Bipolaron confinement in two-dimensional layers

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Widely reported broadening of a bipolaron formation region in two dimensions should be revised in view of a concrete mechanism of electron confinement to a two-dimensional layer.

Recently, there has been renewed interest in the bipolaron problem triggered by a possibility of a bipolaronic mechanism of the high-T_c superconductivity considered in literature. In the context of large bipolarons such a mechanism was studied by Vinetskii and Pashitskii.[1] Later analogous ideas were significantly developed by Emin and Hillery.[2,3] The existence and stability of bipolarons being a prerequisite of such theories depends on values of coupling constants and of phonon frequencies.

Besides, the modern art of creating new materials such as thin films and quantum wires makes it possible to confine moving electrons to two or even one dimensions. The conclusion that a bipolaron formation makes easier in spaces of lower dimensions was made in many recent papers. The goal of the present paper is to show that this statement has to be taken *cum grano salis* because it depends on a concrete *physical* mechanism of the electron confinement. We give here *examples* of how the two-dimensional (2D) structures can be treated for adequate calculations of coupling constants and phonon frequencies.

The Fröhlich Hamiltonian for two electrons interacting with a phonon field is written as follows:

$$H = \frac{\mathbf{p}_1^2}{2m} + \frac{\mathbf{p}_2^2}{2m} + \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}}\, a_{\mathbf{k}}^{\dagger} a_{\mathbf{k}} + U(|\,\mathbf{r}_1 - \mathbf{r}_2\,|) + \sum_{\mathbf{k}} \left[a_{\mathbf{k}}\, V_{\mathbf{k}}\, \left(e^{i\mathbf{k}\mathbf{r}_1} + e^{i\mathbf{k}\mathbf{r}_2}\right) + \text{H.c.}\right], \tag{1}$$

where $\mathbf{r}_i$ ($\mathbf{p}_i$) are the position (momentum) operators of the ith electron, m is the electron band mass, $a_{\mathbf{k}}^{\dagger}$ ($a_{\mathbf{k}}$) are the creation (annihilation) operators of phonons with the wave vector $\mathbf{k}$ and frequency $\omega_{\mathbf{k}}$. The potential $U(|\,\mathbf{r}_1 - \mathbf{r}_2\,|)$ stands for the direct (Coulomb) interaction between electrons, the quantities $V_{\mathbf{k}}$ are the Fourier transforms of the electron-phonon interaction. A conventional model people use for optical phonons is based on the so-called Einstein dispersion law $\omega_{\mathbf{k}} = \omega_D$. Here D denotes the number of space dimensions to which electron movement is confined.

In any case the real physical space remains three dimensional. The direct interaction of electrons is supposed to be of the Coulomb type in an arbitrary number of space dimensions:

$$U(|\,\mathbf{r}_1 - \mathbf{r}_2\,|) = \hbar\omega_D \frac{U_D}{|\,\mathbf{r}_1 - \mathbf{r}_2\,|}\sqrt{\frac{\hbar}{m\omega_D}}, \tag{2}$$

where we introduce a dimensionless Coulomb coupling constant U_D.

Following Ref. 4 one can represent the electron-phonon interaction in the D-dimensional space as follows:

$$V_{\mathbf{k}} = \frac{-i\hbar\omega_D}{k^{D-1}}\left[\frac{\alpha_D}{V}\sqrt{\frac{\hbar}{2m\omega_D}}\left(2\sqrt{\pi}\right)^{D-1}\Gamma\left(\frac{D-1}{2}\right)\right]^{\frac{1}{2}}, \tag{3}$$

where V is the volume of a D-dimensional "crystal" and α_D is a coupling constant of the electron-phonon interaction.

At $D = 3$ Eqs. (1)–(3) lead to the standard Fröhlich-type bipolaron Hamiltonian with $\omega_{3D} = \omega_{LO}$ and conventional coupling constants

$$\alpha_{3D} = \alpha = \frac{e^2}{2\hbar\omega_{LO}}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)\sqrt{\frac{2m\omega_{LO}}{\hbar}} = \alpha_{em}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)\sqrt{\frac{mc^2}{2\hbar\omega_{LO}}} \tag{4}$$

and

$$U_{3D} = U = \frac{e^2}{\hbar\omega_{LO}\epsilon_\infty}\sqrt{\frac{m\omega_{LO}}{\hbar}} = \frac{\sqrt{2}\alpha}{1-\eta}, \qquad \eta = \epsilon_\infty/\epsilon_0. \tag{5}$$

Here e is the electron charge, $\alpha_{em} = e^2/\hbar c$ is the electromagnetic fine structure constant and ϵ_∞ (ϵ_0) are the high frequency (static) dielectric constants. The ratio U/α is evidently not less than $\sqrt{2}$ which defines the physical region of the bipolaron parameters.

