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Polaron density of states of AlAs/GaAs/AlAs and PbS/PbTe/PbS type quantum well

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Polaron energy spectrum of AlAs/GaAs/AlAs and PbS/PbTe/PbS quasi two-dimensional heterostructure as a function of the wave-vector is investigated based on the adiabatic approximation and the Ritz variational technique. The electron interaction with confined, interface and half-space phonons is taken into account. A comparative analysis of the polaron energy spectrum in heterostructures with a finite and infinite breakdown of energy bands at the interface is performed by means of the Li-Lou-Pines variational method. The polaron density of states dependence as a function of energies with the values less than phonon energies is studied. The contribution of each phonon branch to the density of states is determined. A comparative analysis is made for two AlAs/GaAs/AlAs and PbS/PbTe/PbS heterostructures.

Key words: *polaron, heterostructure, quantum well, density of states*

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Recently various low-dimensional structures such as film systems [1–13], superlattices [14], quantum wires [14–16] and quantum dots [17–22] have been widely investigated both experimentally and theoretically. These heterosystems are of great interest mainly due to their unique physical properties which can be used in the electronic and opto-electronic devices.

AlAs/GaAs/AlAs and PbS/PbTe/PbS with one-dimensional quantum well (QW) are among the most highly used low-dimensional heterostructures. The restriction of quasi-particle motion in one direction (perpendicular to the interface) causes an essential difference (in comparison with a massive crystal) not only in the energy spectrum of non-interactive quasi-particles, but also in the values of the interaction energy. Particularly, one can see the changes in the electron, phonon and polaron spectra, which, in its turn, effects the optical and kinetic properties of such structures.

The theory of polaron states has been developed in many papers [3,4,23,24], where various calculation methods and heterostructure models were used. However, most investigations studied a polaron dependence of the main parameters (effective masses, dielectric permittivities, QW widths, etc.) at the minimum of the conduction band. Therefore, in performing theoretical interpretation of the experimental data it is assumed that the polaron dispersion law has a parabolic form just like the electron one. And the difference is observed only in the values of effective mass [23]. However, the electron-phonon interaction depends on the wave vector and this should effect the nature of the polaron distribution law.

The object of this paper is to investigate the polaron dispersion law in AlAs/GaAs/AlAs, PbS/PbTe/PbS heterostructures for different values of QW width. A contribution of various phonon branches to the formation of the polaron dispersion law is determined. The polaron density of states dependence on the energy values is defined based on the calculations performed.

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1. Electron-phonon interaction in a quasi-two-dimensional system. The Hamiltonian

The structure of QW is investigated based on the two polar materials. A square well model is used here. Let z-axis be perpendicular to the surfaces of QW. The Hamiltonian of a well electron interacting with optical phonons in the effective mass approximation and non-degenerate is as follows

$$\hat{H} = \frac{\hat{p}_{||}^2}{2m_{\mathrm{e}}} + \frac{\hat{p}_z^2}{2m_{\mathrm{e}}} + V(z) + \hat{H}_{\mathrm{ph}} + \hat{H}_{\mathrm{int}}\,, \tag{1}$$

where $\hat{\mathbf{p}}_{||}$ and $\hat{\mathbf{p}}_z$ are electron momentum operators in xy-plane and in z- direction respectively, $V(z)$ is electron potential energy in the nanoheterostructure, m_{e} is a corresponding effective mass of electron

$$m_{\mathrm{e}}(z) = \begin{cases} m_1, & 0 < z < L\,, \\ m_2, & z \leqslant 0,\ z \geqslant L\,. \end{cases} \tag{2}$$

In the case of a finite quantum well (FQW) $V(z)$ is as follows:

$$V(z) = \begin{cases} 0, & 0 < z < L\,, \\ V_0, & z \leqslant 0,\ z \geqslant L\,. \end{cases} \tag{3}$$

