Discrete-breather-assisted charge transport along DNA-like molecular wires

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Mobile discrete breathers (MDBs) are here suggested as localized excitations underlying the trapping and transport of charged particles (electron or hole) along a DNA-like molecular wire with anchored ends such as attached to two electrodes. For illustration the Peyrard-Bishop-Dauxois-Holstein (PBDH) model is used. MDBs are excited by imposing appropriate disturbances to velocities or space positions of adjacent nucleotide pairs or lattice units of the wire. They can be directed either towards or away from the wire hence transverse to it. Numerical computer simulations show that a rather stable quasiparticle MDB + electron is possible when just a few of the nucleotide pairs near one of the fixed ends of the wire are excited. For the process to be effective, the charge, e.g., the electron, must be initially placed around the disturbed region of the molecule. Once the MDB + electron quasiparticle is formed it may be transported to quite a long distance up to ca. 60–70 nm in real space. Our findings show that such process does not demand intervention of an externally applied electric field and hence it may be considered as alternative to the polaron transport process.

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I. INTRODUCTION

It is customary to assume polaron transport when, say, an excess electron is injected into a crystal and there is an applied external electric field [1–15]. A similar approach has been used to account for possible charge transport in DNA and the like [16–31]. Indeed, it has been advocated that a DNA-like molecule can be used as a basic element for a molecular wire in nanobioelectronics [32–35]. However, polaron transport is not the only possible way to transfer charges along, say, molecular wires. This was made clear in the case of conducting polymers (aka synthetic metals) and other systems [22,23,27,36–54]. In particular, it has been proposed a field-free charge transport process based upon the genuine nonlinear dynamics of the crystal lattice with results applicable to, e.g., DNA-like molecular wires [55,56]. We know that in one-dimensional crystal lattices of units-oscillators of appropriate dynamics, the nonlinearity of the on-site potential along with the nonlinearity of intersite interaction combined with the dispersion resulting from the lattice discreteness fosters localization of deformation excitations in the form of solitons or discrete breathers (DB aka intrinsic localized modes). Even more, localized modes, may occur either in the absence of on-site dynamics or in the absence of nonlinear intersite dynamics (albeit with harmonic ones) [57,58]. For example, it has been shown that in a chain where «angular» disturbances can be created and where on-site potentials are absent there is chance for the formation of lattice solitons [59,60]. For DNA-based and the like molecular wires, a charge is expected to be transported by profiting of suitable perturbations of the radii of base pairs, even when the nucleotides play identical symmetric motions about an equilibrium point created by a strong enough on-site potential. Discrete breathers [54,57,58,61–65] are nonlinear localized excitations fitting these conditions and, indeed, in DNA-like molecular wires have been shown forming bound states DB electron as polaro-breathers [21–31,39,54,57,58,61–69]. Note that the latter, based on the polaron effect, comes from the lattice disturbing action of the added, excess electron to the wire as first discussed by Landau and Pekar [1–6]. In modern parlance we say that the nonlinear interaction of the electron-phonon interaction defines the Landau quasiparticle as charge carrier. Another case is that of a heated wire when thermally excited DB may also trap electrons. In such a case transport may be hindered as too many lattice excitations can be created with the electron wandering from one to another of them thus leading to a kind of diffusion process demanding, needed less to say, the action of an external electric field to provide definite motion of the electron along the wire. Yet another attractive idea is to externally excite a mobile DB (MDB) or a lattice soliton by an appropriate action, on position or momentum or in both, on units of the molecular wire. In DNA-like wires this could allow a group of adjacent nucleotides to be able to capture, bind and transport electrons along them. The process may lead to a steady or a long transient quasiparticle with a lifetime long enough to produce the transport of the electron from one site to another given acceptor site far away from the former [61–74].

In this paper we study the interaction of an electron with a MDB, excited in a small group of neighboring base pairs near one of fixed ends of the molecular wire due to initial nucleotide displacements or perturbations of their velocity. In Sec. II we introduce the model we consider. It builds upon a Peyrard-Bishop-Dauxois-Holstein model (PBDH) assuming there are only

changes of base pair/unit radii and no angular displacements [10,70] (see also Refs. [16,17,32,55,56,71–73]). In our computer experiments we vary the number of excited units, their location, excitation energy, and initial shape of electron wave function to determine conditions for the formation of stable (multistable) charged quasiparticles that is mobile breather plus trapped electron. As a breather can be excited by perturbations of transverse velocity or momentum or by transverse displacements of positions of equilibrium interbase distances (thus changing the transverse position of units, in the Watson-Crick-like pairs) we examine effects of the displacements from the wire axis independently from the displacements in the reverse direction (towards its axis). Section III is devoted to the case when disturbances are imposed on velocities of units while in Sec. IV the excitation is produced by their space displacements. In Sec. V an illustration is provided about the role of temperature upon excitation of MDB and subsequent trapping and transport processes. Finally, in Sec. VI a few remarks are provided supporting the relevance that the proposed MDB-assisted charge transport offers to molecular electronics.