Coupling constants α and U are well-defined parameters which can be measured experimentally. Dealing with artificial structures of lower dimensions one has to be careful with a definition of analogous parameters. Often people suppose that $\alpha_D = \alpha$ and $U_D = U$ and make some conclusions based on this assumption, which is not necessarily true. Here we clarify the point that electron-phonon and Coulomb coupling constants depend on a concrete mechanism of a realization of *physically* two-dimensional space.

In order to give an insight in the origin and the physical meaning of the 2D-bipolaron problem we shall consider how can it be deduced rigorously from that in real

multilayer structures, starting with a consistent derivation of the Hamiltonians describing both inter-electron[5,6] and electron-phonon interaction[7] for such structures. We restrict ourselves to a three-layer structure (1|2|3) consisting of semiconducting or dielectric media with the geometry and material parameters shown in Fig. 1. It is a simplified representation of high-T_c systems.

For the sake of definiteness, let the electrons be in a central layer at the positions $\mathbf{r}_n = (\boldsymbol{\rho}_n, z_n)$, $n = 1,2$. The potential energy of the direct electron-electron interaction depending on the 2D vector $\boldsymbol{\rho} = \boldsymbol{\rho}_2 - \boldsymbol{\rho}_1$ of relative position is[6]

$$U(\rho, z_1, z_2) = \frac{e^2}{\epsilon_{2,\infty}} \int_0^\infty J_0(k\rho) \Bigg\{ \exp(-k|z_1 - z_2|) + \frac{1}{\epsilon_{2,\infty}^2 + \epsilon_{2,\infty} \coth(kl)(\epsilon_{1,\infty} + \epsilon_{3,\infty}) + \epsilon_{1,\infty}\epsilon_{3,\infty}} \frac{1}{\sinh(kl)}$$
$$\times \Big[e^{-kl}(\epsilon_{2,\infty} - \epsilon_{1,\infty})(\epsilon_{2,\infty} - \epsilon_{3,\infty}) \cosh[k(z_1 - z_2)] + (\epsilon_{2,\infty}^2 - \epsilon_{1,\infty}\epsilon_{3,\infty}) \cosh[k(z_1 + z_2 - \tilde{z}_1 - \tilde{z}_2)]$$
$$+ \epsilon_{2,\infty}(\epsilon_{1,\infty} - \epsilon_{3,\infty}) \sinh[k(z_1 + z_2 - \tilde{z}_1 - \tilde{z}_2)] \Big] \Bigg\} dk, \tag{6}$$

where $J_0(x)$ is the Bessel function. Besides the aforesaid modification of the interaction between electrons, in a multilayer structure there appears another phenomenon, *self-action*, namely, each of electrons interacts with the rapid polarization induced by itself. The potential energy of the self-action for the ith electron can be written in the form

$$U_{\mathrm{SA}}(z_n) = \frac{e^2}{2\epsilon_{2,\infty}} \int_0^\infty \frac{1}{\epsilon_{2,\infty}^2 + \epsilon_{2,\infty} \coth(kl)(\epsilon_{1,\infty} + \epsilon_{3,\infty}) + \epsilon_{1,\infty}\epsilon_{3,\infty}} \frac{1}{\sinh(kl)} \Big[e^{-kl}(\epsilon_{2,\infty} - \epsilon_{1,\infty})(\epsilon_{2,\infty} - \epsilon_{3,\infty})$$
$$+ (\epsilon_{2,\infty}^2 - \epsilon_{1,\infty}\epsilon_{3,\infty}) \cosh[k(2z_n - \tilde{z}_1 - \tilde{z}_2)] + \epsilon_{2,\infty}(\epsilon_{1,\infty} - \epsilon_{3,\infty}) \sinh[k(2z_n - \tilde{z}_1 - \tilde{z}_2)] \Big] dk, \quad n = 1,2. \tag{7}$$

The phonon Hamiltonians as well as those describing the electron-phonon interaction in multilayer structures with an arbitrary number of layers were obtained in Ref. 7. They reflect a drastic reconstruction of the phonon spectrum in such structures in comparison to that of uniform media, including appearance of *interface* phonons related to the waves propagating perpendicularly to the growth axis with amplitudes decreasing when moving sufficiently far away from a boundary plane [cf. (28) below]. Generally speaking, both interface and confined LO modes are available for the carriers to couple with. The confined LO modes were described in a number of papers.[8–18] As it was shown in Ref. 19, various approaches differ from each other by the choice of the additional boundary conditions imposed on the polarization, resulting in different spatial patterns of the confined phonon modes.

