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Large acoustic polaron states and bifurcation in three coupled parallel molecular chains

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ABSTRACT

We consider the properties of the large acoustic polarons in a media composed of three parallel coupled identical macromolecular chains in an equilateral triangular arrangement. The existence of the truly three-dimensional large polarons has been demonstrated. Their appearance demands the complex interference of the effects of the reduced dimensionality, the nature and strength of the interchain coupling and particular geometrical arrangement of molecular chains. Different types of solutions were found and criteria for their existence were formulated in terms of the dimensionless interchain coupling parameter.

1. Introduction

The studies of the electronic properties of the substances consisting of just a few coupled chains of linearly arranged atoms, molecules or molecular groups, are of the particular practical and scientific interest. The practical interest stems from the potentially widespread use of the quasi–one–dimensional (Q1D) media, such as DNA, conjugated polymers, highly conducting organic salts, as the molecular wires in design and fabrication of the micro and nano-sized electronic devices [1–5]. On the fundamental side, primary interest represents the understanding in which way the interplay of the two opposing trends, reduced dimensionality and the interchain coupling, affects the electronic properties of the Q1D media. On one hand, excess charge or energy carriers in low dimensional (1D in particular) systems, should always be accompanied by the local distortion of the surrounding crystal lattice [6–8]. Therefore, it is expected that the transfer processes would be achieved by means of the polaron mechanism. On the other hand, realistic Q1D media do not behave as the ideal 1D systems because of the inevitable interchain coupling which tends to destabilize the polaron and to prevent its confinement to a single chain [9,10]. For that reason, the elucidation of the possible mechanisms for charge transport in these media has not been unequivocally successful so far. Especially challenging situation arises in the adiabatic limit when electron bandwidth highly exceeds the maximal phonon energy and effectively 1D polaron occupies the large number of lattice sites. Its energy lies below the bottom of the conduction band, while its transport properties cannot be understood on the basis of the band theory [11–15]. In particular, large polaron behave as a classical (Newtonian) particles and propagate along the chain over the large distances in a form of solitary wave preserving their shape for a long time with minimal losses of energy [6–8,11–15].

In the realistic conditions, the interchain coupling may substantially affect the large polaron dynamics. Nevertheless, it cannot fully destabilize polaron, instead, it produces substantially new properties of charge carriers [16–32]. In the case of two coupled chains two different types of polaron solutions were observed [23,32]: below the critical interchain coupling, polaron is located at one of the chains (asymmetric polaron); when coupling parameter exceeds the critical value, symmetric solutions, corresponding to a polaron equally shared among the chains, appear.

In the case of more (3,4...) coupled chains, situation is much more complex and besides the strength of the interchain coupling, polaron features are determined by their particular spatial arrangement which may be pretty diverse in the dependence of their number. Thus for example, three coupled parallel chains could be either confined to a single plane (coplanar structure), or arranged in a triangular form. In both variants, molecules (molecular groups)

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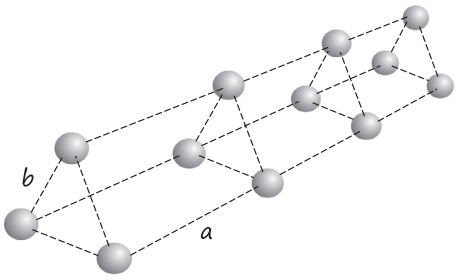

Fig. 1. Spatial arrangement of the molecular chains in model system considered here, b is the distance between chains.

may be positioned exactly opposite to each other, or may be somewhat shifted along the chain. Finally, some substances, α-helix, for example, consist of spirally twisted chain of hydrogen-bonded peptide group which may be viewed as three interlacing chains. In all mentioned cases polaron may have specific properties which demand separate investigation.

In the recent article [33] we have considered structure composed of three coplanar chain and found that polaron features in these media substantially differ from those predicted for the polarons in the two-chain media [18–20,22–24,27–32] or in the infinite 2D systems [6–8,34]. That is, the appearance of the effectively 2D polarons was predicted. Their longitudinal radius highly exceeds the lattice constant along the chain, while the transverse one ranges from zero, in the absence of the interchain coupling, to approximately twice of the separation between the chains when the interchain coupling strength tends towards the infinity. They represent both energetically and dynamically stable configuration. The increase of the interchain coupling strength enhances their stability so that they may be comparably more stable than the pure 1D polarons.

