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===== TRANSLATIONS OF PUBLISHED ARTICLES =====

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Trapping and Transport of Charges in DNA by Mobile Discrete Breathers

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Abstract. Numerical simulation of trapping and transport of a charged particle (electron or hole) by mobile discrete breathers (mobile DB, MDB) in DNA molecule has been provided. Mobile DBs have been excited by disturbance of displacements or velocities of adjacent nucleotide pairs dislocated near one of fixed ends of the molecule. It is shown that effective forming of a stable quasi-particle “MDB + electron” occurs when a few of nucleotide pairs at the end of DNA are excited. Breathers may be excited by disturbances of displacements and velocities directed both to axis and from axis of the molecule. A wave function of an electron must be located initially in a region of disturbance of the molecule. It has been found that a metastable quasi-particle may be transported at a distance up to 200 of a rise per base pair. The mechanism of transport of a charged particle presented is not in need of an external electric field and may be considered as an alternative one to the polaronic mechanism.

Key words: nanobioelectronics, DNA, mobile discrete breathers (MDB), quasi-particles, Peyrard-Bishop-Dauxois-Holstein model.

INTRODUCTION

Earlier, we have demonstrated that a DNA molecule can be used as a base element in nanobioelectronics [1–4]. We may consider it as some molecular wire enabling integration of various elements of biomolecules chains (theoretical justification of electron logic elements construction is presented in [2, 4]). However, a traditional polaronic mechanism [5–10] is not the only possible way to transfer charges in DNA. Recent days brought us the intense debates on a mechanism of charge transport «exploiting» the nonlinear properties of DNA molecule without application of an external (dragging) electric field for its realization [11, 12]. We know that in the chains of elements-oscillators of various nature, non-linearity of the elements by themselves occurring due to nonparabolicity of the *on-site* potential, along with the nonlinearity of inter-element integration combined with the dispersion resulting from the discreteness of the system (chain of the neighboring elements) leads to the localization of the chain perturbations. The localized perturbations may be of the soliton or breather [13] type, in accordance with the interrelation of the parameters. For example, the «angular» disturbances, where an *on-site* potential is absent, form the solitons [14]. However, a charge is transported due to interrelations between external particles (electrons or holes) and perturbations of radii of base pairs, in any of which the nucleotides are ambivalent about an equilibrium point created by a strong *on-site* potential. Therefore, within a DNA molecule, an electron binds to

the breather-type local perturbations. DNA discrete breathers can be of two types: non-mobile and mobile. The breathers of the first type can be excited in a DNA molecule at weak stacking interactions, while the moving breathers, in such a case, can be excited only at the fronts of highly-energetic bubbles [11, 12]. They can trap a charge and move it but at short distances (~ 10 inter-pair distances). The mobile breathers can be excited without essential energy expenses, when a bond strength exceeds some threshold [15–18, 11, 12]. The binding force sets the width of a transmission band for an oscillator chain, therefore, a criterion of mobile breathers formability can be formulated as a restriction to the width of a transmission band at a set frequency of free nucleotide oscillations or to the value of maximal (upper critical) frequency $\omega_{\text{bond cr}}$ [13] of a transmission band. For a Peyrard–Bishop model [19], this criterion is formulated at [18], and in a Dauxois corrected form it can be written as $\omega_{\text{bond}} > \omega_{\text{bond cr}} = 0.354 / (1 + \rho)^{1/2}$, where ρ determines a value of nonlinear correction in the potential of the stacking interaction (see below). In many cases, when DNA does not meet this criterion (refer to [1, 11, 12], for examples), mobile breather-like perturbations occur, as mentioned above, only in a form of «ingredients» of complex highly-energetic fluctuations as, for example, at the fronts of highly energetic bubbles [11, 12]. However, such a mode of excitation distorts a molecule heavily, while a bubble excitation needs high energy. Therefore, excitation of low-energetic autonomous mobile breathers seems a mode of choice [20], since these breathers, as it appears from the results of our preliminary studies [11, 12], can trap electrons and form mobile quasiparticles with them. Such a way resembles the way of a soliton formation [21], except that here the external charged particle cooperates not with a supersonic soliton, but with a discrete mobile breather [19, 22].

More and more current theoretical and experimental studies of various DNA modifications are focused on the investigation of the properties of charge transfer. These studies examine details of mechanisms of electrons interactions with base chain perturbations [23–25], calculate the IU characteristics of a DNA molecule [26, 27], analyze the ways to control charge transport characteristics [28, 29], examine the environmental effects [30], consider complex DNA-involving modifications as a perspective [31–36], and describe various applied problems [37].

This very paper examines an interaction of an electron with a mobile breather, excited in a small group of neighboring base pairs near one of fixed ends of a molecule due to initial nucleotide displacements or perturbations of their speed. The study method is a computer modeling techniques within the frame of a «two-dimensional» Peyrard–Bishop–Dauxois–Holstein model (PBDH) [21, 22, 5, 6, 12] that considers only changes of base pair radii and no angular displacements. The computer experiments vary numbers of excited pairs, their location, excitation energy, and initial shape of electron wave function to determine conditions for formation of stable charged quasiparticles «mobile breather plus trapped electron», enabling charge transfer along a molecule without exposure to an external electric field. We suppose that a breather can be established by initial perturbations of speed or by displacements of equilibrium inter-base distances in the Watson-Crick pairs, and, at that, examine effects of the displacements from a molecule axis independently from the displacements at a reverse direction (towards its axis). One more point of the analysis is a way of excitation, when all particles in a group get the same initial perturbations (technologically more realizable [20]), and a more complex case, when particles in a group have different speeds or displacements.