In the dielectric continuum model, the Hamiltonian of phonon system in the presentation of occupation numbers is written down [2,3]:

$$\hat{H}_{\mathrm{ph}} = \hat{H}_{\mathrm{C}} + \hat{H}_{\mathrm{I}} + \hat{H}_{\mathrm{H}\pm}, \quad \hat{H}_{\mathrm{I}} = \hat{H}_{\mathrm{A}\pm} + \hat{H}_{\mathrm{S}\pm}\,, \tag{4}$$

where

$$\hat{H}_{\mathrm{C}} = \sum_{\mathbf{q},\,m} \hbar\omega_{\mathrm{L1}}(\mathbf{q})\, b_m^{+}(\mathbf{q})\, b_m(\mathbf{q}), \quad m = 1, 2, 3, \ldots \tag{5}$$

is the Hamiltonian of confined phonons,

$$\hat{H}_{\mathrm{I}} = \sum_{\mathbf{q}} \hbar\omega_{\mathrm{S}\pm}(\mathbf{q})\, b_{\mathrm{S}\pm}^{+}(\mathbf{q})\, b_{\mathrm{S}\pm}(\mathbf{q}) + \sum_{\mathbf{q}} \hbar\omega_{\mathrm{A}\pm}(\mathbf{q})\, b_{\mathrm{A}\pm}^{+}(\mathbf{q})\, b_{\mathrm{A}\pm}(\mathbf{q}) \tag{6}$$

is the Hamiltonian of interface phonons, whereas frequencies $\omega_{\mathrm{S}\pm}$, $\omega_{\mathrm{A}\pm}$ are determined from the dispersion equation

$$\omega_{\mathrm{S}\pm} : \varepsilon_{\infty\,1} \frac{\omega^2 - \omega_{\mathrm{L}\,1}^2}{\omega^2 - \omega_{\mathrm{T}\,1}^2} \mathrm{th}\left(\frac{1}{2} qL\right) + \varepsilon_{\infty\,2} \frac{\omega^2 - \omega_{\mathrm{L}\,2}^2}{\omega^2 - \omega_{\mathrm{T}\,2}^2} = 0,$$

$$\omega_{\mathrm{A}\pm} : \varepsilon_{\infty\,1} \frac{\omega^2 - \omega_{\mathrm{L}\,1}^2}{\omega^2 - \omega_{\mathrm{T}\,1}^2} \mathrm{ch}\left(\frac{1}{2} qL\right) + \varepsilon_{\infty\,2} \frac{\omega^2 - \omega_{\mathrm{L}\,2}^2}{\omega^2 - \omega_{\mathrm{T}\,2}^2} = 0. \tag{7}$$

Frequencies of transverse optical phonons of massive crystals of the *i-th* medium are is follows: $\omega_{\mathrm{T}i} = \omega_{\mathrm{L}i}\sqrt{\frac{\varepsilon_{i\infty}}{\varepsilon_{i0}}}$, $(i = 1,\,2)$.

$$\hat{H}_{\mathrm{H}\pm} = \sum_{\mathbf{q}} \hbar\omega_{\mathrm{L2}}(\mathbf{q})\, b_{\mathrm{H}\pm}^{+}(\mathbf{q})\, b_{\mathrm{H}\pm}(\mathbf{q}) \tag{8}$$

is the Hamiltonian of half-space optical phonons of the external medium.

The electron-phonon interaction operator in the presentation of occupation numbers with respect to phonon variables for confined phonons ($\hat{H}_{\mathrm{ep,C}}$), interface phonons ($\hat{H}_{\mathrm{ep,I}} = \hat{H}_{\mathrm{ep,S}\pm} +$

$\hat{H}_{\mathrm{ep,A}\pm}$) and half-space phonons ($\hat{H}_{\mathrm{ep,H}\pm}$) is written down, respectively

$$\begin{aligned}\hat{H}_{\mathrm{ep,C}} &= -\sum_{m}\sum_{\mathbf{q}}\left(\frac{4\pi\hbar\omega_{\mathrm{L1}}e^{2}}{V\tilde{\varepsilon}}\right)^{1/2}\frac{\sin\left(\frac{\pi m}{L}z\right)}{\left(q^{2}+\left(\frac{\pi m}{L}\right)^{2}\right)^{1/2}}\left[b_{m}(\mathbf{q})\mathrm{e}^{\mathbf{iqr}}+b_{m}^{+}(\mathbf{q})\mathrm{e}^{-\mathbf{iqr}}\right],\\ &\ \frac{1}{\tilde{\varepsilon}}=\frac{1}{\varepsilon_{\infty}}-\frac{1}{\varepsilon_{0}}\,,\end{aligned}\tag{9}$$