II. PEYRARD-BISHOP-DAUXOIS-HOLSTEIN (PBDH) MODEL-MOLECULAR WIRE

The building blocks of our extension of the Peyrard-Bishop-Dauxois-Holstein (PBDH) model are the Peyrard-Bishop-Dauxois Hamiltonian [67,71] (describing crystal lattice classical dynamics) and the Holstein Hamiltonian [10] (accounting for electron quantum dynamics). To be specific the bond between nucleotides (all of them are taken identical) in each base pair is described by the anharmonic Morse potential

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

and the stacking interaction between neighboring base pairs is

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

D, σ, K, ρ, and α are all taken real and positive, and the variables y_n denote positive or negative displacements of the nth base pair from its equilibrium positions.

Then our DNA-like molecular wire Hamiltonian is

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

where M is the nucleotide mass, w_n, v_n, displacements of two bases in the nth pair from an equilibrium position, a dot over a quantity denotes time derivative, and corresponding values include velocity of nucleotides in the nth base pair, α_n is the charge energy at the nth site, ν_{nm} are coefficients of hopping and/or jumping integrals, χ characterizes the bond between an external charge and the wire.

For convenience we introduce the compound variables

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

and we consider symmetrical motions ($v_n \approx -w_n$). As the electron obeys the discrete Schrödinger equation on the lattice its wave function is sought in the form

$$|\Psi\rangle = \sum_n c_n(t)\,|n\rangle. \tag{5}$$

In view of the above, the nucleotide motions obey the combined evolution equations

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

$$i\hbar\frac{dc_n}{dt} - \alpha_n c_n + \sum_m \nu_{nm}c_m = -\sqrt{2}\cdot\chi y_n c_n. \tag{7}$$

Further, for a homogenous molecule we set ($\alpha_n \equiv 0$) and reduce (7) to

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

which defines c_n. We shall be using values of the parameters ν and χ obtained from comparison with experiment for small displacements y_n, when the harmonic approximation is applicable, and the PBDH model reduces to just the Holstein dynamics [10,75]. When ν and χ are both positive we have the so-called minimal nonlinear model DNA [29,56,76], and the evolution equations reduce to

$$\ddot{q}_n + \Gamma\dot{q}_n = e^{-q_n}(e^{-q_n} - 1) + \omega_{\text{bond}}^2(q_{n+1} - 2q_n + q_{n-1}) + \rho f_n(y_{n-1,n,n+1}) + \chi_{\text{h}}|c_n|^2 \tag{9}$$

$$\dot{c}_n = i\tau_e(c_{n+1} + c_{n-1}) + i\chi_{\text{el}}q_n c_n, \tag{10}$$

together with the expression for the electron energy (in $\hbar\omega_M$ units) [56]:

$$E_{\text{el}} = -\tau_e\sum_n\left(c_n^*(c_{n-1} + c_{n+1})\right) - \chi_{\text{el}}\sum_n q_n|c_n|^2, \tag{11}$$

and, needless to say, the probability density normalization requirement:

$$\sum_{n=1}^N |c_n|^2 = 1. \tag{12}$$

In the Eqs. (9)–(12) $q_n = \sigma y_n$ denote the dimensionless displacement of the nth nucleotide from its equilibrium position. Now dots above quantities denote derivative with respect to the dimensionless time $\tau = \omega_{\text{M}}t$, thus providing a numerical velocity. The quantity $\omega_{\text{M}} = (2D\sigma^2/M)^{1/2}$ describes the frequency of linear oscillations in the Morse potential well and $\omega_{\text{bond}} = (K/M)^{1/2}/\omega_{\text{M}}$ is the dimensionless frequency of small linear nucleotide oscillations. The groups

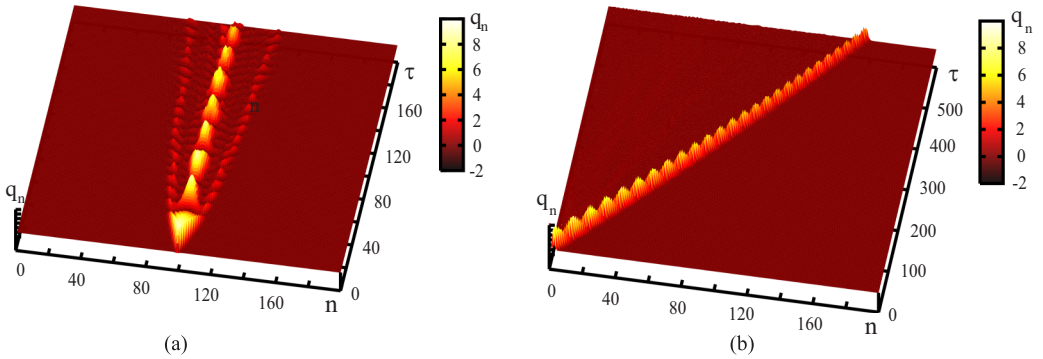

FIG. 1. DNA-like molecular wire with anchored ends ($N = 200$ nucleotides/units). Excitation of pinned and mobile discrete breathers depicted by the evolution of displacements of particles $q_n(\tau)$. (a) Excitation by momentum or velocity kicks, directed towards the axis of the wire, for two adjacent particles located far from ends, $v_{99}(0) = v_{100}(0) = -4$, all other $v_n(0) = 0$, and all $q_n(0) = 0$. (b) The same when excitation is realized near a fixed end, $v_2(0) = v_3(0) = -4$, all other $v_n(0) = 0$, $q_n(0) = 0$. The actual compression of the molecule is about $q_{\min}/R_0 (q_{\min} < 0)$ which does not exceed 4.5% and its expansion $q_{\max}/R_0$ does not exceed 18%. Here $q_{\min}$ and $q_{\max}$ are the respective minimal and maximal deviations of particles from their equilibrium positions.