1. MATHEMATIC MODEL OF PEYRARD-BISHOP-DAUXOIS-HOLSTEIN (PBDH) FOR INVESTIGATIONS OF INTERACTIONS BETWEEN ELECTRON EXCITATION AND DNA MOLECULE PERTURBATIONS

A Peyrard–Bishop–Dauxois–Holstein quantal-mechanic model (PBDH) is a combination of a Holstein “strong link” [22] and of Peyrard–Bishop–Dauxois non-linear [19] models. A

simple description of perturbation dynamics in a chain of base pairs that interact with an electron is changed here to a more correct, analyzed in [19]. First of all, a link in each base pair is described with a nonlinear Morse potential

$$V_n = D(e^{-2\sigma y_n} - 2e^{-\sigma y_n}) \quad , \quad (1)$$

and, second, a stacking interaction between neighboring base pairs is set by a nonlinear link, corresponding to an interaction potential

$$W_n = \frac{K}{2}(y_n - y_{n-1})^2 \left[1 + \rho e^{-\alpha(y_n + y_{n-1})} \right]. \quad (2)$$

Here, the positive Morse parameters, D and σ , set depth of its potential depression and coefficient of stiffness, respectively; the positive K parameter is a coefficient of stacking potential stiffness, and, the same positive, parameters ρ and α designate nonlinearity of force of base pairs stacking interaction. Variables y_n describe displacements of an n -th base pair from its equilibrium positions.

A model Hamiltonian is written as

$$\begin{aligned} \hat{H} = & \sum_n \alpha_n |n\rangle \langle n| - \sum_{n,m} v_{nm} |n\rangle \langle m| + \chi \sum_n (w_n - v_n) |n\rangle \langle n| + \\ & + \sum_n \left[\frac{1}{2} M (\dot{w}_n^2 + \dot{v}_n^2) + V_n(w_n, v_n) + W_n(w_{n,n-1}, v_{n,n-1}) \right] \end{aligned} \quad (3)$$

where M is a nucleotide mass (all nucleotides in this uniform molecule are considered as identical), w_n, v_n – displacements of two bases in the n -th pair from an equilibrium position, a point means a time derivative, and corresponding values include speeds of nucleotides in the n -th base pair, α_n is a charge energy at the n -th site, v_{nm} are coefficients of «jumping» integrals, χ is a constant of a link between an external charge and a chain.

With the variables [19]

$$x_n = (w_n + v_n) / \sqrt{2}, \quad y_n = (w_n - v_n) / \sqrt{2}, \quad (4)$$

considering a symmetrical motion of the nucleotides ($v_n \approx -w_n$), and assuming that an electron wave function is sought in the form

$$|\Psi\rangle = \sum_n c_n(t) |n\rangle \quad (5)$$

nucleotide motions following from equation (3), and the discrete Schrödinger equation for an electron look as follows

$$M \frac{d^2 y_n}{dt^2} + K \{ (2y_n - y_{n-1} - y_{n+1}) + \rho f_n(y_{n-1,n,n+1}) \} + \frac{\partial V(y_n)}{\partial y_n} + \sqrt{2} \cdot \chi |c_n|^2 = 0 \quad (6)$$

$$i\hbar \frac{dc_n}{dt} = \alpha_n c_n - \sum_m v_{nm} c_m + \sqrt{2} \cdot \chi y_n c_n \quad (7)$$

From the last, for *polyG/polyC* of the homogenous molecule in approximation of the nearest neighbors we get ($\alpha_n \equiv 0$)

$$i\hbar \frac{dc_n}{dt} = -v(c_{n+1} + c_{n-1}) + \sqrt{2} \cdot \chi y_n c_n. \quad (8)$$

Note that values of the parameters v and χ were set from the comparison with an experiment for small displacements y_n , when a harmonic approximation is applicable, and the PBDH model goes into the Holstein model [38]. In the Holstein model the signs v and χ are incidental, because in the harmonic approximation a substitution of v with $-v$ corresponds to a

substitution of the wave functions c_n with $\exp(in\pi) \cdot c_n$, and a substitution of χ with $-\chi$ corresponds to a substitution of y_n with $-y_n$. In the PBDH model under consideration, Morse potentials and potentials of the stacking interactions are not anymore symmetrical relatively the substitution of y_n with $-y_n$.

Since a coefficient v , the same as a coefficient χ , can be both of positive and of negative signs [8], we shall write the final equations (7)–(8) as:

$$\ddot{q}_n + \Gamma \dot{q}_n = e^{-q_n} (e^{-q_n} - 1) + \omega_{\text{bond}}^2 \left\{ (q_{n+1} - 2q_n + q_{n-1}) + \rho f_n(y_{n-1,n,n+1}) \right\} \mp |\chi_h| |c_n|^2 \quad (9)$$

$$\dot{c}_n = \pm i |\tau_e| (c_{n+1} + c_{n-1}) \mp i |\chi_{\text{el}}| q_n c_n \quad (10)$$

and supplement them with an expression for an electron energy (in the units $\hbar\omega_M$) [8]:

$$E_{\text{el}} = \mp 2|\tau_e| \left| \sum_n \text{Re}(c_n c_{n-1}^*) \right| \pm |\chi_{\text{el}}| \sum_n q_n |c_n|^2. \quad (11)$$