The Hamiltonian of interface phonons is

$$\sum_{\mathbf{k},j} \hbar\Omega_{\mathbf{k},j}\, a_{\mathbf{k},j}^\dagger a_{\mathbf{k},j}, \tag{8}$$

where $\mathbf{k}$ is a 2D wave vector and an integer j labels the interface vibration branches possessing eigenfrequencies $\Omega_{\mathbf{k},j}$. In particular, for various versions of the structure shown in Fig. 1 these Hamiltonians were obtained in Refs. 7, 20 and 21 and in the most general case when all three layers are polar in a recent paper.[22] For the sake of simplicity, we shall confine ourselves to a symmetrical structure containing polar outer media and a nonpolar central layer, where there are two branches of the interface phonons with eigenfrequencies:

$$\Omega_{\mathbf{k},j}^2 = \omega_{1,\mathrm{TO}}^2 \frac{\epsilon_{1,0}^{(j)}(k)}{\epsilon_{1,\infty}^{(j)}(k)}, \quad j = 1,2. \tag{9}$$

Here the effective dielectric functions

$$\epsilon_{1,0}^{(1)}(k) = \epsilon_{1,0} + \epsilon_{2,\infty} \coth\left(\frac{kl}{2}\right),$$
$$\epsilon_{1,0}^{(2)}(k) = \epsilon_{1,0} + \epsilon_{2,\infty} \tanh\left(\frac{kl}{2}\right),$$
$$\epsilon_{1,\infty}^{(1)}(k) = \epsilon_{1,\infty} + \epsilon_{2,\infty} \coth\left(\frac{kl}{2}\right),$$
$$\epsilon_{1,\infty}^{(2)}(k) = \epsilon_{1,\infty} + \epsilon_{2,\infty} \tanh\left(\frac{kl}{2}\right) \tag{10}$$

determine the dispersion laws. The contribution of bulk-like (confined) vibrations will disappear in the assumed case of a nonpolar middle layer. Thus, an electron interacts only with interface phonons. We choose this model on purpose to demonstrate the physical principle that *different mechanisms of confinement lead to various coupling constants*. The Hamiltonian of the interaction of electrons with the interface phonons is

$$\sum_{n=1,2} \sum_{\mathbf{k},j} \left[a_{\mathbf{k},j}\, V_{\mathbf{k},j}\, e^{i\mathbf{k}\boldsymbol{\rho}_n} + \mathrm{H.c.} \right] g_{\mathbf{k},j}(z_n), \tag{11}$$

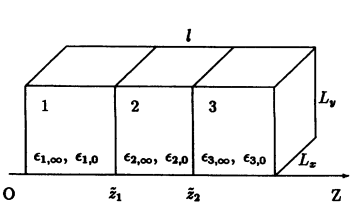

FIG. 1. A scheme of a multilayer structure. OZ is a growth axis and L_x, L_y are the sizes of a sample in a transverse plane, while $l = \tilde{z}_2 - \tilde{z}_1$ is a thickness of a middle layer.

where the functions

$$g_{\mathbf{k},1}(z) = \frac{\sinh\{k[z-(\tilde{z}_1+\tilde{z}_2)/2]\}}{\sinh(kl/2)},$$
$$g_{\mathbf{k},2}(z) = \frac{\cosh\{k[z-(\tilde{z}_1+\tilde{z}_2)/2]\}}{\cosh(kl/2)} \tag{12}$$

allow one to classify the first and second branches as describing asymmetrical and symmetrical potentials, respectively. The amplitudes in Eq. (11) may be represented in the form of Eq. (3) at $D = 2$:

$$V_{\mathbf{k},j} = -i\hbar\Omega_{\mathbf{k},j}\left(\frac{2\pi\alpha_{\mathbf{k},j}}{L_xL_yk}\sqrt{\frac{\hbar}{2m\Omega_{\mathbf{k},j}}}\right)^{\frac{1}{2}}, \tag{13}$$

where (L_xL_y) is the cross-sectional area of a structure and $\alpha_{\mathbf{k},j}$ is the effective dimensionless coupling *function* of the interaction with the jth branch of interface vibrations

$$\alpha_{\mathbf{k},j} = \frac{e^2}{2\hbar\Omega_{\mathbf{k},j}}\left(\frac{1}{\epsilon^{(j)}_{1,\infty}(k)}-\frac{1}{\epsilon^{(j)}_{1,0}(k)}\right)\sqrt{\frac{2m\Omega_{\mathbf{k},j}}{\hbar}}. \tag{14}$$