$\chi_h = \sqrt{2}\chi/2\sigma D$ and $\chi_{\rm el} = \sqrt{2}\chi/\hbar\omega_{\rm M}\sigma = \chi_h(2D/\hbar\omega_{\rm M})$ define parameters accounting for the interaction between the electron and the lattice. $\tau_e = \nu/\hbar\omega_{\rm M}$ is the ratio between typical times of evolution of the electron wave function and that of the lattice dynamics. Finally, the function f_n describes the nonlinearity of the interaction force [55,56]:

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

The coefficient α is now also rescaled ($\alpha \to \alpha/\sigma$) due to introduction of the dimensionless displacement q. Γ is a friction coefficient included into equations to account for various possible losses of energy when units are in motion.

From (11) it follows that, when $\chi = 0$, the electron has zero energy being localized at one single site, while when being localized in a cluster of k sites with, in particular, uniform distribution of probability density $|c_n|^2$ in the cluster, it has the energy:

$$E_{\rm el} = -2\tau_e \frac{k-1}{k} \sum_n \cos(\varphi_n - \varphi_{n-1}). \quad (14)$$

Note that the sign of (14) depends on the distribution of phases φ_n of the components $c_n = |c_n|\exp(i\varphi_n)$. Hence, there is minimal electron energy when all phases φ_n coincide,

$$E_{\rm el} = -2\tau_e \frac{k-1}{k} \to -2\tau_e|_{k\gg 1}, \quad (15)$$

whereas there is maximal electron energy $2\tau_e$, when $\varphi_n = \varphi_{n-1} \pm \pi$, and also $E_{\rm el} \to 0$ if phases of the wave-function components are distributed chaotically.

For a localized distribution (small k) the value of electron energy is between these critical values evolving in time to a distributed state. However, the energy of a localized state may be less than $-2\tau_e$ if the electron interacts with a localized excitation in a lattice for which the second term in Eq. (11) is larger than the first one as we shall see below.

With a suitable choice of initial states and boundary conditions for an anchored molecular wire ($q_{1,N} = v_{1,N} = 0$), the Eqs. (9)–(10) have been numerically integrated using a fourth-order Runge-Kutta method. This permits determination of displacements (of coordinates) $q_n(\tau)$, velocities $v_n(\tau)$, and (probability density) wave function components $c_n(\tau)$. For

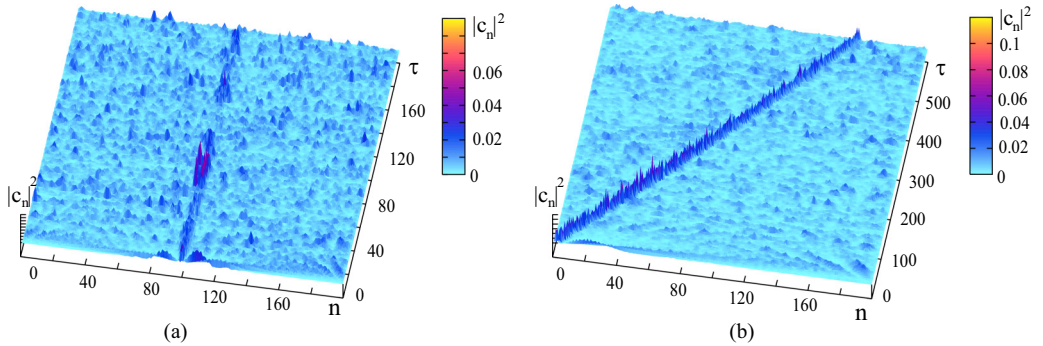

FIG. 2. DNA-like molecular wire with anchored ends ($N = 200$ nucleotides/units). Evolution of electron probability densities $|c_n(\tau)|^2$ when simultaneously there is breather excitation: left panel corresponds to the case of Fig. 1(a) and right panel to that of Fig. 1(b), respectively. $\omega_{\rm bond} = 0.4$, $\tau_e = 18$, $\chi_h \approx -0.5$, $\chi_{\rm el} \approx -6$, $\rho = 0.5$, $\alpha = 0.08$, $\Gamma = 0.001$.