$$\begin{aligned}\hat{H}_{\mathrm{ep,S}\pm} &= \left(\sum_{\mathbf{q}}\left(\frac{2\pi\cdot\hbar\omega_{\mathrm{S}+}\mathrm{e}^{2}}{S}\right)^{1/2}\left(\beta_{1}^{-1}\left(\hbar\omega_{\mathrm{S}+}\right)\mathrm{th}\left(\frac{1}{2}qL\right)+\beta_{2}^{-1}\left(\hbar\omega_{\mathrm{S}+}\right)\right)^{-1/2}\right.\\ &\quad\left.\times\frac{1}{\sqrt{2q}}\phi_{\mathrm{S}}(q,z)\left(b_{\mathrm{S}+}(\mathbf{q})\mathrm{e}^{\mathbf{iq\cdot r}}+b_{\mathrm{S}+}^{+}(\mathbf{q})\mathrm{e}^{-\mathbf{iq\cdot r}}\right)\right)\\ &+\left(\sum_{\mathbf{q}}\left(\frac{2\pi\cdot\hbar\omega_{\mathrm{S}-}\mathrm{e}^{2}}{S}\right)^{1/2}\left(\beta_{1}^{-1}\left(\hbar\omega_{\mathrm{S}-}\right)\mathrm{th}\left(\frac{1}{2}qL\right)+\beta_{2}^{-1}\left(\hbar\omega_{\mathrm{S}-}\right)\right)^{-1/2}\right.\\ &\quad\left.\times\frac{1}{\sqrt{2q}}\phi_{\mathrm{S}}(q,z)\left(b_{\mathrm{S}-}(\mathbf{q})\mathrm{e}^{\mathbf{iq\cdot r}}+b_{\mathrm{S}-}^{+}(\mathbf{q})\mathrm{e}^{-\mathbf{iq\cdot r}}\right)\right),\end{aligned}\tag{10}$$

$$\begin{aligned}\hat{H}_{\mathrm{ep,A}\pm} &= \left(\sum_{\mathbf{q}}\left(\frac{2\pi\cdot\hbar\omega_{\mathrm{A}+}\mathrm{e}^{2}}{S}\right)^{1/2}\left(\beta_{1}^{-1}\left(\hbar\omega_{\mathrm{A}+}\right)\mathrm{ch}\left(\frac{1}{2}qL\right)+\beta_{2}^{-1}\left(\hbar\omega_{\mathrm{A}+}\right)\right)^{-1/2}\right.\\ &\quad\left.\times\frac{1}{\sqrt{2q}}\phi_{\mathrm{A}}(q,z)\left(b_{\mathrm{A}+}(\mathbf{q})\mathrm{e}^{\mathbf{iq\cdot r}}+b_{\mathrm{A}+}^{+}(\mathbf{q})\mathrm{e}^{-\mathbf{iq\cdot r}}\right)\right)\\ &\quad+\left(\sum_{\mathbf{q}}\left(\frac{2\pi\cdot\hbar\omega_{\mathrm{A}-}\mathrm{e}^{2}}{S}\right)^{1/2}\left(\beta_{1}^{-1}\left(\hbar\omega_{\mathrm{A}-}\right)\mathrm{ch}\left(\frac{1}{2}qL\right)+\beta_{2}^{-1}\left(\hbar\omega_{\mathrm{A}-}\right)\right)^{-1/2}\right.\\ &\quad\left.\times\frac{1}{\sqrt{2q}}\phi_{\mathrm{A}}(q,z)\left(b_{\mathrm{A}-}(\mathbf{q})\mathrm{e}^{\mathbf{iq\cdot r}}+b_{\mathrm{A}-}^{+}(\mathbf{q})\mathrm{e}^{-\mathbf{iq\cdot r}}\right)\right).\end{aligned}\tag{11}$$