We stress that concrete forms of the above interactions depend substantially on physical mechanisms of the electron confinement. Two of them, which are of the most practical importance, will be considered below as examples.

Quantum-well confinement. In a quantum-well structure electrons are confined to a central layer due to a big gap between the bottoms of conduction bands in the neighboring materials. Under the condition of a thin layer $kl \ll 1$ (which corresponds to the situation when the radii R of the polaronic or bipolaronic states are much greater than the thickness l) we straightforwardly get from Eq. (6) a 2D Coulomb interaction

$$U(\rho) = \frac{e^2}{\rho(\epsilon_{1,\infty}+\epsilon_{3,\infty})/2} \tag{15}$$

screened by the *mean* dielectric permittivity of the two outer layers. If they are made of the same material, $\epsilon_{1,\infty} = \epsilon_{3,\infty}$, it follows from Eq. (15) that

$$U(\rho) = \frac{e^2}{\rho\epsilon_{1,\infty}}. \tag{16}$$

In the case under consideration of a thin middle layer we successively find the interface phonon eigenfrequencies (9)

$$\lim_{kl\to 0}\Omega_{\mathbf{k},1} = \omega_{1,\mathrm{TO}}, \quad \lim_{kl\to 0}\Omega_{\mathbf{k},2} = \omega_{1,\mathrm{LO}}, \tag{17}$$

the functions (12) describing the z dependence of the interaction amplitudes

$$\lim_{kl\to 0} g_{\mathbf{k},1}(z) = \frac{z-(\tilde{z}_1+\tilde{z}_2)/2}{l/2},$$
$$\lim_{kl\to 0} g_{\mathbf{k},2}(z) = 1, \tag{18}$$

and the electron-phonon coupling amplitudes (14)

$$\lim_{kl\to 0}\alpha_{\mathbf{k},1} = 0,$$
$$\lim_{kl\to 0}\alpha_{\mathbf{k},2} = \alpha_{3D} = \frac{e^2}{2\hbar\omega_{1,\mathrm{LO}}\epsilon^*}\sqrt{\frac{2m\omega_{1,\mathrm{LO}}}{\hbar}},$$
$$\epsilon^* = \frac{1}{\epsilon_{1,\infty}}-\frac{1}{\epsilon_{1,0}}. \tag{19}$$

This means that the first phonon branch is inactive in the electron-phonon interaction. Thus, the Hamiltonian (11) takes on the form

$$\sum_{n=1,2}\sum_{\mathbf{k}}\left[b_{\mathbf{k}}V_{\mathbf{k}}e^{i\mathbf{k}\rho_n}+b^{\dagger}_{\mathbf{k}}V^*_{\mathbf{k}}e^{-i\mathbf{k}\rho_n}\right], \tag{20}$$

with the amplitudes

$$V_{\mathbf{k}} = -i\hbar\omega_{2D}\left(\frac{2\pi\alpha_{2D}}{L_xL_yk}\sqrt{\frac{\hbar}{2m\omega_{2D}}}\right)^{1/2}, \tag{21}$$

wherein both the phonon eigenfrequency and the effective coupling constant coincide with those in a 3D crystal of the first material:

$$\omega_{2D} = \omega_{1,\mathrm{LO}}, \quad \alpha_{2D} = \alpha_{3D}. \tag{22}$$

Just these relations were implied by the authors of Ref. 4. Thus, we find them to be adequate for the electronic confinement to a superthin quantum well. Introducing a notation U_D for the 2D Coulomb potential in a conventional way [compare with Eq. (2)]

$$U(\rho) = \hbar\omega_{2D}\frac{U_{2D}}{\rho}\sqrt{\frac{\hbar}{m\omega_{2D}}}, \tag{23}$$

for U_{2D} we obtain the same expression Eq. (5) as for the 3D case with ϵ and α being related to the first material.