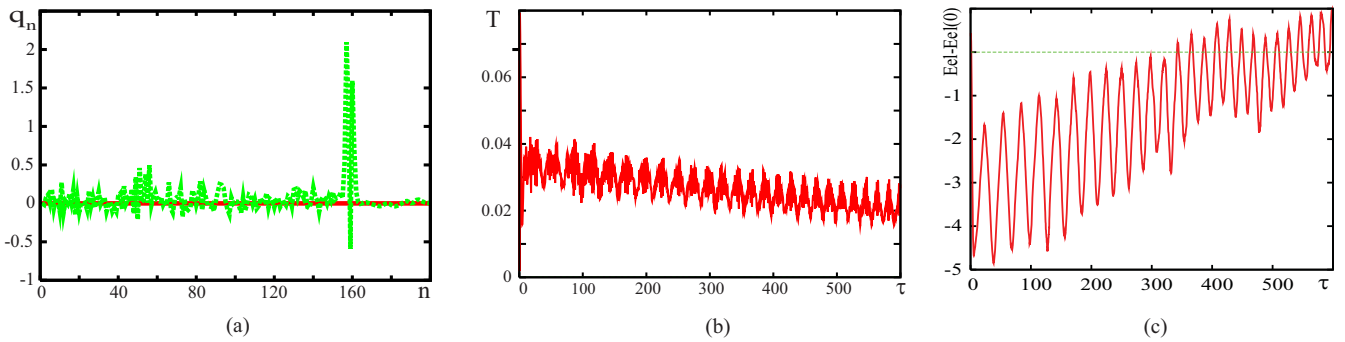

FIG. 3. DNA-like molecular wire with anchored ends ($N = 200$ nucleotides/units). For the case presented in Figs. 1(b) and 2(b): (a) unit displacements q_n at time instant $\tau = 600$, (b) kinetic energy of particles in time $T(\tau)$, averaged over N sites, and (c) energy of the electron relative to its initial value, $E_{el}(\tau)$–$E_{el}(0)$.

illustration, we use in simulations a set of dimensionless parameters, which provide efficient conditions for the phenomena studied $\omega_M \approx 7.1 \times 10^{12}\,c^{-1}$, $\tau_e = v/\hbar\omega_M \approx 18$, $\chi_h \approx 0.5$, $\chi_{el} \approx 6$, $\omega_{bond} \approx 0.4$, and a dimensionless radius of the unperturbed molecule $R_0 = 44.5$. In dimensional units they correspond to the physical parameters in the range of those considered in, e.g., [56,71,72,77,78]: $D = 0.03\,eV$, $\sigma = 4.45\,Å^{-1}$, $m = 210\,Dalton$, $\chi = 0.13\,eV/A$, $v = 0.084\,eV$, and the stiffness of stacking interaction equal to 0.17 eV/Å. As time unit we use $\Delta t = 1/\omega_M = 0.14 \times 10^{-12}\,s$, as length unit for the measurement of lateral displacements $\Delta y = \sigma^{-1} = 2.2 \times 10^{-11}\,m$ and as velocity unit of the motion of the nucleotides $\Delta y/\Delta t \approx 161\,m/s$. The velocity of the breather and the charged quasiparticle displacement along the wire's 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 the numerical velocity is measured by amounts Δn of interbase distances, passed in the numerical time interval τ (on the hypothesis that the motion is uniform).$\alpha = 0.35\,(Å)^{-1}$ (as numerical 0.08) and friction coefficient 0.001.

Now our aim is the determination and analysis of conditions for the creation of a MDB due to initial perturbation of velocities or space coordinates of nucleotides in several neighboring pairs of the DNA molecular wire, and the eventual trapping and transport of an electron with energy close to the upper bound of the conductivity band.

III. EXCITATION OF DISCRETE BREATHERS BY PERTURBING THE VELOCITY OF A FEW UNITS IN THE WIRE AND ELECTRON TRAPPING CONSEQUENCES

Figure 1 illustrates the results of appropriately identically disturbing the velocity of two nucleotides. Figure 1(a) corresponds to the case of a pinned DB while Fig. 1(b) is that of a MDB. As the imposed velocity disturbances are the same, the drastically different consequences prove the relevance of the choice of their location. Now we inject the excess electron nearby the same locations where those breathers are being excited. Figure 2 depicts the time evolution of the electron probability densities $|c_n|^2$ along the molecular wire when the electron is initially placed distributed at eight sites: $c^2_{n0} = 1/8$, $\Delta\varphi_0 = 0$, $n = 96$–103 for Fig. 1(a), and $n = 5$–12 for Fig 1(b).