In this paper we study further the polaron properties in a three chain Q1D media. We consider an extra electron in a 3D structure composed of three parallel coupled identical macromolecular chains in an equilateral triangular arrangement with molecules positioned exactly opposite to each other, as presented at Fig. 1. Each chain is composed of $N \gg 1$ molecules (molecular groups). As a theoretical framework we adopt the model based on an ordinary 1D electron–phonon Hamiltonian with additional term which accounts for the interchain coupling of the electronic excitation on adjacent chains. Only the coupling with acoustic modes will be considered. Phonons are considered to be purely one dimensional and they will be accounted in the harmonic approximation.

Provided that the system parameters satisfy adiabatic condition, dynamics of the excess charge and energy carriers strongly interacting with lattice modes, may be described within the semiclassical variational theory of Pekar [6]. At this stage we shall skip all unessential formal aspect, which were elaborated in details in our previous publications [32,33], and we start employing the set of coupled nonlinear Schrödinger equations (NSE) for polaron wave functions on particular chains [32,33]:

$$i\hbar\frac{\partial\Psi_j}{\partial t}+Ja^2\frac{\partial^2\Psi_j}{\partial x^2}+G(\mathrm{v})\left|\Psi_j\right|^2\Psi_j-L\left(\Psi_{j+1}+\Psi_{j-1}\right)=0. \tag{1}$$

Here j enumerates macromolecular chains, which are directed along the x-axis. Due to the supposed cyclic structure, polaron wave functions have to satisfy the following conditions:

$$\Psi_0=\Psi_3,\ \text{and}\ \Psi_4=\Psi_1. \tag{2}$$

The nonlinearity factor of NSE is $G(\mathrm{v})=4E_B/(1-\frac{\mathrm{v}^2}{c_0^2})$, with v being the polaron velocity; $c_0=a\omega_0$ denotes speed of sound, while a stands for the lattice constant.

Lattice dynamics is determined by the maximal phonon frequency $\omega_0=\sqrt{\kappa/M}$, where κ is the stiffness of the particular chain, and M is molecular mass. Electron–phonon interaction is characterized by the so-called small-polaron binding energy $E_B=4\chi^2/M\omega_0^2$ (χ is the electron–phonon coupling parameter).

Electronic subsystem is characterized by the intrachain J and the interchain L electronic excitation transfer integrals. Depending on the particular physical context, the signs of J and L may be either positive or negative. In the processes of the charge transfer (electron or hole migration in conducting polymers, DNA, etc.) both intrachain (J) and interchain (L) are commonly taken as positive [35,36]. In the case of charge transfer in Peierls dielectrics it is commonly taken that $L<0$. Nevertheless, in some cases, L is of the opposite sign or may even alternate along the chain: $L\to L+(-1)^nL'$ [18].

In the case of the intramolecular energy transfer [16,17,22,25] dipole–dipole interaction is responsible for both intra- and interchain coupling and the signs of corresponding exchange integrals are determined by the dipole orientation. We assume that within the single chain dipoles are all aligned and $J>0$. On the other hand, dipoles at different chains are either parallel ($L<0$) or anti-parallel ($L>0$).

Detailed discussion on the validity of semiclassical *ansatz* would be superfluous, instead we briefly summarize the criteria when it holds:

$$2J\gg E_B\gg\hbar\omega_0 \tag{3}$$

The above relation should be understood as follows [6,7,37,38]: the condition $2J\gg\hbar\omega_0$ provides the applicability of semiclassical approximation, while $E_B\gg\hbar\omega_0$ corresponds to the strong coupling regime; finally, $2J\gg E_B$ provides that polaron size significantly exceeds lattice constant.

