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Influence of quantum lattice fluctuations on the stability of large polarons in anisotropic electron-phonon systems

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We discuss the stability of large polarons in anisotropic media taking into account small-polaron narrowing of the electron band. It was shown that electron-phonon interaction may cause an additional anisotropy of the electron overlap integrals. Large-polaron stability in realistic substances is interpreted in terms of these results.

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Electron- (exciton-, etc.) phonon interaction in many quasi-one-dimensional (1D) substances is rather strong. For these reasons it has been argued that the large polarons or solitons may have a crucial role in charge and energy transfer in highly conducting organic salts (TTF-TCQN, etc.) (Ref. 1) and linear conjugated polymers {*trans*-polyacetylene [*trans*-$(\mathrm{CH})_x$]},[2] and biological macromolecules (α-helix and DNA) (Refs. 3–6). This belief is founded upon the quite general theoretical arguments which imply that the self-trapping (ST) in higher dimensional systems with short-ranged electron-phonon interaction qualitatively differs from that in pure 1D where polarons will always be formed.[7–11] Its radius depends on system parameters and stable, mobile large polarons arise when electron bandwidth exceeds small-polaron binding energy. However, these predictions were based upon the idealized 1D models which may be unsatisfactory for realistic systems. Namely, as shown some time ago,[12,13] even very small anisotropy of electronic subsystem may violate large-polaron stability. In particular, Pertzsch and Rössler[12] found, employing the continuum model, that, irrespectively of the degree of anisotropy, there is no substantial difference between ST in anisotropic and isotropic media so that the existence of the stable large polaron may be just the artefact of the 1D models. Later, Emin[13] examined the ST in molecular chains taking into account interchain coupling. Employing similar continuum theory he found that pure 1D behavior requires the ratio of the anisotropy of transfer integrals at least three orders- of magnitude. However, according to band structure calculations,[1,2] degree of the anisotropy of transfer integrals ranges from 10 to 10^2 which is considerably lower than that required by Emin's criterion, so it seems that large polarons cannot be formed in realistic quasi-1D solids.

Nevertheless, experiments including the infrared absorption,[14] charge carrier mobility measurements,[15] and resonant Raman spectra[16] of conjugated polymers strongly support polaron presence in these materials.

This could be the consequence of the fact that the existence of chain endings, conjugation breaks, and defects can stabilize polarons.[17]

Moreover, electron-phonon interaction may cause an additional anisotropy of electron bands due to the exponential reduction of the electronic transfer integrals.[18] This effect is maximal in the nonadiabatic limit, when electron bandwidth is small as compared with the characteristic phonon frequency, and determines small-polaron properties. Nevertheless, recent studies[19–21] have shown that it may emerge even in the adiabatic regime and therefore could give rise to a large polaron stability. This possibility will be examined in the present paper.

In what follows we shall restrict ourselves to electron interacting with the dispersionless optical phonon through the short-ranged interaction and therefore our analysis will be carried on upon Holstein's molecular crystal model Hamiltonian which reads as follows:[8]

$$H = -\sum_{\mathbf{n},\mathbf{g}} J_{|\mathbf{g}|} A^{\dagger}_{\mathbf{n}} A_{\mathbf{n}+\mathbf{g}} + \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} b^{\dagger}_{\mathbf{q}} b_{\mathbf{q}} + \frac{1}{\sqrt{N}} \sum_{\mathbf{q},\mathbf{n}} F_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{R}_{\mathbf{n}}} A^{\dagger}_{\mathbf{n}} A_{\mathbf{n}} (b_{\mathbf{q}} + b^{\dagger}_{-\mathbf{q}}). \qquad (1)$$

Here $\mathbf{n},\mathbf{g}$ labels lattice sites while the summation over $\mathbf{g}$ extends to adjacent sites in each direction. As usual, $J_{|\mathbf{g}|}$ denotes the intersite transfer integral, operator $A^{\dagger}_{\mathbf{n}}(A_{\mathbf{n}})$ describes the presence (absence) of the electron on the nth lattice site; $b^{\dagger}_{\mathbf{q}}(b_{\mathbf{q}})$ creates (annihilates) phonon quanta with the frequency $\omega_{\mathbf{q}} \equiv \omega_0$; $F_{\mathbf{q}} \equiv F = \text{const}$ denotes the electron-phonon coupling parameter.