As expected there is electron trapping in both cases as a consequence of the dominant role played by the nonlinear lattice excitation (recall initial disturbance only on velocities of the two units). Also as expected the compound DB + electron remains pinned in the first case whereas it is a moving quasiparticle in the second case. The latter, indeed, provides charge transport for over 150 units along the molecular wire. Figure 3(a) shows that the MDB keeps its form for very long time leaving the lattice only weakly disturbed behind it. Its energy decays albeit slowly as seen in Fig. 3(b). We also observe that the amplitudes of units' oscillations involved in the quasiparticle decrease as well. The energy of the electron

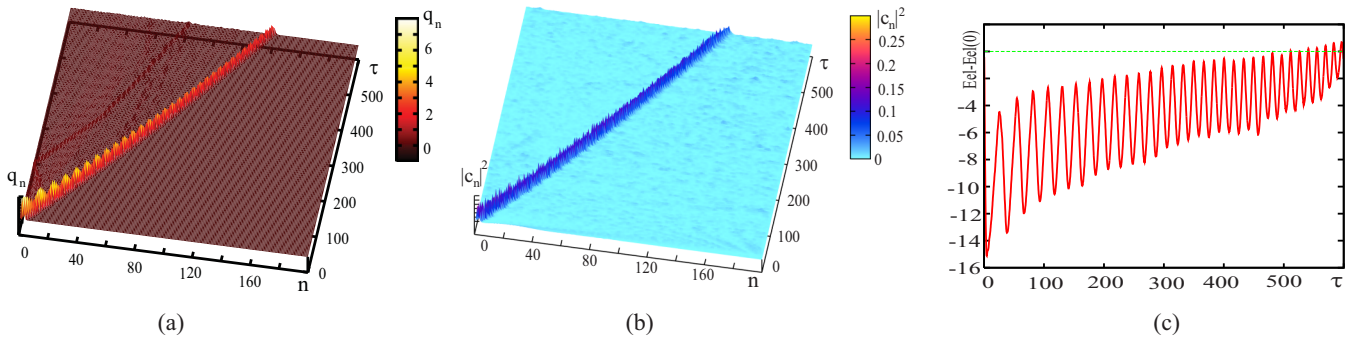

FIG. 4. DNA-like molecular wire with anchored ends ($N = 200$ nucleotides/units). The same as in Figs. 1–3 but for positive initial disturbance of velocity of two units: $v_2(0) = v_3(0) = 3.5$, all other $v_n(0) = 0$, $q_n(0) = 0$ for all n. (a) unit displacements $q_n(\tau)$, (b) electron probability densities $|c_n|^2(\tau)$, and (c) $E_{el}(\tau)$–$E_{el}(0)$.

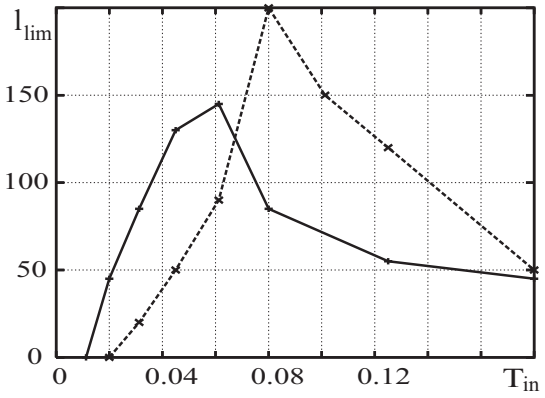

FIG. 5. DNA-like molecular wire with anchored ends ($N = 200$ nucleotides/units). Electron path length, $l_{\rm lim}$, against kinetic energy of initial excitation by external kicks for two particles, directed away from the axis (left curve, $v_n(0) > 0$) and towards the axis [right curve, $v_n(0) < 0$] with parameter values corresponding to those of Figs. 1–4.

$E_{\rm el}(t)$ falls at first below its initial value $E_{\rm el}(0)$ due to being trapped by the breather as shown in Fig. 3(c). Subsequently, however, the energy grows in the mean because the positive displacements prevail for anharmonic oscillations of the units with the Morse on-site potential. Eventually, the electron energy oscillates, following the breather oscillations. We have also observed that the electron always tends to a polaron state, whose structure does not correspond to that of the breather. Yet such decaying process can take very long time and it must go via a stage of destruction of the breather, after the latter being unable to continue the trapping of the electron. Similar results, as those presented in Figs. 1–3, are observed for breather excitation due to positive initial disturbances at two sites [from the axis, $v_n(0) > 0$] as Fig. 4 shows.

By varying the initial velocities $v_2(0) = v_3(0)$, for both positive and negative values, we obtain the dependence of the length of the electron path $l_{\rm lim}$ on the kinetic energy of the initial excitation $T_{\rm in} = (1/N)\sum v_n(0)^2/2$ (Fig. 5). It appears that its maximum value is reached in a limited range of energy of initial excitations though the value $l_{\rm lim} > 100$ sites may be reached for quite a wide range of initial kinetic energy values. Clearly, the quasiparticle formation takes place in a limited range of initial energy for both cases with ranges of energy for negative and positive kicks close to each other. Nevertheless, the excitation by kicks directed from the axis may be considered as more effective because the electron trapping with the same path is possible at lower energies.