We discuss one of the limiting 2D cases when electrons move in a superthin layer between two polar media. In the intermediate region of thicknesses

$$l < R < l\frac{\epsilon^2_{2,\infty}+\epsilon_{1,\infty}\epsilon_{3,\infty}}{\epsilon_{2,\infty}(\epsilon_{1,\infty}+\epsilon_{3,\infty})} \tag{24}$$

the general formula (6) leads to a logarithmic law (see Ref. 20). In a real case of finite thickness of a layer which contains electrons there exists a continuous link with another limiting case. The latter, which we discuss now, corresponds to electrons moving near an interface between two thick slabs.

Image-potential confinement. In the opposite limiting case of a thick middle layer $kl \gg 1$ (which really means that the radii R of the polaronic or bipolaronic states are small in comparison with l) the interaction (6) for electrons in the vicinity of a boundary, say, $z_n \sim \tilde{z}_1$, turns to the 2D Coulomb potential energy

$$U(\rho) = \frac{e^2}{\rho(\epsilon_{1,\infty}+\epsilon_{2,\infty})/2}, \tag{25}$$

wherein the screening is described by the mean dielectric permittivity of the media adjacent to the boundary. If thickness of the second layer increases, then Eq. (7) leads to the *image*-potential energy for the electron in

the second substance not far from the interface (1|2):

$$U_{\mathrm{SA}}(z_n) = \frac{e^2}{\epsilon_{2,\infty}} \frac{\epsilon_{2,\infty} - \epsilon_{1,\infty}}{\epsilon_{2,\infty} + \epsilon_{1,\infty}} \frac{1}{4(z_n - \tilde{z}_1)}, \quad z_n > \tilde{z}_1. \tag{26}$$

Taking account of the polaronic effect was shown[20] to make the boundary value of the self-action potential at $z_n = \tilde{z}_1$ finite. The most important for our present discussion feature of this potential is its attractive nature if the inequality $\epsilon_{2,\infty} < \epsilon_{1,\infty}$ is satisfied (this condition holds true, e.g., for a particular case when a dielectric layer borders on vacuum[23]). Thus, in the vicinity of a boundary between two substances possessing substantially different values of dielectric permittivity in a multilayer structure, electrons suffer a strong attraction to the interface. This attraction confines them to a certain region near the interface, the extent of which along the growth axis may be controlled by the geometric and material parameters of the structure[20] and hence may be made small. In such a case the electronic motion again appears to be effectively two dimensional. In the case of a thick middle layer the eigenfrequencies occur to be degenerate:

$$\lim_{kl\to\infty} \Omega_{\mathbf{k},j} = \omega_{2\mathrm{D}} = \omega_{1,\mathrm{TO}} \sqrt{\frac{\epsilon_{1,0} + \epsilon_{2,\infty}}{\epsilon_{1,\infty} + \epsilon_{2,\infty}}}, \quad j = 1, 2. \tag{27}$$

Supposing electrons to be near the boundary (1|2), we are to pass to the limit $\tilde{z}_2 \to \infty$, which makes the functions (12) identical:

$$\lim_{kl\to\infty} g_{\mathbf{k},j}(z) = g_{\mathbf{k}}(z) = \exp[-k(z - \tilde{z}_1)], \quad j = 1, 2. \tag{28}$$

Therefore under a canonical transformation

$$b_{\mathbf{k}} = \frac{a_{\mathbf{k},1} + a_{\mathbf{k},2}}{\sqrt{2}}, \qquad b'_{\mathbf{k}} = \frac{a_{\mathbf{k},1} - a_{\mathbf{k},2}}{\sqrt{2}}$$

the Hamiltonian (11) acquires the form independent of the "primed" creation and annihilation operators

$$\sum_{n=1,2} \sum_{\mathbf{k}} \left[b_{\mathbf{k}} V_{\mathbf{k}} e^{i\mathbf{k}\rho_n} + b^{\dagger}_{\mathbf{k}} V^{*}_{\mathbf{k}} e^{-i\mathbf{k}\rho_n} \right] g_{\mathbf{k}}(z_n), \tag{29}$$

with the amplitudes (21) and the effective coupling constant

$$\alpha_{2\mathrm{D}} = \frac{e^2}{2\hbar\omega_{2\mathrm{D}}\epsilon^{**}} \sqrt{\frac{2m\omega_{2\mathrm{D}}}{\hbar}},$$