To achieve the above proposed goal we shall utilize the variational method of Brown and Ivić[20] which enables for accounting of quantum effects on large-polaron properties. Thus we choose the normalized trial state in the form of

$$|\Psi\rangle = \sum_{\mathbf{n}} \Psi_{\mathbf{n}} A^{\dagger}_{\mathbf{n}} |0\rangle_e \otimes |\beta_{\mathbf{n}}\rangle, \qquad \sum_{\mathbf{n}} |\Psi_{\mathbf{n}}|^2 = 1. \qquad (2)$$

Here $\Psi_{\mathbf{n}}$ denotes electron wave function while $|\beta_{\mathbf{n}}\rangle = \exp[\Sigma_{\mathbf{q}}(\beta_{\mathbf{q},\mathbf{n}} b^{\dagger}_{\mathbf{q}} - \beta^{*}_{\mathbf{q},\mathbf{n}} b_{\mathbf{q}})]|0\rangle_{\mathrm{ph}}$ corresponds to a phonon part of trial state. In order to examine quantum effects we decompose $\beta_{\mathbf{q},\mathbf{n}}$ into slow (frozen) and fast components as follows: $\beta_{\mathbf{q},\mathbf{n}} = \beta_{\mathbf{q}} - \frac{1}{\sqrt{N}} f_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{R}_{\mathbf{n}}}$. This yields $|\beta_{\mathbf{n}}\rangle = \exp\varphi \exp\{\Sigma_{\mathbf{q}}[(\beta_{\mathbf{q}} - \frac{1}{\sqrt{N}} f_{\mathbf{q}}) b^{\dagger}_{\mathbf{q}} - \mathrm{H.c.}]\}|0\rangle_{\mathrm{ph}}$. Here coherent phonon amplitude $\beta_{\mathbf{q}}$ characterizes the classical, slow or "frozen," part of lattice distortion which dominates in the adiabatic limit. In the opposite limit the electron is surrounded with short-ranged lattice distortion which follows electron motion instantaneously and causes known exponential narrowing of the electron band. This is characterized by the magnitude of $f_{\mathbf{q}}$ which in the strict antiadiabatic limit approaches $\frac{F_{\mathbf{q}}}{\hbar\omega_{\mathbf{q}}}$ while $\beta_{\mathbf{q}} \to 0$. Finally, φ

$=(1/2)\Sigma_{\mathbf{q}}\beta_{\mathbf{q}}\frac{1}{\sqrt{N}}f_{\mathbf{q}}^{*}e^{-i\mathbf{q}\cdot\mathbf{R}_{\mathbf{n}}}-\text{c.c.}$ denotes phase factor introduced here to eliminate the dependence of the band narrowing factor on coherent phonon amplitude. We shall treat $\beta_{\mathbf{q}}$ and $f_{\mathbf{q}}$ as variational parameters which will be determined demanding stationarity of the functional $\mathcal{H}=\langle\Psi|H|\Psi\rangle$. Here we first eliminate $\beta_{\mathbf{q}}$ by virtue of equation $\frac{\partial\mathcal{H}}{\partial\beta_{\mathbf{q}}}=0$,

$$\mathcal{H}=-\frac{1}{N}\sum_{\mathbf{q}}[F_{\mathbf{q}}(f_{\mathbf{q}}+f_{-\mathbf{q}}^{*})-\hbar\omega_{\mathbf{q}}|f_{\mathbf{q}}|^{2}]\sum_{\mathbf{n}}|\Psi_{\mathbf{n}}|^{2}$$