$\phi_{\mathrm{S}}\left(q,z\right)$, $\phi_{\mathrm{A}}\left(q,z\right)$ and $\beta_{n}\left(\omega\right)$ functions are determined as follows

$$\phi_{\mathrm{S}}\left(q,z\right)=\begin{cases}\mathrm{e}^{qz}, & z\leqslant 0,\\ \mathrm{ch}\left(qz-q\frac{L}{2}\right)/\mathrm{ch}\left(\frac{1}{2}qL\right), & 0\leqslant z\leqslant L\,,\\ \mathrm{e}^{-q(z-L)}, & z\geqslant L,\end{cases}\tag{12}$$

$$\phi_{\mathrm{A}}\left(q,z\right)=\begin{cases}-\mathrm{e}^{qz}, & z\leqslant 0,\\ \mathrm{sh}\left(qz-q\frac{L}{2}\right)/\mathrm{sh}\left(\frac{1}{2}L\right), & 0\leqslant z\leqslant L\,,\\ \mathrm{e}^{-q(z-L)}, & z\geqslant L,\end{cases}\tag{13}$$

$$\beta_{n}\left(\omega\right)=\left(\frac{1}{\varepsilon_{\infty\,n}}-\frac{1}{\varepsilon_{0\,n}}\right)\frac{\omega_{\mathrm{L}\,n}^{2}}{\omega^{2}}\left(\frac{\omega^{2}-\omega_{\mathrm{T}\,n}^{2}}{\omega_{\mathrm{L}\,n}^{2}-\omega_{\mathrm{T}\,n}^{2}}\right)^{2}.\tag{14}$$

$$\begin{aligned}\hat{H}_{\mathrm{ep,H}\pm} &= -\sum_{\mathbf{q}_{z}>0}\sum_{\mathbf{q}}\left(\frac{2\pi\,\hbar\omega_{\mathrm{L2}}\mathrm{e}^{2}}{L^{3}\tilde{\varepsilon}}\right)^{1/2}\frac{2\sin\left(q_{z}(z-a)\right)}{\left(q^{2}+q_{z}^{2}\right)^{1/2}}\left(b_{\mathrm{H}+,q_{z}}(\mathbf{q})\mathrm{e}^{\mathbf{iq\cdot r}}+b_{\mathrm{H}+,q_{z}}^{+}(\mathbf{q})\mathrm{e}^{-\mathbf{iq\cdot r}}\right)\\ &\quad-\sum_{\mathbf{q}_{z}>0}\sum_{\mathbf{q}}\left(\frac{2\pi\,\hbar\omega_{\mathrm{L2}}\mathrm{e}^{2}}{L^{3}\tilde{\varepsilon}}\right)^{1/2}\frac{2\sin\left(q_{z}z\right)}{\left(q^{2}+q_{z}^{2}\right)^{1/2}}\left(b_{\mathrm{H}-,q_{z}}\left(\mathbf{q}\right)\mathrm{e}^{\mathbf{iq\cdot r}}+b_{\mathrm{H}-,q_{z}}^{+}\left(\mathbf{q}\right)\mathrm{e}^{\mathbf{iq\cdot r}}\right).\end{aligned}\tag{15}$$

The Li-Lou-Pines method is used here in to determine a polaron energy. It was taken into account that the considered system contains fast and slow subsystems [12]. The electron motion in the direction perpendicular to the interface represents a fast subsystem. Therefore we use the adiabatic approximation here. The Hamiltonian under consideration (1) is averaged over the wave functions of the ground stationary state for the motion along OZ axis

$$\hat{\mathrm{H}}_{\mathrm{ef}} = \langle \psi_1(z) | \hat{\mathrm{H}} | \psi_1(z) \rangle, \tag{16}$$

where the function $\psi_n(z)$ is a solution of the Schrödinger equation

$$\left[-\frac{\hbar^2}{2} \frac{\mathrm{d}}{\mathrm{d}z} \frac{1}{m_{\mathrm{e}}} \frac{\mathrm{d}}{\mathrm{d}z} + V(z) \right] \psi_n(z) = E_n \psi_n(z), \quad n = 1, 2, 3, \ldots \tag{17}$$