$$\frac{1}{\epsilon^{**}} = \frac{1}{(\epsilon_{1,\infty} + \epsilon_{2,\infty})/2} - \frac{1}{(\epsilon_{1,0} + \epsilon_{2,\infty})/2} \tag{30}$$

resulting from Eq. (14). Then the expression for the Coulomb coupling constant of Eq. (23) follows from Eqs. (25) and (30):

$$U_{2\mathrm{D}} = \frac{\sqrt{2}\alpha_{2\mathrm{D}}}{1 - \eta_{2\mathrm{D}}}, \qquad \eta_{2\mathrm{D}} = \frac{\epsilon_{1,\infty} + \epsilon_{2,\infty}}{\epsilon_{1,0} + \epsilon_{2,\infty}}. \tag{31}$$

In case a polar substance contacts with vacuum, $\epsilon_{2,\infty} = 1$, Eqs. (21) and (30) reproduce the known amplitude of the interaction of electrons with interface phonons obtained in Ref. 23; other papers on the subject are cited in Ref. 20. When neglecting the motion of electrons along the growth axis ($z_n = \tilde{z}_1$), we finally obtain from Eq. (29) the 2D electron-phonon interaction Hamiltonian (20), wherein the limiting interface phonon eigenfrequency (27) as well as the effective coupling constant (30) depend both on dielectric permittivities of the polar medium and on a dielectric constant of the electron-containing substance. In these circumstances under the inequality $\epsilon_{1,\infty} \gg \epsilon_{2,\infty}$ from the above-displayed results it follows obviously that

$$\omega_{2\mathrm{D}} \to \omega_{1,\mathrm{LO}}, \quad \alpha_{2\mathrm{D}} \to 2\alpha_{3\mathrm{D}}, \quad \eta_{2D} \to \eta = \frac{\epsilon_{1,\infty}}{\epsilon_{1,0}}. \tag{32}$$

Thus, the only difference with the quantum-well confinement is an effective increase of the electron-phonon coupling constant.

In a 3D space bipolarons can be formed if the electron-phonon interaction is strong enough to overcome the Coulomb repulsion. To formulate this statement numerically, it is convenient to consider a phase plane of physical parameters—Coulomb and electron-phonon coupling constants (U, α).[25] Surely, bipolarons cannot be formed at any given value of α if a Coulomb repulsion coupling constant is large enough: $U > U_c(\alpha)$. Thus, a bipolaron formation region is restricted on a phase diagram by a curve $U_c(\alpha)$ and a line $U = \sqrt{2}\alpha$ which is the border of a physical region [see Eq. (5)]. The situation is shown in Fig. 2.

Two parameters α_c and η_c, whose meaning is obvious from Fig. 2, are of importance. The best results for the 3D case are as follows: α_c lies in a range 5.4–7.3

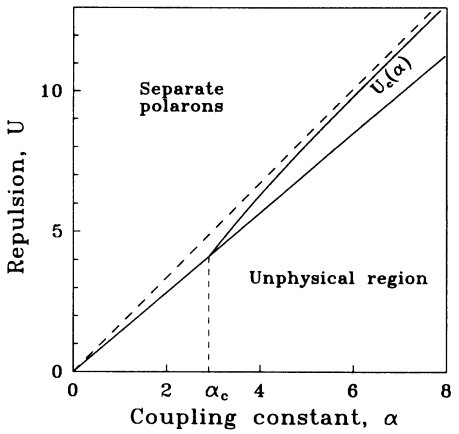

FIG. 2. Phase diagram of a bipolaron formation region. Critical value $U_c(\alpha)$ of the Coulomb coupling constant is presented as a solid curve. A dashed line represents its asymptotes $U = \sqrt{2}\alpha/(1 - \eta_c)$. The sector above the solid line $U = \sqrt{2}\alpha$ corresponds to the physical values of parameters. A space between the solid lines is a bipolaron formation region. In this plot we use results for 2D bipolarons: $\alpha_c = 2.9$ (Ref. 25) and $\eta_c = 0.158$ (Ref. 30).

(Refs. 24–27) η_c is about 0.12–0.14 (Refs. 24 and 28–30). Analogous results (including phase diagram) were obtained in the 2D case with $\alpha_{2D,c} = 2.9$ in Ref. 25 (2 in Ref. 26) and $\eta_{2D,c} = 0.158$ (Ref. 30). Herefrom people concluded that a bipolaron formation region is enlarged in 2D.

