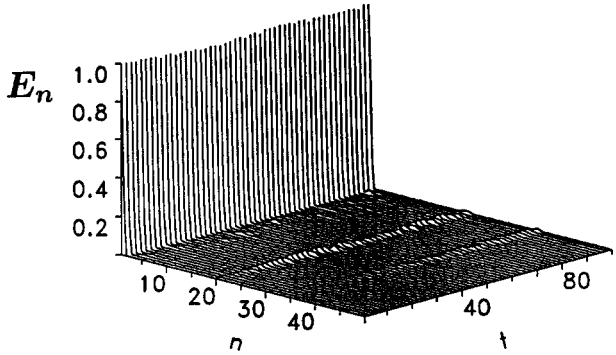

Figure 9. The time dependence of energy distribution E_n between the different states n for the same values of the field parameters as in Figure 8.

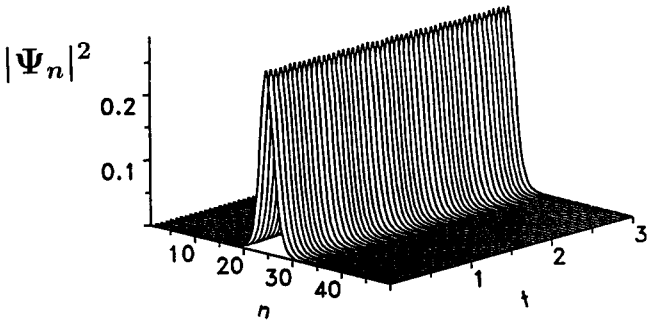

Figure 10. Variation with time of the probability of a quasiparticle excitation in site n, $|\Psi_n|^2$, in an external field of amplitude $A = 0.9$ and frequency $\omega = 10$.

The dynamics of a soliton in a field of amplitude $A = 0.9$ and frequency $\omega = 0.5$ is displayed in Figure 3 and confirms soliton stability even at such a large value of perturbation. The oscillations of the soliton c.o.m. around the unperturbed position in the middle of the chain and the emission of two sound waves which move in opposite directions, are clearly seen at the shorter time interval represented

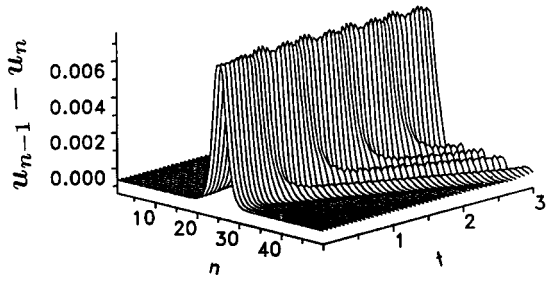

Figure 11. The time dependence of the difference of the neighboring molecule displacements $u_{n-1} - u_n$ at the same values of the field parameters as in Figure 10.

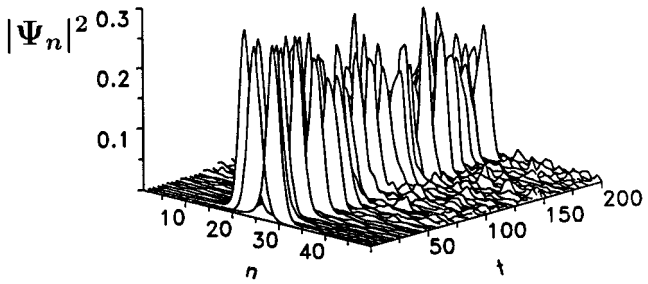

Figure 12. Variation with time of the probability of a quasiparticle excitation in site n, $|\Psi_n|^2$, in an external field of amplitude $A = 1.2$ and frequency $\omega = 0.56$.

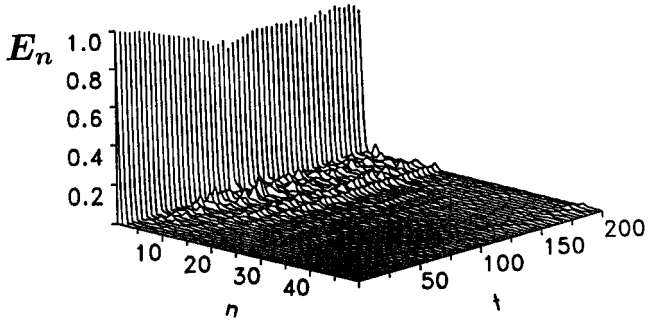

Figure 13. The time dependence of energy distribution E_n between the different states n for the same values of the field parameters as in Figure 12.