If the quantum well is in the form of (3), then the wave function of a particle in FQW is presented as follows

$$\psi_n(z) = \begin{cases} A\mathrm{e}^{\kappa z}, & z < 0, \\ \alpha \sin(\chi z) + \beta \cos(\chi z), & 0 \leqslant z \leqslant L, \\ B\mathrm{e}^{-\kappa z + \kappa L}, & z > L, \end{cases} \tag{18}$$

where $\kappa = \sqrt{\frac{2m_2}{\hbar^2}\left(|E - U_0|\right)}$, $\chi = \sqrt{\frac{2m_1}{\hbar^2}(E)}$.

Energy levels of stationary states are found from the dispersion equation

$$\frac{1}{m_2^2}(\kappa L)^2 - \frac{1}{m_1^2}(\chi L)^2 + \left(\frac{2}{m_1 m_2}\right)(\kappa L)\ (\chi L)\,\mathrm{ctg}\,(\chi L) = 0. \tag{19}$$

For the infinite well ($U_0 = \infty$) the wave function and energy are defined by the following equations

$$\psi_n(z) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L} n z\right), \quad E_n = \frac{\hbar^2 \pi^2}{2 m_1 L^2} n^2, \quad n = 1, 2, ...$$

Two unitary subsequent transformations by means of operators are applied to the Hamiltonian (16)

$$\hat{S} = \exp\left[\frac{\mathrm{i}}{\hbar} \left(\mathbf{P} - \sum_{\mathbf{q},\nu} b^{+}_{\mathbf{q},\nu} b_{\mathbf{q},\nu} \hbar \mathbf{q} \right) \mathbf{r} \right], \tag{20}$$

$$\hat{U} = \exp\left\{ \sum_{\mathbf{q},\nu} \left(b^{+}_{\mathbf{q},\nu} f_\nu - b_{\mathbf{q},\nu} f^{*}_\nu \right) \right\}, \tag{21}$$

where ν denotes phonon branches, $\mathbf{P} = \hbar \mathbf{k}$ is polaron impulse.

As far as we know the expressions for unitary transformations of $b_{\mathbf{q},\nu}$ and $b^{+}_{\mathbf{q},\nu}$ [25], after averaging over the vacuum phonon state $|0\rangle$, the energy function of the electron-phonon system is obtained

$$\begin{aligned} \varepsilon(f_\nu) \quad &= \quad \langle 0 | U^{-1} H U | 0 \rangle = E_1 + \frac{P^2}{2m_{\mathrm{e}}} + \sum_{\mathbf{q},\nu} \left\{ V_{\mathbf{q},\nu} M_{11,\nu} f_\nu + V^{*}_{\mathbf{q},\nu} M^{*}_{11,\nu} f^{*}_\nu \right\} \\ &+ \frac{\hbar^2}{2m_{\mathrm{e}}} \left\{ \sum_{\mathbf{q},\nu} |f_\nu|^2 \mathbf{q} \right\}^2 + \sum_{\mathbf{q},\nu} |f_\nu|^2 \left\{ \hbar\omega_\nu - \frac{\mathbf{qP}}{m_{\mathrm{e}}} \hbar + \frac{q^2}{2m_{\mathrm{e}}} \hbar^2 \right\}, \end{aligned} \tag{22}$$

where

$$M_{11,\nu} = \int \psi_1^2(z)\, F_\nu(z)\, \mathrm{d}z. \tag{23}$$

$$V_{\mathbf{q},C} = \frac{\left(\frac{4\pi\, \hbar\omega_{\mathrm{L1}} \mathrm{e}^2}{V \tilde{\varepsilon}} \right)^{1/2}}{\left(q^2 + \left(\frac{\pi m}{L} \right)^2 \right)^{1/2}}, \qquad F_{\mathrm{C}}(z) = \sin\left(\frac{\pi m}{L} z \right), \tag{24}$$