There exists some misunderstanding of the physical meaning of the results obtained for the 2D case. The immediate conclusion that the bipolaron formation region is larger in two dimensions as compared to the 3D case is based on the *assumption* that material characteristics are the same as for 3D samples. We demonstrated that this is true, say, for the quantum-well confinement when the results mentioned above take the form

$$\omega_{2D} = \omega_{LO}, \quad \alpha_{2D} = \alpha_c = 2.9, \quad \epsilon_\infty/\epsilon_0 = 0.158 \quad (33)$$

with parameters related to the outer layer.

Our second example is the image potential confinement when electrons move on the border of polar and nonpolar media. If the dielectric constant of a polar layer is much larger than that of a nonpolar layer, we have the same relations for the phonon frequency and the ratio of the dielectric constants, but $\alpha_{2D} \to 2\alpha_{3D}$. This leads to the critical value

$$\alpha_c = 2.9/2 \approx 1.4. \quad (34)$$

Here α is related to the polar layer and a bipolaron formation is easier than it was supposed before. But we can give an alternative example. Say, we deal with a polar material for which $\epsilon_{1,\infty} = 5$, $\epsilon_{1,0} = 50$. Then $\eta_c = 0.1$ and a bipolaron formation seems to be possible (if one forgets that the criterion was derived for η_{2D}). Suppose, however, that for nonpolar medium we have $\epsilon_{2,\infty} = 5$. Then, as it follows from Eq. (31), $\eta_{2D} = 2/11 \approx 0.18$. This number exceeds the reported critical value $\eta_{2D,c}$.

Thus, in general the relations between parameters are more complicated and could lead both to a *narrowing* and to a *broadening* of a bipolaron formation region. The relation between dielectric constants cannot be represented via the simple ratio $\eta = \epsilon_\infty/\epsilon_0$. At last, a phonon frequency could be changed in a *physically* two-dimensional system. So people should be careful comparing theoretical results with experimental data. Above we presented the formula needed in such cases.

To conclude we note that we do not pretend to give a quantitative description of any concrete multilayer structure. We presented here a model to display a possible role of the interface phonons in the formation of bipolarons which may be relevant to high-T_c superconductivity. Studying some concrete multilayer structure such as GaAs-GaAlAs both types of the phonons, bulklike and interface ones, certainly should be and are in fact considered simultaneously (see, for example, the monograph[20] and papers[31,32]). The spatial pattern of the bulk-type phonon field is sensitive to the additional boundary conditions imposed on the polarization and is therefore "sample specific," while the interface phonon field is shown[19] to be universal (in the sense that it does not depend on the mentioned additional boundary conditions).

Besides, according to our experience, the role of the interaction with the bulklike phonons in comparison with that of the interaction with the interface phonons in polaronic energies[20] and optical coefficients[32] depends strongly on the thickness of the electron-containing layers and is dominant for sufficiently thin layers. When (which is the case of our consideration) electrons are in nonpolar (or weakly polarizable) media, then the dominant role of the interface phonons is in general independent (or almost independent) of the thickness of these electron-containing layers. The diminishing of *this* thickness makes the electrons near the interfaces and thus creates *conditions* favorable for the interaction of electrons with the interface phonons. At the same time, the absolute characteristics of the effects due to the interface phonons evidently decrease with diminishing the thickness of the *polar* (or, correspondingly, strongly polarizable) layers. Certainly, the notion "sufficiently thin" is relative to a given structure and any attempt to formulate it precisely would require a calculation of the bipolaronic spectra with the both types of phonons being taken into consideration (see, for example, papers[31] where a number of concrete structures are discussed).

Keeping in mind results on 2D bipolarons obtained in cited papers, we tried to consider them from a more general point of view. This is why we chose the interface phonon field for the present *qualitative* consideration, calculating the contribution of the interface phonons and demonstrating wherefrom they appear.

Note also that electrons can be confined to 1D space as well. An example of a mechanism is given by a (bi)polaron in a strong magnetic field.[33,34] This mechanism leads to specific links of coupling constants in 3D and 1D. As is clear from our discussion of the 2D case, other confinement mechanisms are also possible. But in contrast with 2D where we concentrated on flat layers, one now needs the theory of (bi)polarons in axial symmetrical layers. This will allow one to take the limit of an infinitely small radius, that is, to study the physical 1D space. Such a theory is now in progress.

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