Here, the upper signs correspond to the positive signs of the values τ_e and χ , respectively, while the lower ones to the negative. The coefficients c_n complementary meet the normalization requirement (prohibition of an electron escape from a molecule):

$$\sum_{n=1}^N |c_n|^2 = 1. \quad (12)$$

In the equations (10)–(12) $q_n = \sigma y_n$ is a numerical displacement of the n -th nucleotide from the equilibrium position, now the point denotes a derivative with respect numerical time $\tau = \omega_M t$, at that the derivative has a meaning of the numerical speed, $\omega_M = (2D\sigma^2 / M)^{1/2}$ is a frequency of linear oscillations of the Morse oscillator corresponding to (9), $\omega_{\text{bond}} = ((K/M) / \omega_M)^{1/2}$ – is a numerical frequency of small linear nucleotide oscillations occurring due to its links with the neighbors, $\chi_h = \sqrt{2}\chi / 2\sigma D$ and $\chi_{\text{el}} = \sqrt{2}\chi / \hbar\omega_M \sigma = \chi_h (2D / \hbar\omega_M)$ are numerical parameters of the link between an electron and a lattice, $\tau_e = v / \hbar\omega_M$ is a numerical parameter setting a relation between typical times of evolution of an electron wave function and dynamics of perturbations within a lattice, and a function f_n describes nonlinearity of the interaction force:

$$f_n = (q_{n+1} - q_n) \left[1 + 0.5\alpha(q_{n+1} - q_n) \right] e^{-\alpha(q_{n+1} + q_n)} + (q_{n-1} - q_n) \left[1 + 0.5\alpha(q_{n-1} - q_n) \right] e^{-\alpha(q_{n-1} + q_n)}. \quad (13)$$

A coefficient α is now also normalized ($\alpha \rightarrow \alpha/\sigma$) due to introduction of a numerical displacement (of a coordinate) q , a friction coefficient Γ is included into equations to consider various losses of particles energy at motion.

From (11) it follows that, when a molecule dynamics does not affect an electron ($\chi = 0$), it has zero energy being localized at one site, while being localized in a cluster from k sites with uniform distribution of probability $|c_n|^2$ in the cluster, it has energy:

$$E_{\text{el}} = \mp 2|\tau_e| \left| \frac{k-1}{k} \cos(\varphi_n - \varphi_{n-1}) \right|. \quad (14)$$

This energy sign depends on the coefficient τ_e sign and distribution of phases of φ_n components $c_n = |c_n| \exp(i\varphi_n)$. For example, at a positive sign τ_e (the upper sign in the (9)–(10) and relation (11)) a minimal electron energy is realized in a distribution with similar phases φ_n :

$$E_{\text{el}} = -2|\tau_e| \left| \frac{k-1}{k} \right| \rightarrow -2|\tau_e|_{k \gg 1}, \quad (15)$$

while a state, in which phases of neighboring components differ by $\Delta\varphi = \pi$, that is,

$$c_n = c_{n_0} e^{i(n-n_0)\Delta\varphi} = (-1)^{n-n_0} c_{n_0}, \quad n = n_0, n_0 + 1, \dots, n_0 + k \quad (16)$$

has a maximal energy (n_0 is a number of the first element of a cluster, and c_{n_0} is a correspondent value of a wave function component)

$$E_{el} = 2|\tau_e| \frac{k-1}{k} \rightarrow 2|\tau_e|_{k \gg 1}. \quad (17)$$

The opposite situation occurs in systems with negative τ_e (a lower sign in equations (9)–(10) and formulas (11), (14)): a maximal electron energy corresponds to a distribution with similar phases, while a minimal electron energy corresponds to a distribution with phases $\Delta\varphi = \pi$. It is evident that energy of other states falls into a range limited with values shown in (15) и (17).

From the presented formulas, we may expect availability of a great many combinations of chain parameters allowing for realization of a mechanism of electron transport due to interactions with chain perturbations. We shall limit this paper with a case of negative τ_e and positive χ , when equations (9), (10) are written as:

$$\dot{c}_n = -i|\tau_e|(c_{n+1} + c_{n-1}) - i|\chi_{el}|q_n c_n \quad (18)$$

$$\ddot{q}_n + \Gamma\dot{q}_n = e^{-q_n}(e^{-q_n} - 1) + \omega_{\text{bond}}^2 \{(q_{n+1} - 2q_n + q_{n-1}) + pf_n(y_{n-1,n,n+1})\} - |\chi_h||c_n|^2, \quad (19)$$

at that, we shall analyze a situation, when a mobile breather traps a highly excited electron introduced into the system (interaction between a low-energy breather with a localized electron leading to formation of the polaron state will be considered in another paper; a system with a positive τ_e , along with an alternate $\chi < 0$ will also be considered in a separate paper).

Equations (18)–(19) with a special selection of initial states (see below) and boundary conditions corresponding to the fixation of a molecule endings ($q_{1,N} = v_{1,N} = 0$) were solved numerically by the Runge–Kutta method of the 4th order with a required precision provided, in particular, by support of constant values of a system integrals. Process of modeling included determination of displacements (of a coordinate) $q_n(\tau)$, speed $v_n(\tau)$ and component of a wave function $c_n(\tau)$.

At selection of a parameter value we considered those realized in real molecules. For example, when we suppose $D = 0.04$ eV, $\sigma = 4.45$ Å⁻¹ [19], $m = 300$ dalton, $\chi = 0.18$ eV/Å, $v = 0.084$ eV [25] (for *polyG/polyC*-chain), $\omega_M \approx 7.1 \times 10^{12}$ c⁻¹, $\tau_e = v/\hbar\omega_M \approx 18$, $\chi_h \approx 0.5$, $\chi_{el} \approx 8.5$. We select stiffness of stacking interaction equal to 0.24 eV/Å, so a corresponding $\omega_{\text{bond}} \approx 0.4$, making formation of mobile breathers possible [13, 20]. A time unit used in the model $\Delta t = 1/\omega_M = 0.14 \times 10^{-12}$ s, length unit for the measurement of lateral displacements $\Delta y = \sigma^{-1} = 2.2 \times 10^{-11}$ m, respectively, unit of nucleotides motion speed $\Delta y/\Delta t \approx 161$ m/s. Speed of a breather and a charged quasiparticle displacement along a molecule axis is measured in the units $d/\Delta t = 2.43 \times 10^3$ m/s at a standard $d = 0.34$ nm, which implies that a numeric speed is measured by amounts Δn of inter-base distances, passed in a numerical time τ (on the hypothesis that the motion is uniform). A selected parameter value was standard: $\alpha = 0.35$ (Å)⁻¹ (as a numerical: -0.08). A selected friction coefficient was 0.001. Values of parameters used in a numerical simulation were selected with consideration of the executed estimations.