$$-\sum_{\mathbf{n},\mathbf{g}}J_{|\mathbf{g}|}e^{-W(\mathbf{g})}\Psi_{n}^{*}\Psi_{\mathbf{n}+\mathbf{g}}+\frac{1}{N}\sum_{\mathbf{m},\mathbf{n}}\mathcal{K}_{\mathbf{m},\mathbf{n}}|\Psi_{\mathbf{m}}|^{2}|\Psi_{\mathbf{n}}|^{2},$$

$$\mathcal{K}_{\mathbf{m},\mathbf{n}}=E_{b}\frac{1}{N}\sum_{\mathbf{q}}\left|1-\frac{\hbar\omega_{\mathbf{q}}f_{\mathbf{q}}}{F_{\mathbf{q}}}\right|^{2}e^{i\mathbf{q}\cdot(\mathbf{R}_{\mathbf{m}}-\mathbf{R}_{\mathbf{m}})}. \tag{3}$$

Here $E_{b}=\frac{F^{2}}{\hbar\omega_{0}}$ denotes small-polaron binding energy; $\mathbf{g}=\{a\mathbf{e}_{\mathbf{x}},b\mathbf{e}_{\mathbf{y}};b\mathbf{e}_{\mathbf{z}}\}$ is the vector connecting neighboring lattice sites.

We are considering a anisotropic crystal consisting of a collection of linear chains oriented along the x axis. Easy transfer along the chains is associated with the nearest-neighbor transfer integral $J_{a}\equiv J_{\parallel}$; the interchain transfer is associated with the transverse transfer integral $J_{b}\equiv J_{\perp}$ and the interchain distance b. Finally, the electron-band-narrowing factor reads

$$W(\mathbf{g})=\frac{1}{N}\sum_{\mathbf{q}}|f_{\mathbf{q}}|^{2}(1-\cos\mathbf{q}\cdot\mathbf{g}). \tag{4}$$

Its evaluation and consequences for polaron dimensions is our main goal hereafter.

Character of ST states is determined by the "dressing" parameter $f_{\mathbf{q}}$. For the particular set of system parameters one must find the optimized value for $f_{\mathbf{q}}$ by minimizing the above functional. In the adiabatic limit, dressing vanishes $(f_{\mathbf{q}}\to 0)$ and a large polaron may arise if a small polaron binding energy does not exceed electron bandwidth. Maximal dressing arises in the opposite limit when $f_{\mathbf{q}}\sim\frac{F_{\mathbf{q}}}{\hbar\omega_{q}}$ and the nonlinear term in (3) vanishes so that ST results in the creation of small-polaron band states. In the practical calculation we shall disregard the dependence of the nonlinear term on dressing parameter since its inclusion[20] only weakly modifies the results of the prior linear polaron theories.[8,9] Therefore, the kernel in (3) may be safely approximated as follows: $\mathcal{K}_{\mathbf{m},\mathbf{n}}\approx E_{b}\delta_{\mathbf{m},\mathbf{n}}$.

Passing to the continuum limit functional $\mathcal{H}$ attains the following form:

$$\mathcal{H}=\varepsilon+a^{2}J_{\parallel}e^{-W_{\parallel}}\int\frac{d\mathbf{r}}{V}|\Psi_{x}(\mathbf{r})|^{2}-E_{b}\int\frac{d\mathbf{r}}{V}|\Psi(\mathbf{r})|^{4}$$

$$+b^{2}J_{\perp}e^{-W_{\perp}}\int\frac{d\mathbf{r}}{V}[|\Psi_{y}(\mathbf{r})|^{2}+|\Psi_{z}(\mathbf{r})|^{2}]. \tag{5}$$

Here $V=ab^{2}$ denotes the volume of the elementary cell, index x,y,z in the subscript refers to derivative with respect to Cartesian coordinates; $\varepsilon=-\frac{1}{N}\Sigma_{\mathbf{q}}[F_{\mathbf{q}}(f_{\mathbf{q}}+f_{-\mathbf{q}}^{*})-\hbar\omega_{\mathbf{q}}|f_{\mathbf{q}}|^{2}]-2\Sigma_{\mathbf{g}}J_{|\mathbf{g}|}e^{-W(|\mathbf{g}|)}$ stands for the polaron shift of the bottom of the electron band. Labels $W_{\parallel}\equiv W_{a}$, $W_{\perp}\equiv W_{b}$ stand for the narrowing of the intrachain and interchain overlap integrals, respectively.