2. Spectra of linear excitations

Following [33] we first discus the spectra of the linear modes. Thus, putting the $G=0$ and taking the solutions in the form

$$\Psi_j(x,t)=A_je^{ikx-(i/\hbar)\varepsilon(k)t} \tag{4}$$

we obtain the following set of the algebraic equations for unknown amplitudes

$$(\varepsilon(k)-Ja^2k^2)A_j-L(A_{j+1}+A_{j-1})=0. \tag{5}$$

Further, we can choose $A_j=e^{i\phi_j}B_j$, where B_j are real. In such a way the last system becomes:

$$(\varepsilon(k)-Ja^2k^2)B_je^{i\phi_j}-L\left[B_{j+1}e^{i\phi_{j+1}}+B_{j-1}e^{i\phi_{j-1}}\right]=0 \tag{6}$$

Now, we multiply each of these equations by $e^{-i\phi_1}$ and separate real from imaginary parts. In such a way we obtain the two sets of equations for polaron amplitudes and phases:

$$(\varepsilon(k)-Ja^2k^2)B_j\cos(\phi_j-\phi_1)-L\sum_{l=\pm1}B_{j+l}\cos(\phi_{j+l}-\phi_1)=0, \tag{7}$$

$$(\varepsilon(k)-Ja^2k^2)B_j\sin(\phi_j-\phi_1)-L\sum_{l=\pm1}B_{j+l}\sin(\phi_{j+l}-\phi_1)=0. \tag{8}$$

The last system is satisfied for all B_i provided that the phase differences are integer multiples of π:

$$\phi_1-\phi_j=s\pi,\ (s=0,1,2,\ldots). \tag{9}$$

System (7) may be viewed as homogeneous system of equations for variables $\mathcal{B}_i=B_i\cos(\phi_1-\phi_i)$. Secular equation yields three solutions, one of which is doubly degenerated:

$$\begin{aligned}\varepsilon_0(k)&=Ja^2k^2+2L,\ \mathcal{B}_1=\mathcal{B}_2=\mathcal{B}_3\equiv\pm\frac{1}{\sqrt{3}},\\ \varepsilon_{1,2}(k)&=Ja^2k^2-L,\ \mathcal{B}_1=\mathcal{B}_2=-\mathcal{B}_3\equiv\pm\frac{1}{\sqrt{3}}.\end{aligned} \tag{10}$$

3. Nonlinear modes

System of Eq. (1) is invariant with respect to the following symmetry transformations:

- Cyclic permutation: $\Psi_1 \mapsto \Psi_2$; $\Psi_2 \mapsto \Psi_3$; $\Psi_3 \mapsto \Psi_1$
- Mirror symmetry: $\Psi_1 \mapsto \Psi_2$; $\Psi_2 \mapsto \Psi_1$; $\Psi_3 \mapsto \Psi_3$,
- Inversion symmetry: $\Psi_1 \mapsto -\Psi_1$; $\Psi_2 \mapsto -\Psi_2$; $\Psi_3 \mapsto -\Psi_3$
- Parity: $x \mapsto -x$.

Also, different combinations of the listed symmetries are possible, for example inversion mirror symmetry: $\Psi_2 \mapsto -\Psi_3$; $\Psi_3 \mapsto -\Psi_2$; $\Psi_1 \mapsto -\Psi_1$.

One of the consequences of the above symmetry relations is the existence of the following simple types of the solutions (which happen to be the only types of the solutions):

- symmetric: $\Psi_1 = \Psi_2 = \Psi_3$
- antisymmetric: $\Psi_1 = -\Psi_2, \Psi_3 = 0$,
- partially symmetric: $\Psi_1 = \Psi_2 \neq \Psi_3$. Apparently, any cyclic permutation of indices yields fully equivalent set of solutions.

In order to determine under which conditions particular type of solution exists, we perform analysis based on the average profile approximation [39–45] and choose the solutions of the system (1) in the following form:

$$\Psi_j(x,t) = A_j(t)\mathrm{e}^{ik(x-x_0-\mathrm{v}t)}\psi(x,t). \tag{11}$$

Here, $\psi(x, t)$ is real function chosen in the form of pure 1D soliton solution:

$$\psi(x,t) = \sqrt{\frac{\mu}{2}}\,\mathrm{sech}\left\{\frac{\mu}{R_0}(x-x_0-\mathrm{v}t)\right\}, \tag{12}$$