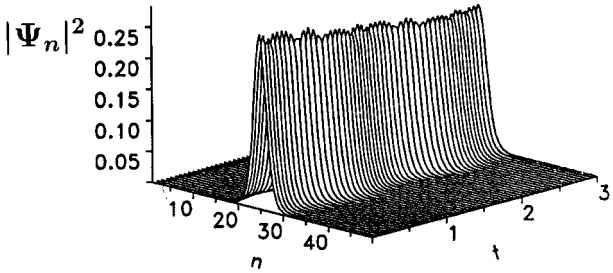

Figure 14. Variation with time of the probability of an amide I excitation in site n, $|\Psi_n|^2$, in an external field of amplitude $A = 50$ and frequency $\omega = 100$.

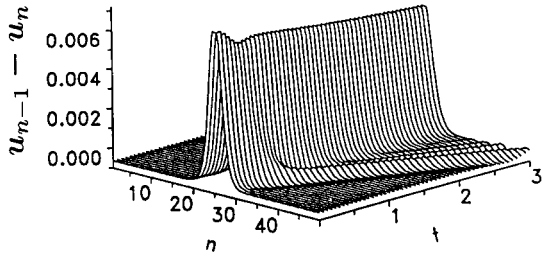

Figure 15. The time dependence of the difference of the neighboring molecule displacements $u_{n-1} - u_n$ at the same values of the field parameters as in Figure 14.

on Figures 4–5. The interference of the two sound waves in Figure 5 is due to the periodic boundary conditions. Worth mentioning is also the very weak time dependence of the soliton amplitude which can be seen in Figures 3–5. As the field frequency increases, the amplitude of soliton c.o.m. oscillations decreases, as shown in Figure 6 and there appears a small probability for the vibration to occupy the excited delocalized energy level corresponding to the energy absorbed from the field, as is seen in Figures 7, for $\omega = 1.5$. With a further frequency increase the second delocalized level (overtone) can be partially occupied as it is shown on Figures 8–9 for $\omega = 2.5$. If the frequency of the field is too large, the overtones lie above the allowed energy levels. The emission of sound waves increases with frequency while the latter is less or comparable to the dynamic resonance frequency. When the field frequency greatly exceeds the dynamic resonance frequency, the sound emission decreases and becomes very similar to that observed at small frequencies of the external field, as shown in Figures 10–11 for $\omega = 10$. Although the amplitude of the oscillations is very small and almost invisible in Figure 10 for the excitation probability, the presence of oscillations can be distinctly seen in the site displacements in the form of emitted sound waves (see Figure 11). At this frequency, the amide I vibration is in the ground localized state and there is no possibility for its transition into an excited delocalized state (we do not present here the corresponding figure for the occupation probability of energy levels since it is of trivial form).

Increasing the EMF amplitude further, the adiabatic approximation breaks down and cannot be used to describe the dynamics. The amplitude of the soliton decreases significantly and tails appear, as it is shown on Figure 12 for $A = 1.2$ and $\omega = 0.56$. The probability of higher level occupation increases with time (see Figure 13) and some features of stochasticity arise in the system. However, from a physical point of view, even under fields of such large amplitude the autolocalized state is stable for long enough to travel along the chain length.

In Figures 14–15 we show the behaviour of the soliton at very high frequencies. At $\omega = 100$ the chain deformation cannot follow the very fast oscillations of the 'light' amide I subsystem, except at the very beginning when the soliton is pushed from its equilibrium position by the external field and with some retardation the deformation wave was pushed over (we have chosen here a large value of A, namely $A = 50$, to make the physical picture more striking). This dynamics agrees well with the analytical asymptotic analysis of the soliton dynamical mass at large frequencies given above in Section 3.

5. Discussion

Comparing the analytical and numerical results, we conclude that they coincide to a great extent at small amplitudes of perturbation, and complement each other at the intermediate and large amplitudes. The numerical analysis has proved the validity of adiabatic perturbation for rather strong perturbations and the exceptional stabil-

ity of the soliton as an autolocalized state in the presence of external EMF. While the oscillatory character of soliton motion can be well described by the analytical approach, the emission of sound waves is much easier to study within by numerical simulations, and especially the interference of sound waves with one another due to the periodic boundary conditions used in the numeric method. In biological systems these finite size effects will be present because of sound reflection from the polypeptide ends.