If $\Psi(\mathbf{r})$ is an exact ground-state (GS) function, $\mathcal{H}$ would be an exact GS energy. However, we do not know an explicit expression for $\Psi(\mathbf{r})$ and therefore we shall try to understand the effects of anisotropy qualitatively employing variational calculations. For that purpose we presume that $\Psi(\mathbf{r})$ is spatially separable and confined in a spatial region with the longitudinal extent of the length $l_{\parallel}$ and width $l_{\perp}$. Next, we introduce the norm-preserving scale change $\Psi(\mathbf{r})\to\frac{1}{R_{\parallel}^{1/2}R_{\perp}}\Psi(x/R_{\parallel};y/R_{\perp},z/R_{\perp})$ in which scaling parameters $R_{\parallel}=l_{\parallel}/a$ and $R_{\perp}=l_{\perp}/b$ have the meaning of dimensionless longitudinal and transverse polaron radius, respectively. They are constrained to be larger or equal to unity because of the validity of the continuum approximation.

In such a way, functional (5) attains the following form:

$$\mathcal{H}(R_{\parallel},R_{\perp})=\varepsilon+\frac{E_{k}^{\parallel}}{R_{\parallel}^{2}}+\frac{E_{k}^{\perp}}{R_{\perp}^{2}}-\frac{E_{p}}{R_{\parallel}R_{\perp}^{2}}. \tag{6}$$

Here we have introduced the appropriate abbreviations for the integrals in (5). Thus, $E_{k}^{\parallel}$ and $E_{k}^{\perp}$ stand for the first and third integral and have the meaning of the kinetic energies of longitudinal and transverse motion, respectively. E_{p} stands for the second integral in (5) and corresponds to a potential energy. For the explicit evaluation of these integrals we took $\Psi(\mathbf{r})=\frac{1}{\sqrt{2}\cosh x/a}e^{-(y^{2}+z^{2})/2b^{2}}$.

GS energy (6) has no stable minimum with respect to $R_{\parallel}$ and $R_{\perp}$ both exceeding unity. This means that the stable large-polaron state which spreads over the region exceeding both interchain separation and lattice constant along the chain does not exist for any set of system parameters.

Let us now examine stability of the large polaron in the anisotropic system $(J_{\perp}\neq 0)$ confined to a single chain so that polaron transverse radius approaches unity $R_{\perp}=1$. Under these circumstances GS energy (6) has a minimum at $R_{\parallel}=4J_{\parallel}e^{-W_{\parallel}}/E_{b}$ which is 2 times the extent of the 1D polaron. Moreover, in contrast to pure 1D systems where such minimum always exists and corresponds to a stable large polaron for $E_{B}\ll 2J_{\parallel}e^{-W_{\parallel}}$, GS energy $\mathcal{H}(R_{\parallel}^{\min})$ is increased by an amount $E_{\perp}^{k}=J_{\perp}e^{-W_{\perp}}$ associated with confining the particle to the chain. Therefore, stability of this state relative to the three-dimensional quasifree state (dressed small polaron) requires that it does not exceed the energy gained by the large-polaron formation, $E_{b}^{2}/(48J_{\parallel}e^{-W_{\parallel}})$. This yields $E_{b}^{2}>48J_{\parallel}J_{\perp}e^{-W_{\parallel}}e^{-W_{\perp}}$. For practical purposes it is more convenient to express this condition in terms of polaron size along the chain $(R_{\parallel}=4J_{\parallel}^{\text{eff}}/E_{b};\ J_{\parallel}^{\text{eff}}=J_{\parallel}e^{-W_{\parallel}})$ as follows:

$$\frac{J_{\parallel}^{eff}}{J_{\perp}^{eff}}>3R_{\parallel}^{2}. \tag{7}$$

This condition is equivalent to Emin's criterion and for polaron extended over 10 lattice sites it demands approximately three orders of magnitude of the anisotropy of the effective transfer integrals. This condition may be fulfilled, in contrast to expectations on the basis of pure semiclassical analysis,[13] if quantum corrections cause different narrowing of the effective transfer integrals, i.e., if $W_\perp > W_\parallel$. For the proper understanding of the role of quantum lattice fluctuations in large-polaron stability on the basis of the above criterion, one must evaluate $W_\parallel$ and $W_\perp$. For that purpose one must find the optimal value of $f_{\mathbf{q}}$ minimizing the GS energy. Note, however, that the potential and longitudinal kinetic energy term are of the same order and $\sim \frac{J_\parallel e^{-W_\parallel}}{R_\parallel^2}$ so that the main contribution comes from ε and $E_k^\perp$. This yields

$$f_{\mathbf{q}} = \frac{F}{\hbar\omega_0}\frac{1}{1 + \sum_{\mathbf{g}} \frac{2\delta_g J_{|\mathbf{g}|}}{\hbar\omega_0} e^{-W(\mathbf{g})} \sin^2 \frac{\mathbf{q}\cdot\mathbf{g}}{2}}. \tag{8}$$

Here $\delta_a = 1, \delta_b = 1/2$. Substitution of the last expression into (4) results in

$$W(\mathbf{g}) = 2S\frac{1}{N}\sum_{\mathbf{q}} \frac{\sin^2 \frac{\mathbf{q}\cdot\mathbf{g}}{2}}{\left(1 + \sum_{\mathbf{g}} \frac{2\delta_g J_{|\mathbf{g}|}}{\hbar\omega_0} e^{-W(\mathbf{g})} \sin^2 \frac{\mathbf{q}\cdot\mathbf{g}}{2}\right)^2}. \tag{9}$$

Here $S = (F/\hbar\omega_0)^2 \equiv E_b/\hbar\omega_0$ denotes the coupling constant introduced in Ref. 8. The above expression represents the set of coupled self-consistent equations for small-polaron screening parameters. It cannot be solved explicitly in terms of $W_\parallel$ and $W_\perp$ as a function of system parameters. However, at this stage we may obtain, in accordance with the assumption about high anisotropy of the electronic system, some reliable approximate results expanding $W(\mathbf{g})$ in powers of the anisotropy parameter $J_\perp/J_\parallel$. Adopting this approximation and substituting the summation over $\mathbf{q}$ by an integration in accordance with the aforementioned rule we obtain

$$W_\parallel \approx S(1 + 2B_\parallel e^{-W_\parallel})^{-3/2} + 4SB_\parallel B_\perp e^{-W_\parallel} e^{-W_\perp},$$

$$W_\perp \approx W_\parallel (1 + B_\parallel e^{-W_\parallel}). \tag{10}$$

Here $B_{\parallel(\perp)} = \frac{2J_{\parallel(\perp)}}{\hbar\omega_0}$ represent longitudinal (transverse) adiabatic parameters. This system of equations does not admit explicit solutions in terms of $W_\parallel$ and $W_\perp$. However, it is possible to express S as a function of $W_\parallel$ taking $B_\parallel$ and $B_\perp$ as parameters. Desired dependence of $W_\parallel$ on system parameters follows simply by inverting the so-obtained solution. Finally, $W_\perp(S; B_\parallel, B_\perp)$ is found combining this result with the second equation in (10).