coefficient $\mu = G/4J$, and polaron quasi-momentum $k = \frac{m^*\mathrm{v}}{\hbar}$ ($m^* = \hbar^2/2Ja^2$) were found after the substitution of (11) into (1), and separating imaginary from the real part. Finally, x_0 is the polaron center of mass coordinate, it is irrelevant in the present context. Polaron amplitudes $A_j(t)$ satisfy the set of difference–differential equations:

$$i\hbar\frac{dA_j}{dt} = aA_j + L\left(A_{j-1} + A_{j+1}\right) - g\left|A_j\right|^2 A_j, \tag{13}$$

where $A_0 = A_3$, $A_4 = A_1$, and

$$a = \frac{m^*v^2}{2} + \frac{G^2(\mathrm{v})}{48J}, \quad g = \frac{G^2(\mathrm{v})}{12J} \tag{14}$$

We look for the stationary solutions of (13) in the form $A_j = \mathrm{e}^{-i\omega t}B_j$, where amplitudes B_j may be chosen as real functions. In this manner we find:

$$(\hbar\omega - a)B_i = L(B_{i+1} + B_{i-1}) - gB_i^3, \tag{15}$$

$$B_1^2 + B_2^2 + B_3^2 = 1. \tag{16}$$

Clearly, $B_0 = B_3$, $B_4 = B_1$.

By the elimination of the $(\hbar\omega - a)$ from (15), it is possible to rearrange this system of equations into the following form:

$$\begin{aligned}
&(B_1 - B_2)[L(B_1 + B_2 + B_3) + gB_1B_2(B_1 + B_2)] = 0,\\
&(B_2 - B_3)[L(B_1 + B_2 + B_3) + gB_2B_3(B_2 + B_3)] = 0,\\
&(B_1 - B_3)[L(B_1 + B_2 + B_3) + gB_1B_3(B_1 + B_3)] = 0.
\end{aligned} \tag{17}$$

Polaron ground state energy corresponds to adiabatic functional [32,33] with $\mathrm{v} = 0$ and reads:

$$\mathcal{E} = 2\lambda(B_1B_2 + B_1B_3 + B_2B_3) - \frac{1}{2}(B_1^4 + B_2^4 + B_3^4) \tag{18}$$

where $\mathcal{E} = \frac{E-a}{g}$ is polaron ground state energy, normalized to g, and $\lambda = \frac{L}{g}$ is interchain coupling parameter, its intensity, $|\lambda|$ represents the strength of the interchain coupling.

3.1. Types of solutions

As mentioned above, the system (17) may have three types of solutions: (a) fully symmetric solution, $B_1 = B_2 = B_3$; (b) partially symmetric solutions, $B_i = B_j \neq B_k$, $(i, j, k = 1, 2, 3;\ i \neq j \neq k)$; and (c) antisymmetric solutions $B_1 = -B_2$, $B_3 = 0$. In further, we investigated all three possibilities.

3.1.1. Symmetric solutions

In accordance with the normalization condition, symmetric solutions are simply

$$B_i = \pm\frac{1}{\sqrt{3}}, \quad \forall i = 1, 2, 3, \tag{19}$$

while the ground state energy is linear in coupling parameter:

$$\mathcal{E}_s = 2\lambda - \frac{1}{6} \tag{20}$$

3.1.2. Antisymmetric solutions

In this case all amplitudes are different: $B_1 \neq B_2 \neq B_3$, so that the system of Eq. (17) becomes:

$$\begin{aligned}
&[L(B_1 + B_2 + B_3) + gB_1B_2(B_1 + B_2)] = 0\\
&[L(B_1 + B_2 + B_3) + gB_2B_3(B_2 + B_3)] = 0\\
&[L(B_1 + B_2 + B_3) + gB_1B_3(B_1 + B_3)] = 0.
\end{aligned} \tag{21}$$

Combining these equations we easily obtain

$$\begin{aligned}
&B_3(B_1 - B_2)(B_1 + B_2 + B_3) = 0.\\
&B_2(B_1 - B_3)(B_1 + B_2 + B_3) = 0.\\
&B_1(B_2 - B_3)(B_1 + B_2 + B_3) = 0.
\end{aligned} \tag{22}$$