IV. EXCITATION OF DISCRETE BREATHERS BY LATTICE DEFORMATION CONSEQUENCE OF INITIAL DISPLACEMENTS OF A FEW UNITS IN THE WIRE AND ELECTRON TRAPPING CONSEQUENCES

Figure 6 illustrates the results of initial displacement of two particles. Noteworthy is that in the present case the characteristics of the electron interaction are slightly different from those analyzed in Sec. II. This is to be expected as now the energy of interaction of the electron with the lattice wire is a part of the energy of a bound electron treated as a quantum particle as the Hamiltonian (3) and Eqs. (11), (14) imply. This part of energy does not depend on disturbances of velocities v_n but it does depend on disturbances of positions of particles q_n. Thus, in the first case, the initial energy of a bound electron depends on the configuration of the wave function only and it is the same value, let $E_{\rm el}(0)$, as in an equilibrium chain independently of initial disturbances of velocities. However, in the last case it depends also on values of the particles' displacements q_n and relative positions of the breather and the electron. The initial energy may be higher or lower relative to $E_{\rm el}(0)$ according to whether the molecule is locally compressed [$q_n(0) < 0$] or locally stretched [$q_n(0) > 0$].

Once more, the lifetime of such a quasiparticle and the length of its path are both significantly long so much that we can safely consider this form of transport as useful for applications. Note that it covers up to about 200 interbase distances corresponding to approximately 60 nm as Figs. 6(a) and 6(b) show. During the trapping, the electron energy falls below its initial value and then oscillates for a long time with the frequency of the breather while slightly increasing in the mean because the breather structure in such a case can robustly bind the electron as depicted in Fig. 6(c).

The dependence of the maximum electron path length $l_{\rm lim}$ on the initial space disturbances $q_2(0) = q_3(0)$ is shown in Fig. 7 together with the initial potential energy (relatively minimal potential energy corresponding to the bottom of the

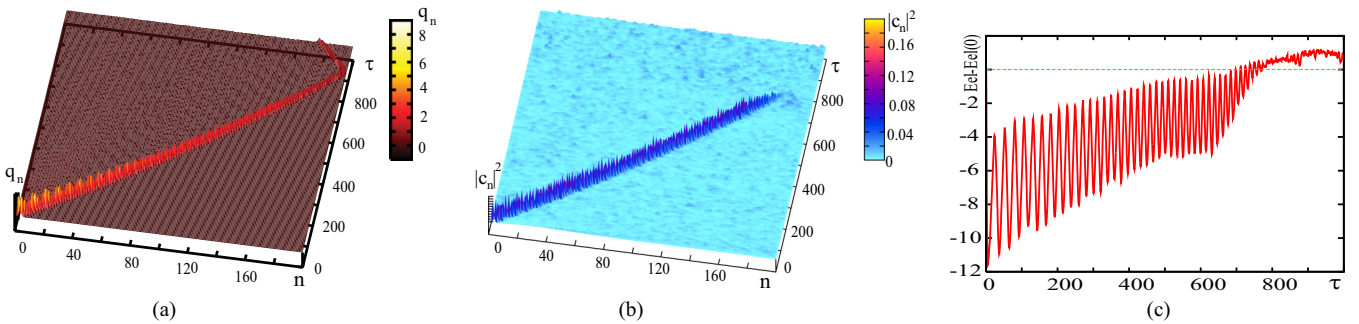

FIG. 6. DNA-like molecular wire with anchored ends ($N = 200$ nucleotides/units). The same as in Fig. 4 when the excitation of the MDB is done by displacing two adjacent particles towards the wire away from their equilibrium positions (negative values): $q_2(0) = q_3(0) = -1.4$ (all others $q_n(0) = 0$) and all $v_n(0) = 0$, $\omega_{\rm bond} = 0.4$, $\tau_e = 18$, $\chi_h \approx -0.5$, $\chi_{\rm el} \approx -6$, $\rho = 0.5$, $\alpha = 0.08$, $\Gamma = 0.001$. Similar results are obtained for positive displacement values.

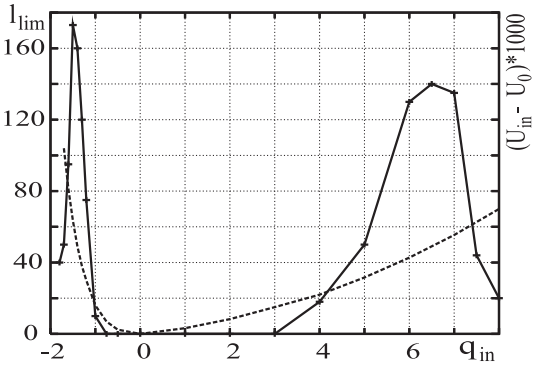

FIG. 7. DNA-like molecular wire with anchored ends ($N = 200$ nucleotides/units). Maximum electron path course, $l_{\rm lim}$ (solid line) and potential energy $(U_{\rm in}–U_0)^*10^3$ (dotted line) against initial displacements $q_{\rm in} = q_2(0) = q_3(0)$ (parameter values as in Fig. 6). The initial compression of the molecule does not exceed 4.5% and its expansion does not exceed 18%.

potential well, $U_{\rm in}–U_0$) as a function of q_{20}. It appears that such maximum length value is again about 200. Besides the trap of the electron takes place for the same range of initial energy as in the case of Sec. II corresponding to disturbances of the velocity of the units. It also appears that the initial disturbance must exceed some critical value for MDB to be formed with eventual electron trapping.