The main aim of the study was determination and analysis of conditions of mobile breathers excitations due to initial perturbation of coordinates and speeds of nucleotides in several neighboring pairs located near one of the fixed ends of the DNA molecule [20], and

trapping and transport of an electron with energy close to an upper bound of the conductivity band, at that, the electron was initially dislocated in the region of the breather excitation.

2. TRANSPORT OF AN ELECTRON BY MOBILE BREATHERS EXCITED WITH INITIAL PERTURBATIONS OF NUCLEOTIDES SPEED

Earlier [20], we demonstrated that in a DNA molecule with fixed ends, mobile breathers can be effectively excited at the expenses of the initial excitation or displacements of several (2–4) particles located near one of the molecule ends, at that, excitations of all particles were expected to be the same. It seems natural to use the same initial conditions for excitations of mobile breathers in order to trap an excited electron (with high energy) introduced in the system and transfer it along the molecule. Indeed, the results of a numerical simulation show that breathers excited with identical perturbations of nucleotides speed can localize a wave function of an electron. However, it was found that a structure of such breathers is far from that optimal for trapping and transfer of an electron.

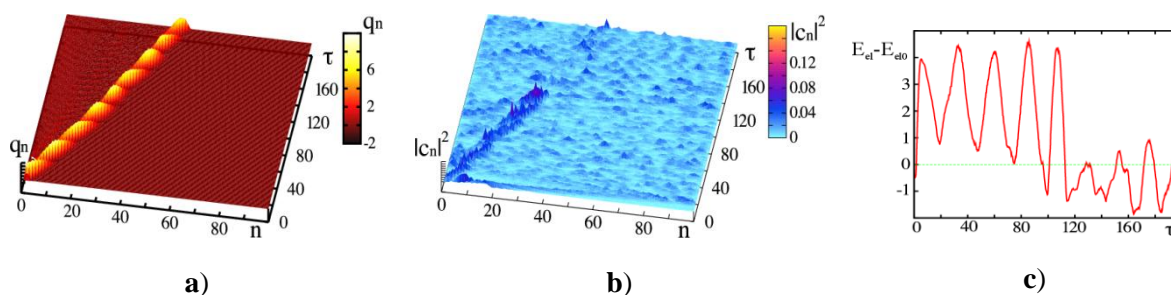


Fig. 1. Mobile breather in the DNA with fixed ends at $v_{20} = v_{30} = -4$, $q_{n0} = 0$. **a)** and **b)** – evolution of coordinates $q_n(\tau)$ distribution and probability of electron presence $|c_n|^2$ at the site with number n , respectively **c)** dependence from electron time energy relatively its initial value $E_{el}(\tau) - E_{el}(0)$. $\omega_{\text{bond}} = 0.4$, $\tau_e = -18$, $\chi_h \approx 0.5$, $\chi_{el} \approx 8.5$, $\rho = 0.5$, $\alpha = 0.08$, $\Gamma = 0.001$, $N = 50$, $\tau_k = 200$.

Figure 1 presents patterns of evolution of particles displacements and of electron time probability function $|c_n|^2$ of breather excitation in response to an initial negative perturbation of two particles speed ($v_{20} = v_{30} = -4$) and to dislocation of an electron with high energy at 8 sites ($c_n^2 = 1/8$, $\Delta\phi = 0$, $n = 4, 5, \dots, 12$).

It is clear that, though an electron is trapped initially by a formed mobile breather, the breather loses it, when its transfer takes a distance about thirty inter-base distances. Energy of the electron falls a little at trapping, lower than a level of its initial high energy, but then quickly increases because the positive displacements prevail at anharmonic oscillations of the particles-oscillators with the Morse *on-site* potential. Then the electron energy oscillates, repeating the breather oscillations, reaches the level of initial energy and goes on decreasing down this level that corresponds to the process of electron delocalization. The results are typical for interaction of an electron with a breather excited with initial identical negative excitations of particles speed. Hence we may conclude that the described breather has not the best structure to form a long-living quasiparticle.

A larger path length may be provided by excitation of mobile breather at the expenses of initial speed perturbations when we realize, for example, the initial positive (from the axis) speed excitation with the profile falling from the end (for example, $v_{20} = 4$, $v_{30} = 2$, $v_{40} = 1$, Fig. 2) and place an excited electron into the same region ($|c_{2,3,4}|^2 = 1/3$, $\Delta\phi = 0$). In such a case, a mobile breather is quickly formed, the breather traps an electron and they together establish a bound state (a quasiparticle). The breather at that is localized at approximately 10 particles, the maximal speed excitation (a breather amplitude) is approximately 1.5 (Fig. 2,b), the breather moves at a speed 0.2 (Figs. 2,a and 2,b). At the moment of trapping, the electron energy jumps again, however it is kept in the potential depression formed by the breather long enough, just leaking away its energy (Fig. 2,e). The breather also loses its energy during

motion, due to friction and deformation of its structure. Finally, the breather loses the electron after transferring it at the distance of approximately 140 inter-pair distances (34 nm) (Figs. 2,b and 2,d), but still moves for some time until the complete delocalization.