After the disregarding the solutions of type $B_i = B_j$, $j \neq i$ which are not in accordance with condition that all solutions are different, we are left with two possibilities:

$$B_i = 0; i = 1, 2, 3 \tag{23}$$

or (and)

$$B_1 + B_2 + B_3 = 0. \tag{24}$$

They are equivalent, as can be seen after the substitution of the last one into the system (17) which then becomes

$$\begin{aligned}
&B_1B_2(B_1 + B_2) = 0,\\
&B_2B_3(B_2 + B_3) = 0,\\
&B_3B_1(B_3 + B_1) = 0.
\end{aligned} \tag{25}$$

By adding and subtracting B_3, B_1 and B_2 respectively in the bracketed terms, we finally got

$$B_1B_2B_3 = 0, \tag{26}$$

$$\begin{aligned}
&B_1 = -B_2,\ B_3 = 0,\\
&B_2 = -B_3\ B_1 = 0,\\
&B_3 = -B_1, B_2 = 0.
\end{aligned} \tag{27}$$

That is, the antisymmetric solutions are:

$$\begin{aligned}
&B_1 = -B_2 \equiv \pm\frac{1}{\sqrt{2}},\ B_3 = 0,\\
&B_2 = -B_3 \equiv \pm\frac{1}{\sqrt{2}},\ B_1 = 0,\\
&B_3 = -B_1 \equiv \pm\frac{1}{\sqrt{2}}, B_2 = 0.
\end{aligned} \tag{28}$$

In this case, polaron ground state energy attains the following form:

$$\mathcal{E}_{as} = -\lambda - \frac{1}{4}. \tag{29}$$

3.1.3. Partially symmetric solutions

Here, we have three equivalent set of solutions: $B_1 = B_3 \neq B_2$; $B_1 = B_2 \neq B_3$; $B_2 = B_3 \neq B_1$. Due to the symmetry with respect to cyclic permutation we may focus to one particular case, say $B_1 = B_3 \neq B_2$, while the remaining ones may be obtained by the permutation of the indices $i = 1, 2, 3$. From (17) we find:

$$\lambda = -\frac{B_1 B_2 (B_1 + B_2)}{2B_1 + B_2}, \tag{30}$$

while, from normalization condition we have:

$$B_2 = \pm\sqrt{1 - 2B_1^2}. \tag{31}$$

The sign $\pm$ can be understood in the sense that the polaron amplitudes B_1 and B_2 may have the same sign or the opposite signs, thus the $+$ $(-)$ sign corresponds to the case $B_1 B_2 > 0$ $(B_1 B_2 < 0)$. Additionally, from (31) one can see that polaron amplitudes B_1 and B_3 may have the values only within the interval $(0, 1/\sqrt{2})$, while the values of amplitude B_2 lie in the interval (0, 1). For further analysis it is useful to introduce new parameter $m \in \left(0, \frac{1}{2}\right)$, such that $B_1 = B_3 = \sqrt{m}$, and $B_2 = \pm\sqrt{1 - 2m}$. In such a way, the dependence of the polaron amplitudes on the strength of the interchain coupling may be written as set of parametric equations:

$$B_1 = B_3 = \sqrt{m}$$

$$B_2 = \sqrt{1 - 2m}$$

$$\lambda = -\sqrt{m(1-2m)} + \frac{m\sqrt{1-2m}}{2\sqrt{m} + \sqrt{1-2m}} \tag{32}$$

for $B_1 B_2 > 0$, and

$$B_1 = B_3 = \sqrt{m}$$

$$B_2 = -\sqrt{1 - 2m}$$

$$\lambda = \sqrt{m(1-2m)} - \frac{m\sqrt{1-2m}}{2\sqrt{m} - \sqrt{1-2m}} \tag{33}$$

for $B_1 B_2 < 0$.

By means of the above results we may express the polaron ground state energy (18) in parametric form as follows:

$$\mathcal{E}_+ = \lambda\left(m + 2\sqrt{m(1-2m)}\right) - \frac{1}{2}\left(1 - 4m + 6m^2\right);\ B_1 B_2 > 0$$

$$\mathcal{E}_- = \lambda\left(m - 2\sqrt{m(1-2m)}\right) - \frac{1}{2}\left(1 - 4m + 6m^2\right);\ B_1 B_2 < 0 \tag{34}$$

4. Analysis of solutions

The results of preceding analysis are presented in Figs. 2–4. In Fig. 2, we have plotted the polaron amplitudes versus coupling parameter for all three types of solutions.