Our results are visualized in Fig. 1 where we have plotted the set of "adiabatic" curves which explicitly display the dependence of the small-polaron narrowing factors in anisotropic media $[W_\parallel = W_\parallel(S)$ and $W_\perp = W_\perp(S)]$ and in pure 1D systems on the coupling constant for a few fixed values of adiabatic parameters and degree of anisotropy $\gamma = J_\parallel/J_\perp$. Our primary goal is the problem of the large-polaron stability in anisotropic media. Therefore, we must choose $B_\parallel \gg 1$ while the allowed values of the coupling constant are restricted to the region in which the condition for the applicability of the continuum approximation, $R_\parallel \gg 1 \Leftrightarrow S \ll B_\parallel$ is satisfied. Thus we plot these curves for $B_\parallel = 10, 20$; and $\gamma = 10, 100$. This is consistent with the estimated values of physical parameters for the number of realistic substances: *trans*-(CH)$_x$ ($J_\parallel \approx 2.5$ eV, $\hbar\omega_0 \sim 0.175$ eV);[2] DNA and α–helix-intrachain transfer integral is of the order of a few tenths of eV, 0.2–0.4 eV (Refs. 4 and 6), while $\omega_0 \sim 10^{13}$ s^{-1} so that $B_\parallel \sim 20-30$. We finally note that our consideration may be relevant for organic conductors such as TTF-TCQN and related substances since some recent findings[22] have shown that the intrachain transfer integral is comparable with that of conducting polymers, i.e., 10 times larger than that usually quoted ($J_\parallel \sim 0.13-0.25$ eV) which is of the same order of typical phonon energies.[1,18]

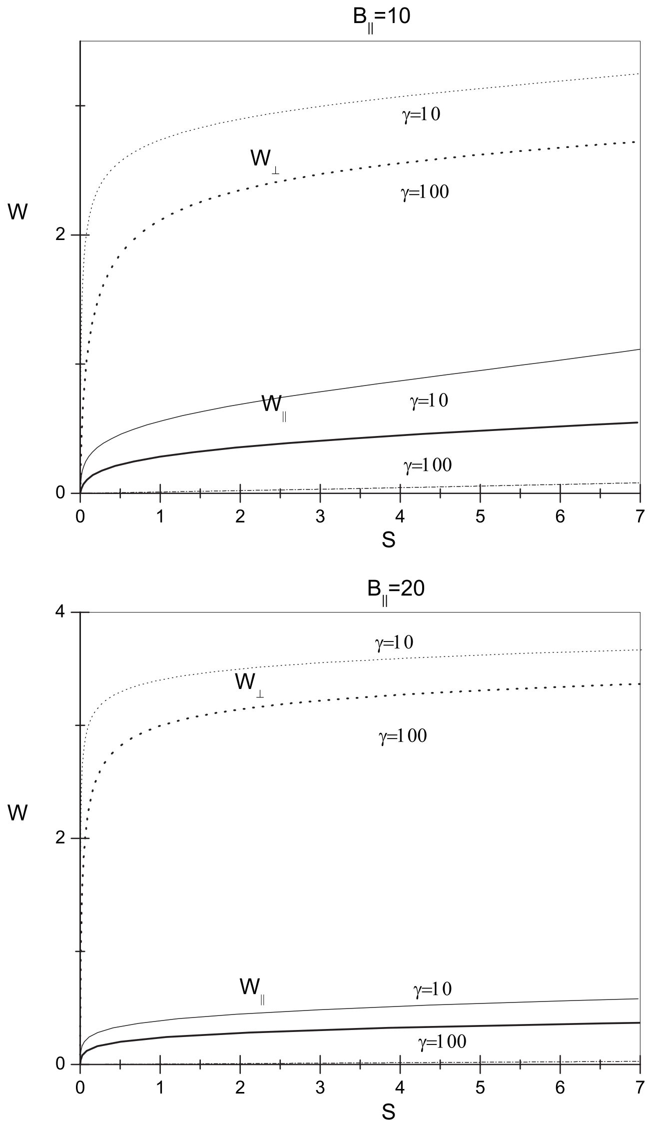

FIG. 1. Longitudinal (full lines) and transverse (dotted lines) polaron screening parameters versus coupling constant for $B_\parallel = 10$ and 20, and $J_\parallel/J_\perp = 10$ (thin lines), and $J_\parallel/J_\perp = 100$ (thick lines). The dashed-dotted line represents the small-polaron screening factor in pure 1D systems.