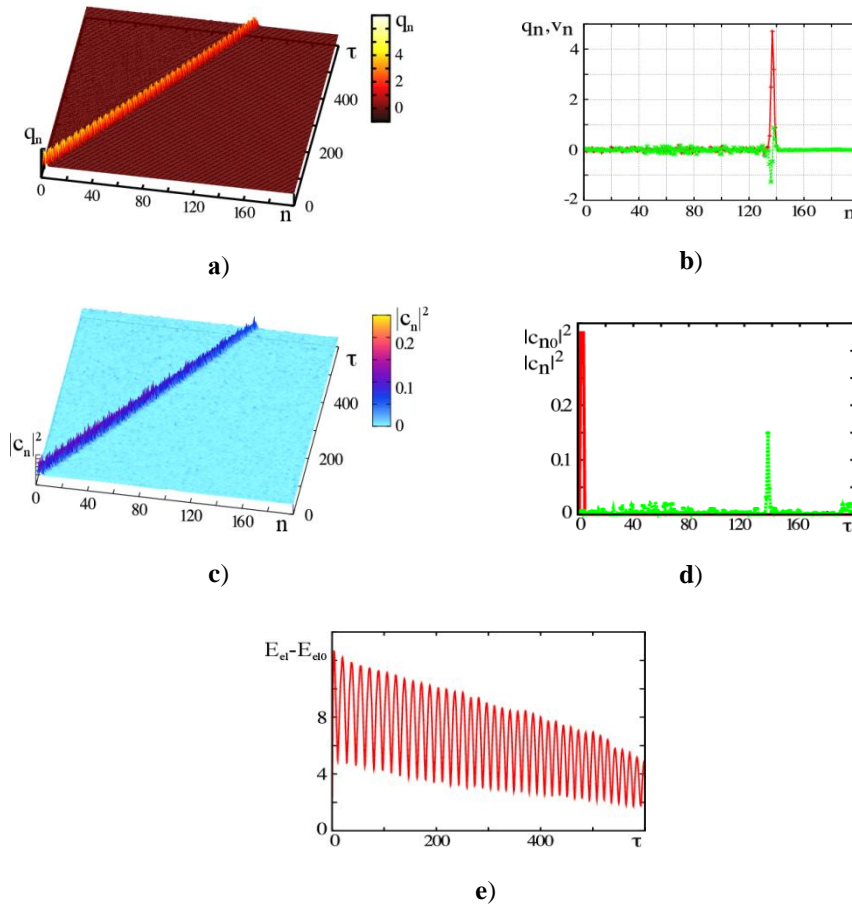


Fig. 2. Mobile breather in the DNA with fixed ends at $v_{20} = 4$, $v_{30} = 2$, $v_{20} = 1$, $q_{n0} = 0$. **a)** and **b)** – evolution of coordinates $q_n(\tau)$ distribution and probability of electron presence $|c_n|^2$ at the site with number n , respectively **c)** distributions of particles displacement from the equilibrium position q_n (red) and of speeds v_n (green) at the last moment of the simulation $\tau_k = 600$, **d)** distribution of probability $|c_n|^2$ at initial, $\tau_k = 0$ (red) and final, $\tau_k = 600$ (green) moments of time, **e)** dependence from electron energy time relatively its initial value $E_{el}(\tau) - E_{el}(0)$. $\omega_{\text{bond}} = 0.4$, $\tau_e = -18$, $\chi_h \approx 0.5$, $\chi_{el} \approx 8.5$, $\rho = 0.5$, $\alpha = 0.08$, $\Gamma = 0.001$, $N = 50$, $\tau_k = 200$.

In this example the energy «pumped» into the chain is rather large. But if it is decreased, while the profile of the initial speed distribution in the cluster from three first non-fixed particles is maintained, according to the determined empiric equation:

$$v_m = A(0.5m^2 - 4.5m + 11), m = 2, 3, 4,$$

where the amplitude factor A determines the level of initial energy $T_{\text{kin}} = (v_2^2 + v_3^2 + v_4^2)/2$, it may be concluded that the breather becomes excited at values of A , variable within rather wide ranges. However, the range of parameter values, at which it can hold an electron localized initially in the region of initial excitation of the molecule, is considerably narrower: $-0.8 < A < 1.1$. This restriction to a value of the parameter A (a value of the initial excitation energy) is determined at the base of the constructed dependence of the charged quasiparticle path length for its lifetime (Fig. 3).

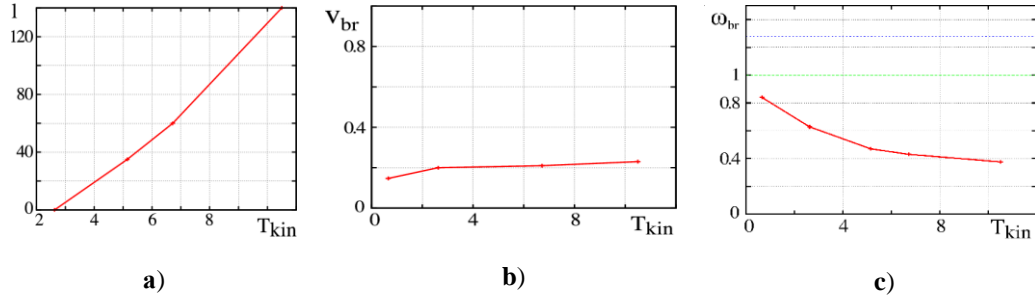


Fig. 3. Dependences from energies of initial excitation T_{kin} of the length of a quasiparticle path (a), breather speed (b) and its frequency (c) for a case presented at Figure 2.

It is clear that a path length grows almost linear with the energy growth (Fig. 2,a), a breather speed is almost constant (Fig. 2,b), and oscillation frequency, remaining lower than a critical speed, falls more than twice (Fig. 2,c) within an analyzed energy range.