Apparently, each particular type of solution exists in the entire range of λ. In particular, apart the narrow region – $-0.254 < \lambda < 0.074$ – system of equations for polaron amplitudes has the threefold solutions: for each λ there are three solutions, one of each type. For $-0.254 < \lambda < 0.074$, the "knot area", all three polaron amplitudes (B_i) have multiple solutions for one value of λ.

To determine the conditions under which each of the above solutions represent the optimal eigenstate of the system, we compare corresponding energies – Fig. 3. The basic requirement for large polaron stability is that its energy lies below the energy of the bottom of the band of linear modes. Among all of the polaron branches only those which minimize the system ground state energy are physically meaningful. Graphical summary is presented in Fig. 4 where we plotted the polaron amplitudes versus the interchain coupling parameter for optimized solutions. Apparently, the antisymmetric solutions are energetically unstable in the whole interval of λ.

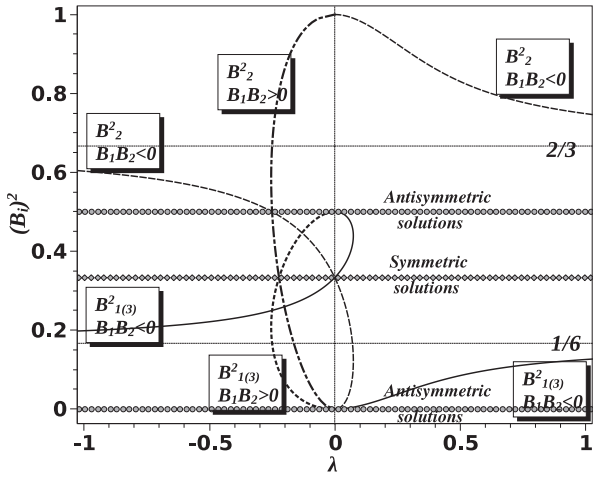

Fig. 2. Polaron amplitudes versus coupling parameter.

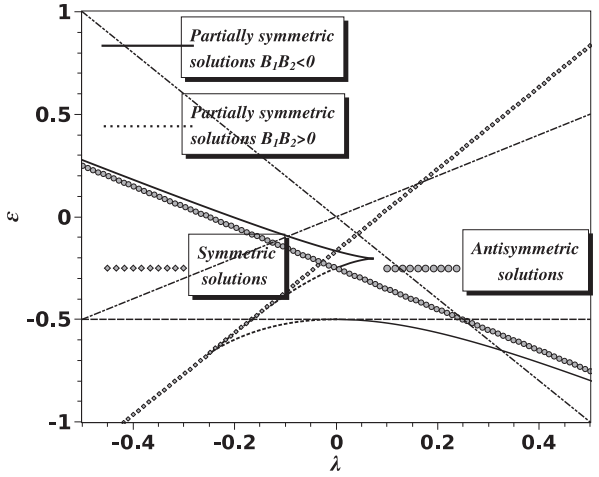

Fig. 3. The dependence of the ground state energy on coupling parameter. Dashed line corresponds to the energy of the pure 1D polaron, while dash-dotted and dash double dotted lines represent the energy of linear modes.

Symmetric polaron minimizes $\mathcal{E}$ for all values of λ up to a lower boundary of the "knot area" ($\lambda_L = -0.254$): that is for $\lambda < \lambda_L$, amplitudes on each chain have the same value and orientation. These solutions are dynamically stable for all $-\infty < \lambda < \lambda_L$ (see the Appendix A).