Both screening factors display qualitatively the same dependence on the coupling constant as in the pure 1D systems. The only difference is in their magnitudes which are noticeably larger than those in the 1D case. Note also that $W_\perp$ is always larger than $W_\parallel$ which increases slowly with the rise of coupling constant. The deviation from the 1D result is determined by the degree of anisotropy and by the value of $B_{\parallel}$. With the increase of $B_{\parallel}$ this deviation gradually disappears and fully vanishes in the extreme adiabatic limit. The influence of anisotropy is noticeable for not too high values of the adiabatic parameter. It is manifested through the increase of the magnitude $W_{\parallel}$ with the decrease of the degree of anisotropy, i.e., when $J_{\perp}$ tends to $J_{\parallel}$. Behavior of $W_{\perp}$ is similar to that of $W_{\parallel}$ but its magnitude is significantly larger in the practically whole region of parameter space of interest. Moreover, its increase in the weak coupling regime is much steeper than that of $W_{\parallel}$, which causes a sharp drop of the effective intersite transfer integral even for the system parameters for which $J_{\parallel}^{\mathrm{eff}} \sim J_{\parallel}$. This is determined by the magnitude of $B_{\parallel}$. For very large values of $B_{\parallel}$ magnitude of $W_{\parallel}$ does not exceed 0.3. In the same time $W_{\perp}$ suddenly jumps approaching large values even in the weak coupling limit. This causes significant reduction, up to 20 times, of the effective transverse transfer integral and provides the fulfillment of the large-polaron stability condition (7).

Our analysis clearly shows that quantum lattice fluctuations may considerably enhance the prospects for large-polaron existence in anisotropic media in contrast to previous predictions.[13] This is the consequence of the additional anisotropy of electronic bands caused by the small-polaron effect. Besides that, we also observe the screening of the intrachain transfer integral. Its reduction is small as compared with the reduction of the transverse term but noticeably larger than that calculated within pure 1D models. This points to the necessity of the accounting of quantum effects in the analysis of the possible role of large polarons in various contexts in realistic conditions. Thus, for example, for the values of system parameters employed here, effective intrachain overlap integral may be reduced up to 23% for $\gamma = 100$ and 30% for $\gamma = 10$. These estimates hold for both values of $B_{\parallel}$ and for values of the coupling constant $S \lesssim B_{\parallel}/5$ which provide the applicability of the continuum approximation. For these reasons the large-polaron effective mass in realistic substances may considerably differ from that calculated within pure 1D models and should be accounted for in the analysis of the large-polaron motion. At this stage we must stress that the direct application of the present results, which were obtained within the static limit, does not introduce any substantial error in the analysis of the features of a moving large polaron. This follows from the comprehensive analysis of Ref. 20, where the results obtained by means of the present method within the static limit are in substantial agreement with quantum Monte Carlo simulations (QMC).[23]

We finally note that our estimates of the additional anisotropy of electron bands are far below that of Gogolin.[18] This discrepancy is the consequence of the fact that Gogolin used the Lang-Firsov[24] method which is satisfactory in the strong coupling nonadiabatic limit while our analysis concerns quite the opposite case, i.e., adiabatic weak coupling limit: the region of parameter space where one can expect formation of a large polaron.

In conclusion we point out that the variational nature of our method imposes certain reserves on the validity of our conclusions. Unfortunately, at present, in the absence of the reliable numerical studies on the subject, we are not in the position to estimate the validity of our approach in the whole parameter space of the system. However, for the values of system parameters where large-polaron existence is expected, adiabatic ($B \gg 1$) "weak" coupling case ($S \ll B$), we believe that our results are reliable enough to give further insight in the issue of the stability of large polaron in chain-like structures in the highly anisotropic case. We base such belief upon the aforementioned agreement of the QMC simulations and results of the present variational method in pure 1D systems.

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