3. ELECTRON TRANSPORT WITH MOBILE BREATHERS EXCITED BY THE INITIAL NUCLEOTIDE DISPLACEMENTS

Breathers formed by the initial displacements of particles and initial perturbations of their speeds have similar characteristics when energies of initial perturbations and degree of localization are approximately the same [20]. However, characteristics of an electron interaction with these two types of breathers are considerably different, since in the first case initial energy of the electron depends only on the configuration of its wave function (formulas (11), (14) does not include speed), while in the second case it depends also on a value of the particles displacement q_n and relative positions of breather and electron. So, when we analyze an electron whose wave function is coincided with breather excited by the positive displacement of the particles, its energy is very high at the beginning (energy of the bond $|\chi_{el}| \left| \sum_n q_n |c_n|^2 \right|$ is added to its own energy $2|\tau_e| \left| \sum_n \text{Re}(c_n c_{n-1}^*) \right|$). During the trapping, the energy jumps down and then oscillates for a long time with a frequency of the breather and a weak decrease in average level (Fig. 4,c), because the breather structure in such a case can reliably hold even such a high energy electron; this is shown by the data of numerical simulation (Fig. 4). Hence, a lifetime of such a quasiparticle is large and a length of its path up to destroy is large also (up to ~ 200 inter-base distances corresponding to approximately 60 nm, Fig. 4,a and 4,b).

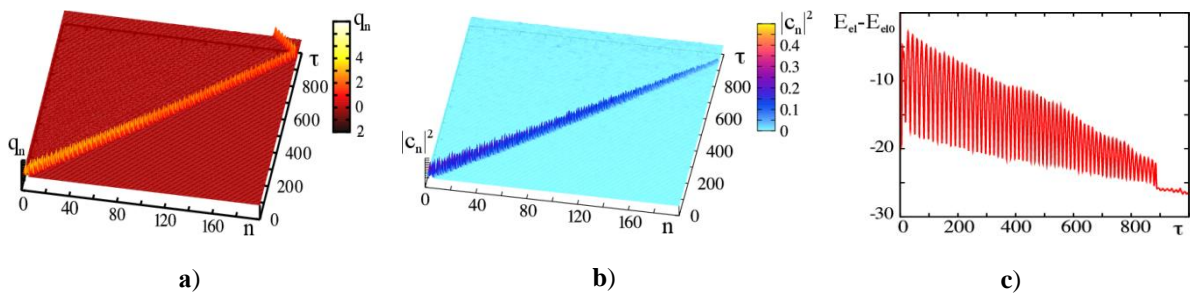


Fig. 4. Mobile breather in the DNA with fixed ends at $q_{20} = q_{30} = 7$, $v_{n0}=0$. **a)** and **b)** – evolution of coordinates $q_n(\tau)$ distribution and probability of electron presence $|c_n|^2$ at the site with number n , respectively, **c)** dependence from electron energy time relatively its initial value $E_{el}(\tau) - E_{el}(0)$. $\omega_{bond} = 0.4$, $\tau_e = -18$, $\chi_h \approx 0.5$, $\chi_{el} \approx 8.5$, $\rho = 0.5$, $\alpha = 0.08$, $\Gamma = 0.001$, $N = 200$, $\tau_k = 1000$.

Of course, with the decrease in the energy of the initial excitation, path length of this high energy quasiparticle falls, nevertheless, it remains rather large, even at moderate values of energy.

At excitation of the breather at the expenses of a molecule «compression» ($q_n < 0$), a bond energy $|\chi_{el}| \left| \sum_n q_n |c_n|^2 \right|$ is deduced from the own energy and, seemingly, a stable quasiparticle should be established. However, let us note that a quasiparticle with high energy electron may be basically instable (metastable), because an electron always streams to the stable polaron state, whose perturbation structure does not correspond to the breather structure. But a process of its transformation into a polaron state can take a long time, and just this time sets lifetime for a metastable quasiparticle and path length. One more determining factor is a level of initial electron energy. In the case analyzed above, at positive initial displacements, it is large and lifetime of a quasiparticle is also large. The same time, at negative initial displacements, it is small and lifetime should be short as was demonstrated by the results of a numeric simulation. At the negative initial displacements ($q_{20} = q_{30} = -1.5$, $v_{n0} = 0$, Fig. 5), giving approximately the same level of energy than in the case analyzed above (Fig. 4), characteristics of the transportation are much worse than at the positive displacements.

They correspond to the characteristics of quasiparticles formed by a breather excited by negative perturbations of energy with the same level of energy (confer Fig. 1 and Fig. 5): electron is trapped with a mobile breather in the same manner, but further it is delocalized at a distance of approximately thirty inter-base distances, an electron energy, the same, first becomes higher than an initial energy level, and then fluctuates, decreasing at an average rate much higher than has an electron in a quasiparticle established by breathers excited by speed of positive perturbations (Fig. 2) or of coordinate (Fig. 4).

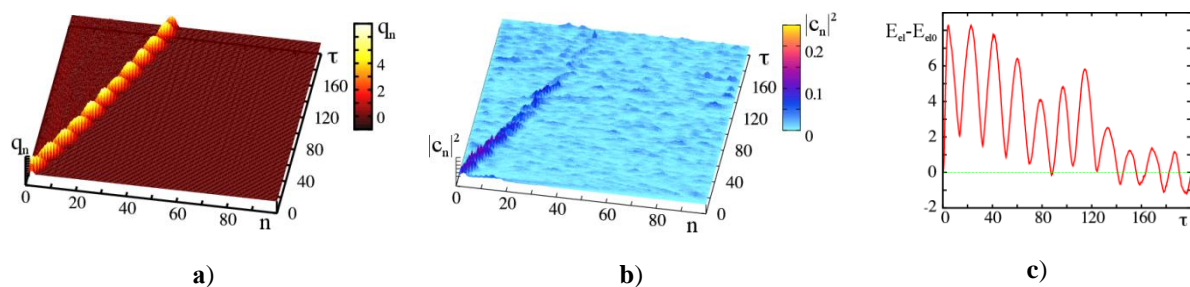


Fig. 5. Mobile breather in the DNA with fixed ends at $q_{20} = q_{30} = -1.4$, $v_{n0}=0$. **a)** and **b)** – evolution of coordinates distribution $q_n(\tau)$ and of probability of electron presence $|c_n|^2$ at the site with number n , respectively **c)** dependence from electron energy time relatively its initial value $E_{el}(\tau) - E_{el}(0)$. $\omega_{bond} = 0.4$, $\tau_e = -18$, $\chi_h \approx 0.5$, $\chi_{el} \approx 8.5$, $\rho = 0.5$, $\alpha = 0.08$, $\Gamma = 0.001$, $N = 100$, $\tau_k = 200$.