Partially symmetric solutions appear when coupling parameter exceeds λ_L. They are energetically the most favorable for $-0.254 < \lambda < 0.36$. When coupling parameter exceeds 0.36 polaron becomes unstable with respect to free (band) states, whose energy lies below the energy of the polaron branch. For coupling parameter from the interval $-0.254 < \lambda < 0$, stable solutions correspond to $B_1 B_2 > 0$; That is, all three amplitudes are aligned. As a function of the coupling parameter, amplitude of $B_{1,3}$ gradually decreases from $1/\sqrt{6}$ towards the zero; in the same time amplitude of B_2 increases from $\sqrt{2/3}$ towards unity. Particular case $\lambda = 0$ corresponds to uncoupled chains and polaron confinement to single chain occurs: amplitudes $B_{1,3}$ disappear, while B_2 approaches unity. After switching on coupling again ($\lambda \geq 0$) amplitudes $B_{1(3)}$ and B_2 become anti-parallel ($B_1 B_2 < 0$). As coupling strength increases $B_{1(3)} \to \pm\sqrt{1/6}$ and $B_2 \to \sqrt{2/3}$. These solutions are stable for all $\lambda \geq 0$.

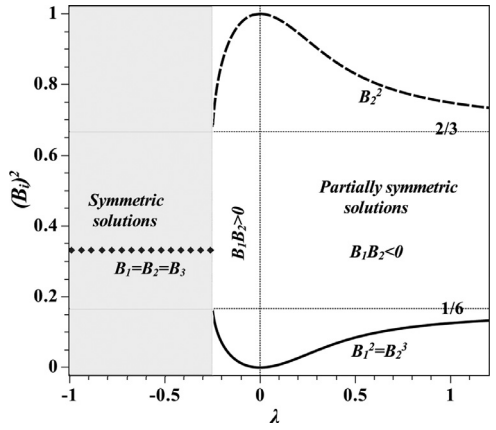

Fig. 4. The dependence of polaron amplitude on the interchain coupling parameter for optimized polaron solutions. Partially symmetric solutions are presented for $B_1 = B_3 \neq B_2$ case. All other cases follow simply after the cyclic permutation of indices.

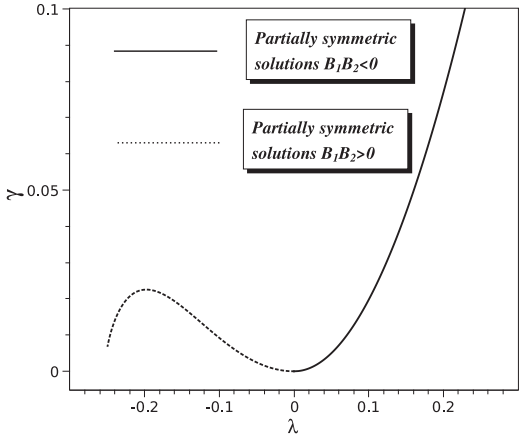

Fig. 5. Left-hand side of the inequality (39) versus coupling parameter.

5. Concluding remarks

The most important result of this study is the demonstration of the possible existence of the truly 3D large polarons in triple chain media. The existence of such quasiparticles is provided by the particular geometrical arrangement of chains (Fig. 1). These entities cannot exist in bulk media, where transverse coupling destabilize effectively 1D polarons, and where only the free (delocalized) and severely localized (small-polaron), may be expected [6–8]. We found that the energies of the symmetric and partially symmetric solutions are always below the energy of pure 1D polaron. Thus, up to $\lambda \sim 0.36$, effectively 3D large polaron is energetically and dynamically more stable with respect to its 1D counterpart.

The properties of these 3D quasiparticles are determined by the nature of the intrachain interaction which is formally determined by the sign of parameter λ. Thus, for $\lambda < \lambda_L$, polaron is equally distributed among the macromolecular chains – $B_1^2 = B_2^2 = B_3^2$. This, effectively 3D entity, possesses relatively large extent in the longitudinal direction ($\sim 1/\mu \gg 1$), while the transverse ones are practically equal to interchain separation. When coupling parameter approaches the critical value $\lambda = -0.254$, we observe the bifurcation from the symmetric to partially symmetric solution: the polaron amplitude increases on one macromolecular chain, while it decreases on other two chains. Naturally, in the absence of coupling ($\lambda = 0$), polaron becomes confined to a single chain. By further increasing of the ratio λ (i.e. for $\lambda > 0$) this essentially 1D polaron gradually becomes truly 3D quasiparticle: it is highly peaked on one chain, while the amplitudes on the other two are comparably smaller. Similarly to the symmetric solutions, partially symmetric ones are truly 3D entities, and irrespectively of the values of system parameters, there is no confinement to a single chain. Increasing of interchain coupling leads to the destabilization of these polarons whose energy for $\lambda > 0.36$, overgrows the energy of band states. In that respect, these polarons fundamentally differs from the ones in the twin-chain structures where, above the bifurcation point, truly 1D polarons, cannot appear.