Note that the curve $l_{\rm lim}(q_{\rm in})$ looks almost symmetric relatively to its maximum for both ranges of positive $[q_2(0) = q_3(0) \approx 6.5]$ and negative $[q_2(0) = q_3(0) \approx –1.6)$ initial space displacements. Apparently, it seems better to use initial disturbances of lower energy values to reach the same value $l_{\rm lim}$. Yet the MDB velocity grows with energy as it is shown in Fig. 8.

The results presented above refer to the values $\chi_h \approx -0.5, \chi_{\rm el} \approx –6$. It seems clear, however, that the actual value of the strength of interaction of the electron with the lattice must significantly affect the feasibility of electron trapping by a MDB. For instance, it may be expected that for too

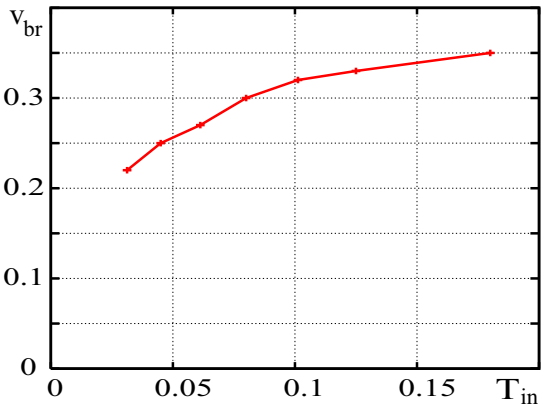

FIG. 8. DNA-like molecular wire with anchored ends ($N = 200$ nucleotides/units). Typical MDB velocity plot (in units of number of bases per dimensionless time) against the energy of the initial excitation in a molecular wire with features presented in Figs. 2 and 3.

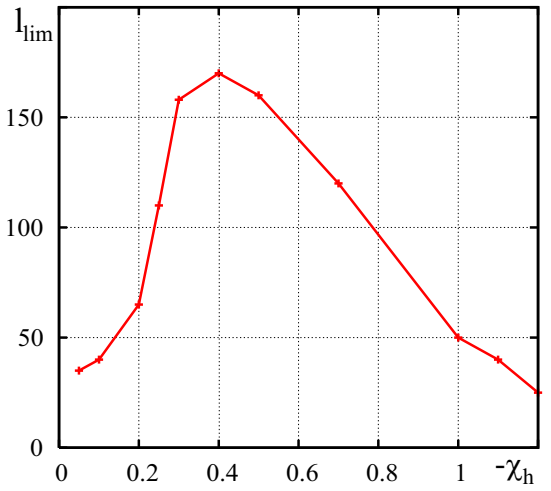

FIG. 9. DNA-like molecular wire with anchored ends ($N = 200$ nucleotides/units). Maximum electron path length, $l_{\rm lim}$ against electron-lattice interaction parameter χ_h(of negative value here). Other parameter values are as in Fig. 6, the parameter $\chi_{\rm el}$ changes as proportional to χ_h.

a small value of such parameter a mobile breather may not be able to keep an electron for a long time. At the other extreme too, a strong interaction may lead to the electron dramatically affecting the lattice so that an incipient MDB would not develop thus aborting the excitation process. In Fig. 9 the dependence of the maximum electron path length, $l_{\rm lim}$, is shown as a function of χ_h for cases corresponding, to parameter values as in Fig. 6. Clearly, on the one hand, there is an optimal value of the electron-lattice interaction parameter when the electron path length appears maximal. On the other hand, there is a wide range of values close to the optimal of χ_h(and, correspondingly, $\chi_{\rm el}$) for the survival of the MDB and the subsequent processes described above.

V. ILLUSTRATION OF THE ROLE OF TEMPERATURE UPON LOCALIZED EXCITATIONS AND SUBSEQUENT TRAPPING AND TRANSPORT PROCESSES

Finally, it seems pertinent to check the effect of temperature on the survival of MDB and the subsequent trapping and transport processes. Just, for illustration Fig. 10 depicts the evolution of electron probability densities $|c_n|^2(\tau)$ in a lattice heated up to $T \sim 200^\circ$ K. It corresponds to augmenting Eq. (9) with the Langevin dynamics a done in Eq. (16). Here D_v is noise intensity and $\xi_n(\tau)$ account for Gaussian white noise sources. Following Einstein, the ratio D_v/Γ defines the temperature of a system. We have:

$$\ddot{q}_n + \Gamma\dot{q}_n = e^{-q_n}(e^{-q_n} - 1) + \omega^2_{\rm bond}(q_{n+1} - 2q_n + q_{n-1}) + \rho f_n(y_{n-1,n,n+1}) + \sqrt{2D_v}\xi_n(\tau). \quad (16)$$

The computer experiment can be done by straightforwardly integrating the full set of equations for the lattice and the electron dynamics with their corresponding coupling or one