Here the logical question comes: on the transportation of a low energy electron. The question is based on the assumption that providing of an initial state of an a low energy electron (with $\Delta\phi = \pi$) gives a possibility to decrease a trap energy. However such a hypothesis is incorrect, because at reasonable values of parameters such an electron cannot be trapped at all. To clarify details of dynamics of electron-chain interactions in various conditions, we made a series of calculations for various values of $\Delta\phi$, within a range $\Delta\phi = 0 - \pi$. The results showed that at fixed values of the other parameters (for example, corresponding to the data presented at Fig. 4), characteristics of breather-electron interaction worsen with the $\Delta\phi$ growth from the zero value. Specifically, for $\Delta\phi = 2$ in the middle of the range, trapping can be observed yet, though with characteristics of transportation worse than at $\Delta\phi = 0$ (Fig. 6), while at $\Delta\phi = 2.5$ it is impossible. It looks like an ineffective trapping could be caused by out-of-phase oscillations of an electron motion and a chain, though this idea requires further examination.

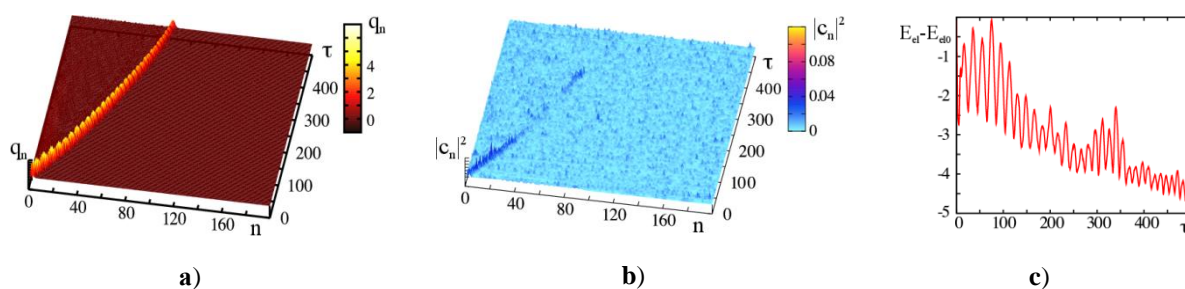


Fig. 6. Mobile breather in the DNA with fixed ends at $q_{20} = q_{30} = 7$, $v_{n0} = 0$, $\Delta\varphi = 2$. **a)** and **b)** – evolution of coordinates distribution $q_n(\tau)$ and probability of electron presence $|c_n|^2$ at the site with number n , respectively, **c)** dependence from electron energy time relatively its initial value $E_{el}(\tau) - E_{el}(0)$. $\omega_{\text{bond}} = 0.4$, $\tau_e = -18$, $\chi_h \approx 0.5$, $\chi_{el} \approx 8.5$, $\rho = 0.5$, $\alpha = 0.08$, $\Gamma = 0.001$, $N = 200$, $\tau_k = 500$.

Nevertheless, it is obvious that the revealed shape of an initial excitation, or displacements, or speed is not the exclusive version. For example, an initial perturbation of speed and displacements may be set in a form close to the form of an established breather from the preceding computer simulations. However, realization of such an initial perturbation in a real system seems a much greater problem in relation to the above described way of excitation of coordinates or of speed of only two or three particles.

CONCLUSION

A computer experiment within the frames of a Peyrard–Bishop–Dauxois–Holstein model demonstrated that mobile discrete breathers excited near one of the fixed ends of a DNA molecule due to a displacement of small nucleotide group from the equilibrium position or perturbation of their speed can trap a highly energetic electron located at the same region. The formed quasiparticle is metastable, however, it can possess high lifetime and move along the molecule at a distance of up to 200 inter-pair distances, i.e., 60–70 nm. The last condition occurs in a case, when the breathers are excited with the perturbations coming from the axis region. A particle lifetime depends strongly on the signs of the interaction parameters, the breather energy, the electron energy, and initial breather – electron collocation; therefore, determination of the laws of interactions between a DNA molecular chain and an electron is, formally, a subject of an optimization problem to be solved later. The described method of an electron transport does not require application of an external electrical field or any effects at the DNA molecule, and it is an alternative to the polaronic mechanism of the charged particles transport in the DNA.

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REFERENCES

1. Shigaev A.S., Ponomarev O.A., Lakhno V.D. *Mathematical Biology and Bioinformatics*. 2013. V. 8. No. 2. P. 553–664 (in Russ.) doi: [10.17537/2013.8.553](https://doi.org/10.17537/2013.8.553)
2. Lakhno V.D. *Int. Quant. Chem.* 2008. V. 108. P. 1970.
3. *Nanobioelectronics – for Electronics, Biology and Medicine*. Edit. by Offenhausser A., Rinaldi R. New York: Springer, 2009. 337 p.
4. Lakhno V.D., Sultanov V.B. *Int. J. Quant. Chem.* 2008. V. 108. P. 1913.
5. Lakhno V.D. *J. Biol. Phys.* 2000. V. 26. P. 133.
6. Fialko N.S., Lakhno V.D. *Phys. Lett. A*. 2000. V. 278. P. 108.
7. Conwell E.M., Rakhmanova S.V. *PNAS*. 2000. V. 97. P. 4556.