$$V_{\mathbf{q},\,S\pm} = \frac{\left(\frac{2\pi\,\hbar\omega_{\mathrm{S}\pm}\mathrm{e}^2}{S}\right)^{1/2}}{\sqrt{\beta_1^{-1}\left(\omega_{\mathrm{S}\pm}\right) th\left(\frac{1}{2}qL\right) + \beta_2^{-1}\left(\omega_{\mathrm{S}\pm}\right)}}\frac{1}{\sqrt{2q}}\,, \tag{25}$$

$$V_{\mathbf{q},\,A\pm} = \frac{\left(\frac{2\pi\,\hbar\omega_{\mathrm{A}\pm}\mathrm{e}^2}{S}\right)^{1/2}}{\sqrt{\beta_1^{-1}\left(\omega_{\mathrm{A}\pm}\right) ch\left(\frac{1}{2}qL\right) + \beta_2^{-1}\left(\omega_{\mathrm{A}\pm}\right)}}\frac{1}{\sqrt{2q}}\,. \tag{26}$$

For the infinite QW

$$F_{\mathrm{S}\pm}\left(z\right) = \frac{\mathrm{ch}\left(qz - q\frac{L}{2}\right)}{\mathrm{ch}\left(\frac{1}{2}qL\right)}\,,\quad F_{\mathrm{A}\pm}\left(z\right) = \frac{\mathrm{sh}\left(qz - q\frac{L}{2}\right)}{\mathrm{sh}\left(\frac{1}{2}qL\right)}\,, \tag{27}$$

and in the case of a finite QW $F_{\mathrm{S}\pm}\left(z\right)$, $F_{\mathrm{A}\pm}\left(z\right)$ is written down (12) and (13), respectively.

Confined phonons are only with the QW, that is ([23])

$$H_{\mathrm{C}}\left(z\right) = \begin{cases} 1, & \text{if}\quad 0 \leqslant z \leqslant L, \\ 0, & \text{otherwise}\,. \end{cases}$$

In the case of FQW there is another phonon type, represented by half-space phonons for which

$$V_{\mathbf{q},\,H\pm} = \frac{2\left(\frac{2\pi\,\hbar\omega_{\mathrm{L}2}\mathrm{e}^2}{L^3\tilde{\varepsilon}_2}\right)^{1/2}}{\left(q^2+q_z^2\right)^{1/2}}\,,\quad F_{\mathrm{H}+}\left(z\right) = \sin\left(q_z(z-a)\right),\quad F_{\mathrm{H}-}\left(z\right) = \sin\left(q_z z\right),$$

$$H_{\mathrm{H}+}\left(z\right) = \begin{cases} 1, & \text{if } z \geqslant a, \\ 0, & \text{otherwise,} \end{cases}\qquad H_{\mathrm{H}-}\left(z\right) = \begin{cases} 1, & \text{if } z \leqslant 0, \\ 0, & \text{otherwise.} \end{cases}$$

E_1 is the electron ground state energy.

Minimizing $\varepsilon(f)$ over f_ν and f_ν^*, and using $\mathbf{P} = \hbar\mathbf{k}$, one can get a polaron energy of the heterosystem

$$\begin{aligned} E_{\mathrm{pol}}(k) &= E_1 + \frac{\hbar^2k^2}{2m_{\mathrm{e}}}\left(1 + \sum_\nu \eta_\nu^2\right) + \sum_{\mathbf{q},\,\nu}\frac{-2\cdot|V_{\mathbf{q},\,\nu}|^2|M_{11,\,\nu}|^2}{\hbar\omega_\nu - \frac{\hbar\mathbf{qP}}{m_{\mathrm{e}}}\left(1-\eta_\nu\right) + \frac{\hbar^2q^2}{2m_{\mathrm{e}}}} \\ &\quad + \sum_{\mathbf{q}}\frac{|V_{\mathbf{q},\,\nu}|^2|M_{11,\,\nu}|^2\cdot\left\{\hbar\omega_\nu - \frac{\hbar\mathbf{qP}}{m_{\mathrm{e}}} + \frac{\hbar^2q^2}{2m_{\mathrm{e}}}\right\}}{\left\{\hbar\omega_\nu - \frac{\hbar\mathbf{qP}}{m_{\mathrm{e}}}\left(1-\eta_\nu\right) + \frac{\hbar^2q^2}{2m_{\mathrm{e}}}\right\}}, \end{aligned} \tag{28}$$