Polaron motion may substantially affect its character and stability. Due to the quasi-relativistic dependence of the nonlinear parameter $G(v)$ on polaron velocity, effective interchain coupling decreases as v approaches the speed of sound. This enhances the polaron confinement to a single chain and supports its stability: the energy of faster polaron is deeper below the bottom of the energy of band states.

The current simple model encompasses only the most essential physical ground governing the transport processes in some realistic Q1D media. The establishment of the quantitative correspondence with experimental data and possible implementation in nano- or micro-electronic devices, should be based on more elaborate ground.

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Appendix A. Polaron stability – the linear mode analysis

In order to analyse dynamical stability, we perform the standard linear perturbation theory [46]. Only the symmetric and partially symmetric solutions were considered; the antisymmetric ones were not considered since their energy always lies above the energies of these two types.

Following the standard procedure [32,46], we linearize system of equation for polaron amplitudes assuming $A_i(t) = (B_i + \delta A(t))e^{i\omega t}$. Here, $\delta A_i(t)$ denote the small corrections of the polaron amplitudes for which we got the following system of evolution equations:

$$\frac{d}{dt}\begin{pmatrix} Re\ \delta A(t) \\ Im\ \delta A(t) \end{pmatrix} = \begin{pmatrix} 0 & \mathcal{B} \\ \mathcal{A} & 0 \end{pmatrix}\begin{pmatrix} Re\ \delta A(t) \\ Im\ \delta A(t) \end{pmatrix}$$

Here, the following abbreviations were introduced:

$$Re\ \ \delta A(t) = \begin{pmatrix} Re\ \delta A_1(t) \\ Re\ \delta A_2(t) \end{pmatrix},\quad Im\ \ \delta A(t) = \begin{pmatrix} Im\ \delta A_1(t) \\ Im\ \delta A_2(t) \end{pmatrix}. \tag{35}$$

Now, we chose "small corrections" in the form:

$$\delta A_j(t) = \delta A_j(0) \cdot e^{\frac{\nu}{\hbar}t}, \tag{36}$$

where ν is the instability growth rate, while $\delta A_j(0)$ denote the stationary part of solution.

Instability growth rate (ν) was found from the condition that the above system has the non-trivial solutions. Stable solutions correspond to vanishing or pure imaginary instability growth.

(a) Symmetric solutions $B_1 = B_2 = B_3 = \pm 1/\sqrt{3}$

In this case we have $\mathcal{A} = 2gB_1^2$ and $\mathcal{B} = 0$ while the instability growth rate ($\nu \equiv 0$): i.e., symmetric solutions are always dynamically **stable**.

(b) Partially symmetric solutions $B_1 = B_3 \neq B_2$

In this case $\mathcal{A}, \mathcal{B}$ represents 2×2 matrices given by

$$\mathcal{A} = \begin{pmatrix} L\frac{B_2}{B_1} + 2gB_1^2 & -L \\ -2L & 2L\frac{B_1}{B_2} + 2gB_2^2 \end{pmatrix}$$
$$\mathcal{B} = \begin{pmatrix} -L\frac{B_2}{B_1} & L \\ 2L & -2L\frac{B_1}{B_2} \end{pmatrix} \tag{37}$$

Secular equation for ν is simply

$$\frac{\nu^2}{g^2} + \frac{L}{g}\frac{6B_1^3B_2^3 + \frac{L}{g}}{B_1^2B_2^2} = 0, \tag{38}$$

Apparently, stable solutions corresponds to :

$$\gamma \equiv \left(\frac{L}{g}\right)^2 + 6B_1^3B_2^3\frac{L}{g} > 0. \tag{39}$$

As illustrated in Fig. 5, the above condition is satisfied for all λ for which partially symmetric solutions minimizes polaron energy. That is, they are both energetically and dynamically stable.

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