8. Lakhno V.D., Korshunova A.N. *Mathematical Biology and Bioinformatics*. 2010. V. 5. P. 1. doi: [10.17537/2010.5.1](https://doi.org/10.17537/2010.5.1)
9. Lakhno V.D., Fialko N.S. *Glass. Phys. & Chemistry*. 2011. V. 37. P. 51.
10. Lakhno V.D., Fialko N.S. *Russian J. Phys. Chem. A*. 2012. V. 86. P. 832.
11. Lakhno V.D., Chetverikov A.P. *Mathematical Biology and Bioinformatics*. 2014. V. 9. No. 1. P. 4–19 (in Russ.). doi: [10.17537/2014.9.4](https://doi.org/10.17537/2014.9.4)
12. Chetverikov A.P., Ebeling W., Lakhno V.D., Shigaev A.S., Velarde M.G. *Eur. Phys. J. B*. 2016. V. 89. P. 101. doi: [10.1140/epjb/e2016-60949-1](https://doi.org/10.1140/epjb/e2016-60949-1)
13. Velarde M.G., Chetverikov A.P., Ebeling W., Dmitriev S.V., Lakhno V.D. *Eur. Phys. J. B*. 2016. V. 89. P. 233. doi: [10.1140/epjb/e2016-70489-3](https://doi.org/10.1140/epjb/e2016-70489-3)
14. Yakushevich L.I. *Nonlinear Physics of DNA*. Weinheim: Wiley-VCH Verlag GmbH & Co. KGaA, 2005. (Wiley Series in Nonlinear Science).
15. Cheng D., Aubry S., Tsironis G.P. *PRB*. 1996. V. 77. P. 4776.
16. Aubry S., Cretegny T. *Physica D: Nonlinear Phenomena*. 1998. V. 119. № 1. P. 34.
17. Cuevas J., Starikov E.B., Archilla J.F.R., Hennig D. *Mod. Phys. Lett. B*. 2011. doi: [10.1142/S0217984904007840](https://doi.org/10.1142/S0217984904007840)
18. Fakhretdinov M.I., Zakiryanov F.K. *ZhTF*. 2013. V. 83. P. 1–5 (in Russ.).
19. Dauxois T., Peyrard M., Bishop A.R. *Phys. Rev. E*. 1993. V. 47. P. 2755–2758.
20. Chetverikov A.P., Sergeev K.S., Lakhno V.D. *Mathematical Biology and Bioinformatics*. 2017. V. 12. No. 2. P. 375–384 (in Russ.). doi: [10.17537/2017.12.375](https://doi.org/10.17537/2017.12.375)
21. Chetverikov A.P., Ebeling W., Velarde M.G. *Eur. Phys. J. B*. 2006. V. 51. P. 87–99.
22. Holstein T. *Ann. Phys.* 1959. V. 8. P. 343.
23. Li G., Govind N., Ratner M.A., Cramer C.J., Gagliardi L. *J. of Physical Chemistry Letters*. 2015. V. 6. P. 4889–4897.
24. Yoo-Konga S., Liewriana W. *Eur. Phys. J. E*. 2015. P. 1–14.
25. Xiang L., Palma J.L., Bruot C., Mujica V., Ratner M.A., Tao N. *Nature Chemistry*. 2015. P. 221–226. doi: [10.1038/nchem.2183](https://doi.org/10.1038/nchem.2183)
26. Zhang Y., Zhu W.-H., Ding G.-H., Dong B., Wang X.F. *Nanotechnology*. 2015. P. 1–14.
27. De Moura F.A.B.F., Lyra M.L., de Almeida M.L., Ourique G.S., Fulco U.L., Albuquerque E.L. *Physics Letters A*. 2016. V. 380. No. 42. P. 3559–3563.
28. Artes J.M., Li Y., Qi J., Anantram M.P., Hihath J. *Nature Communications*. 2015. P. 1–8. doi: [10.1038/ncomms9870](https://doi.org/10.1038/ncomms9870)
29. Xiang L., Palma J.L., Li Y., Mujica V., Ratner M.A., Tao N. *Nature Communications*. 2017. P. 1–10. doi: [10.1038/ncomms14471](https://doi.org/10.1038/ncomms14471)
30. Wolter M., Elstner M., Kubar T. *Chem. Phys.* 2013. V. 139. P. 125102. doi: [10.1063/1.4821594](https://doi.org/10.1063/1.4821594)
31. Behnia S., Fathizadeh S., Akhshani A. *J. Phys. Chem. C*. 2016. V. 120. P. 2973–2983.
32. De Almeida M.L., Ourique G.S., Fulco U.L., Albuquerque E.L., de Moura F.A.B.F., Lyra M.L. *Chemical Physics*. 2016. P. 1–10. doi: [10.1016/j.chemphys.2016.05.020](https://doi.org/10.1016/j.chemphys.2016.05.020)
33. Gu L., Fu H.H. *New J. Phys.* 2016. V. 18. P. 053032.
34. Li Y., Artés J.M., Qi J., Morelan I.A., Feldstein P., Anantram M.P., Hihath J. *J. Phys. Chem. Lett.* 2016. V. 7. Iss. 10. P. 1888–1894. doi: [10.1021/acs.jpcllett.6b00749](https://doi.org/10.1021/acs.jpcllett.6b00749)
35. Zhu X., Liu S., Cao J., Mao X., Li G. *Scientific Reports*. 2016. P. 1–9. doi: [10.1038/srep19515](https://doi.org/10.1038/srep19515)
36. Liu C., Xiang L., Zhang Y., Zhang P., Beratan D.N., Y. Li, Tao N. *Nature Chemistry*. 2016. V. 8. P. 941–945. doi: [10.1038/NCHEM.2545](https://doi.org/10.1038/NCHEM.2545)
37. Arnold A.R., Grodick M.A., Barton J.K. *Cell Chemical Biology*. 2016. V. 23. P. 183–197. doi: [10.1016/j.chembiol.2015.11.010](https://doi.org/10.1016/j.chembiol.2015.11.010)
38. Shigaev A.S., Ponomarev O.A., Lakhno V.D. *Chemical Physics Letters*. 2011. V. 513. P. 276–279.

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