where

$$\eta_\nu\mathbf{P} = \sum_{\mathbf{q}}|f_{\mathrm{min},\,\nu}|^2\hbar\mathbf{q}\,,\qquad f_{\mathrm{min},\,\nu} = -\frac{V_{\mathbf{q},\,\nu}^*M_{11,\,\nu}^*}{\hbar\omega_\nu + \frac{\hbar^2q^2}{2m_{\mathrm{e}}} - \frac{\hbar^2}{m_{\mathrm{e}}}\mathbf{kq}\left(1-\eta_\nu\right)}\,.$$

Expression (28) defines the polaron energy dependence on the wave vector which is actually the polaron dispersion law.

Calculations are also performed without use of the adiabatic approximation. The difference is that we do not distinguish between slow and fast motion of electrons in different directions. Then two subsequent transformations are applied to Hamiltonian (1) using the operators (20), (21), and after averaging over the vacuum phonon state $|0\rangle$ the following Hamiltonian is obtained

$$\begin{aligned} \hat{H} &= V\left(z\right) + \frac{\hbar^2}{2m_{\mathrm{e}}}k^2 - \sum_{\mathbf{q},m}V_{\mathbf{q},\,\nu}F_\nu\left(z\right)\left(f_\nu + f_\nu^*\right) + \frac{\hbar^2}{2m_{\mathrm{e}}}\left(\sum_{\mathbf{q}}|f_\nu|^2\mathbf{q}\right)^2 \\ &\quad + \sum_{\mathbf{q}}|f_\nu|^2\left(\hbar\omega - \frac{\hbar}{m_{\mathrm{e}}}\left(\hbar\mathbf{k}\right)\mathbf{q} + \frac{\hbar^2}{2m_{\mathrm{e}}}q^2\right). \end{aligned} \tag{29}$$

Minimizing $\varepsilon(f)$ (29) over f_ν and f_ν^*, and using $\mathbf{P} = \hbar\mathbf{k}$ we get:

$$\hat{H} = V(z) + \frac{\hbar^2 k^2}{2m_{\mathrm{e}}}\left(1 + \sum_\nu \eta_\nu^2\right) - \sum_{\mathbf{q},\nu} \frac{2 \cdot |V_{\mathbf{q},\nu}|^2 |F_\nu(z)|^2}{\hbar\omega_\nu - \frac{\hbar\mathbf{qP}}{m_{\mathrm{e}}}(1-\eta_\nu) + \frac{\hbar^2 q^2}{2m_{\mathrm{e}}}} + \sum_{\mathbf{q},\nu} \frac{|V_{\mathbf{q},\nu}|^2 |F_\nu(z)|^2 \cdot \left\{\hbar\omega_\nu - \frac{\hbar\mathbf{qP}}{m_{\mathrm{e}}} + \frac{\hbar^2 q^2}{2m_{\mathrm{e}}}\right\}}{\left\{\hbar\omega_\nu - \frac{\hbar\mathbf{qP}}{m_{\mathrm{e}}}(1-\eta_\nu) + \frac{\hbar^2 q^2}{2m_{\mathrm{e}}}\right\}}. \tag{30}$$

We may conveniently introduce the parameter η_ν in formula (30) according to [23] defined by

$$\eta_\nu \mathbf{P} = \sum_{\mathbf{q}} |f_{\min,\nu}|^2 \hbar\mathbf{q}, \qquad f_{\min,\nu} = \frac{V^*_{\mathbf{q},\nu} F_\nu(z)}{\hbar\omega_\nu + \frac{\hbar^2 q^2}{2m_{\mathrm{e}}} - \frac{\hbar^2}{m_{\mathrm{e}}}\mathbf{kq}(1-\eta_\nu)}.$$

The next stage of problem solving is to find a solution of the Schrödinger equation with Hamiltonian (30. The problem is solved using the Ritz variational method. A trial wave function of the ground state of the system is expressed as follows

$$\psi(z) = A \cdot \mathrm{e}^{-\alpha\left(z - \frac{L}{2}\right)^2}, \tag{31}$$

where α is a variational parameter, $A = \sqrt[4]{\frac{2\alpha}{\pi}}$ is a normalizing constant.