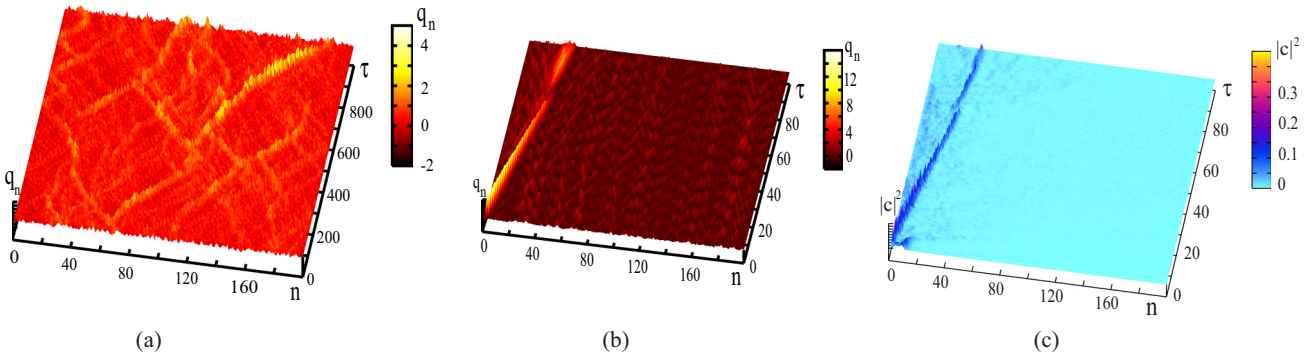

FIG. 10. DNA-like molecular wire with anchored ends ($N = 200$ nucleotides/units). Space and time evolution of lattice units and electron probability densities $|c_n(\tau)|^2$ when, simultaneously, there is MDB excitation by momentum or velocity kicks, directed towards the axis of the wire, for two adjacent particles located near the extreme left end, as in Figs. 1 and 2. Left panel: evolution of lattice units for a heated wire when the maximum of q_n does not exceed 5 and a bunch of MDB excitations are observed. Central panel: similar case when the maximum of q_n does not exceed 16 yet with a value significantly higher than the level of thermal fluctuations thus providing stability to the excitation. Right panel: for the conditions of the central panel it shows the corresponding evolution of a trapped electron illustrated by the evolution of the electron probability densities $|c_n(\tau)|^2$. Parameter values: $\omega_{\text{bond}} = 0.4$, $\tau_e = 18$, $\chi_h \approx -0.5$, $\chi_{\text{el}} \approx -6$, $\rho = 0.5$, $\alpha = 0.08$) but with $v_2(0) = v_3(0) = -5$, $\Gamma = 0.0005$, in a previously heated lattice.

step at a time. We have chosen to use the second approach. First we use Eq. (16) to heat up the lattice and then we look for the MDB and by adding the electron for the compound quasiparticle electron MDB. The parameter values are those used for Fig. 1 but, for easiness of the computations, with slightly higher values of the initial velocities, $v_2(0) = v_3(0) = -5$. It seems clear that excitation of MDB, electron trapping, and transport are feasible at such temperature. The MDB, either alone or carrying an electron, traverses the lattice weakly interacting with the latter's thermal excitations. As expected, the velocity of the electron-lattice quasiparticle compound is slightly less than the corresponding value at zero K. In a subsequent paper, we plan to fully explore the role of temperature by enlarging its range of values.

VI. CONCLUDING REMARKS

Polaron transport is not the only possible way to transfer charges along, say, molecular crystal wires. This was made clear in the case of conducting polymers, DNA-like molecular wires, and other dynamically similar systems. Further, for certain nonlinear systems it has been suggested a field-free charge transport process based upon the possibility of charge surfing on lattice solitons or mobile discrete breathers (a clear case of mechanical control of charges at the nanolevel). For modeling DNA-like molecular wires a valuable dynamical system is the mixed classical-quantum Peyrard-Bishop-Dauxois-Holstein model. Here we have presented results of computer simulations using such a model. First we have shown how mobile discrete breathers can be excited in such a model either by locally altering velocities of lattice units or nucleotides or by displacing such units from their original equilibrium positions in an appropriate albeit generic manner. We have found that localizing initial disturbances near the anchoring ends of the model molecular crystal lattice seems to be the easiest and best choice for creating such mobile excitations. Indeed, we have seen that when localizing initial disturbances far away from the anchoring ends of the wire the tendency is to excite pinned breathers. Then we have shown how discrete breathers, mobile and otherwise, are capable of trapping injected excess charges. This trapping mechanism relies on the anharmonicity of the interaction potential used for intersite and on-site interactions. Once a charge, say, an electron, is trapped by the breather the formed compound quasiparticle can play a role similar to the polaron. It can move together with the trapped charge along the molecular wire with a significantly long lifetime over a wire length of up to 200 interunit distances, i.e., approximately 60–70 nm. The simplest case considered here is that when only two nucleotide pairs are excited identically, but other cases are expected to produce similar results. Noteworthy is that the proposed charge transport process does not require application of an external electrical field. Thus it appears as a clear and useful extension of the polaron transport. Building upon the Peyrard-Bishop-Dauxois-Holstein model we can conclude that DNA-like molecular wires could be used as conducting nanowires of great potential for molecular electronics.

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