We note that the electromagnetic radiation is shown to have a specific influence on electrosolitons which, we believe, could be responsible for the observed effects of EMF on charge transport in biological systems. Thus, this theory predicts that these effects 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 [30].

As it was shown in Section 3, the effects of EMFs on electrosolitons is particularly intense at two characteristic frequencies, ω_{dyn} and ω_{diss}, determined by Equations (3.21) and (3.34), respectively, but in a qualitatively different manner. The dynamic resonant frequency of the field, ω_{dyn}, is connected with the absorption by electrosolitons of energy from the field and the following generation of acoustic waves. This process is the most intense at the field frequency $\omega_{dyn} = 1.3\omega_0$ 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 (see (3.21)). The generation of acoustic waves in the polypeptide chain can result not only in the obvious local heating of the system, but also in sound waves that propagate along the α-helix as in a channel carrying some additional information. Moreover, the generation of sound can qualitatively change some functional processes connected with conformal states of macromolecules or their fragments, since electromagnetic radiation of the corresponding frequencies causes the oscillations of electrosolitons including oscillations of chain distortion. In this respect it is worth mentioning the function of calcium channels, namely, their opening and closing, which depends on the channel conformation, and to cite the experimental results about the strong influence of EMF on calcium balance [31, 32].

Another type of EMF bioeffect takes place at $\omega \approx \omega_{diss}$, namely, when the frequency of electromagnetic radiation corresponds to the splitting energy of the electrosoliton level from the band bottom, i.e. when the quantum transition of the electrosoliton into the delocalized band state occurs. As a result, the electromagnetic radiation of the corresponding frequencies can, with finite probability, destroy the electrosoliton completely. In this case the coherent charge transport in the system becomes far less effective, if possible at all.

It is worth mentioning here that the soliton mechanism is not the sole possible mechanism for charge and energy transport in biosystems. In such rich structures as biosystems, under different conditions and for different biological ‘aims’, different mechanisms can complement one another. But whenever this occurs in α-helical molecules, it is necessary to take into account that these molecules are formed by

weak hydrogen bonds, hence, the electron-phonon interactions are essential and cannot be neglected. In low-dimensional systems the electron-phonon coupling under certain conditions can result in the autolocalization of quasiparticles, and this is the case when the soliton mechanism arises. Among other advantages of this mechanism (see [9], e.g.) there is the fact that molecular solitons carry the information from one place of the cell to another without losing or changing it, since they propagate in the system without spreading or changing shape and velocity, even after collisions with other solitons or thermal phonons.

In conclusion, we note that the present paper describes the main but not all of the features of EMF bioeffects in the framework of the soliton concept for energy and charge transport in biosystems. As was mentioned in Section 4, for our calculations we started from an initial state in the form of the exact minimum energy one-quantum state of the unperturbed Davydov model. This state describes the autolocalized soliton state and our approach corresponds to the adiabatic switching of the perturbation and it is investigated here only in the case of zero soliton velocity. It should also be interesting to investigate the dependence of these results on initial conditions and soliton velocity. Here we should mention also that charge transport in biological systems can be provided by bisolitons which are bound states of two electrosolitons with opposite spins [15, 16] and one can expect that the spectrum of bisoliton interaction with electromagnetic radiation to be richer than that of a single electrosoliton.

Another limitation of the present study is that we have considered the system at zero temperature, while all biological processes take place at physiological temperatures. Temperature has significant influence on soliton state properties [24, 33] and it can lead not only to a temperature dependence of the absorption line characteristics in (2.15), but also to more significant effects on soliton dynamics under EMF.

Finally, the single band model (2.1) is oversimplified for the description of charge and energy transport along α-helical protein molecules. There are three chains of peptide groups in the α-helical structure and, therefore, there are three energetic bands for quasiparticles. With allowance for helical structure, soliton states become more complicated [34, 35, 36, 37] which will lead to more complex spectra for the soliton response to an external EMF. All the missing factors mentioned will introduce new features in the biological effects of EMF and we intend to investigate their role in forthcoming papers.

Acknowledgements

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