According to the variational technique, the following functional is found

$$\int_{-\infty}^{\infty} \psi^*(z)\,\hat{H}\psi(z)\,\mathrm{d}z = E_{\mathrm{pol}}(\alpha). \tag{32}$$

The polaron energy is determined as the minimum of function $E_{\mathrm{pol}}(\alpha)$. The calculations are performed for two heterostructures AlAs/GaAs/AlAs, PbS/PbTe/PbS, for which the weak and transition electron-phonon coupling is realized.

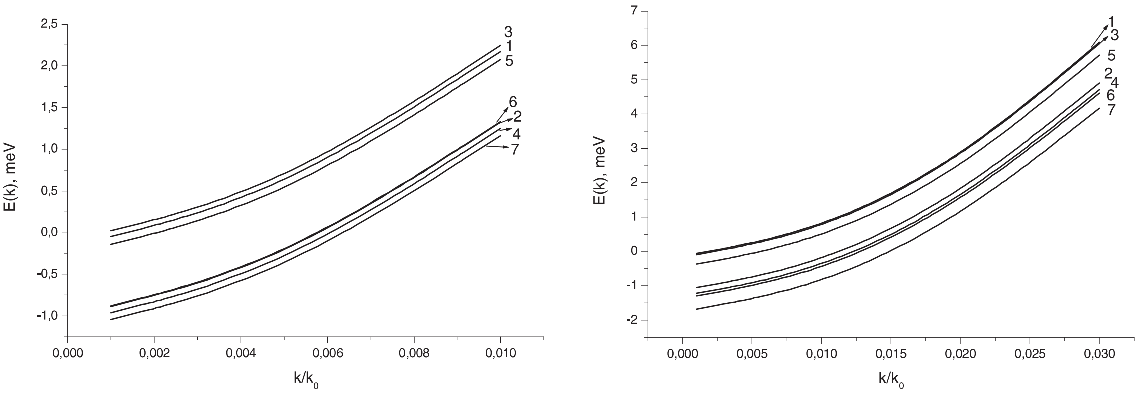
2. Numerical calculations. The analysis of the obtained results

Using expression (28) a polaron energy in the heterostructure can be calculated. The polaron dispersion relations

$$E(k) = E_{\mathrm{pol}}(k) - E_1$$

with consideration of various phonon branches in heterosystems AlAs/GaAs/AlAs and PbS/PbTe/PbS, in the cases of the finite and infinite QW's are shown in figures 1a and 1b. Herein, we take GaAs for material 1 and AlAs for material 2. Material parameters are taken to be $m_{\mathrm{e}} = 0.067m_0$, $\hbar\omega_{\mathrm{L}} = 36.2meV$, $\hbar\omega_{\mathrm{T}} = 33.3meV$, $\varepsilon_\infty = 10.9$ for GaAs. For AlAs, we take $m_{\mathrm{e}} = 0.124m_0$, $\hbar\omega_{\mathrm{L}} = 50.1meV$, $\hbar\omega_{\mathrm{T}} = 44.8meV$, $\varepsilon_\infty = 8.16$. Then, we take PbTe for material 1 and PbS for material 2. Material parameters are taken to be $m_{\mathrm{e}} = 0.22m_0$, $\hbar\omega_{\mathrm{L}} = 13.6meV$, $\hbar\omega_{\mathrm{T}} = 3.9meV$, $\varepsilon_\infty = 33$ for PbTe. For PbS, we take $m_{\mathrm{e}} = 0.124m_0$, $\hbar\omega_{\mathrm{L}} = 50.1meV$, $\hbar\omega_{\mathrm{T}} = 44.8meV$, $\varepsilon_\infty = 8.16$.

From the figures it is seen that the energy of polarons in the PbS/PbTe/PbS heterosystem is less (the binding energy is greater) than in the AlAs/GaAs/AlAs structure for every value of the wave vector (k/k_0, $k_0 = \pi/a$, a is a lattice parameter) which is related to the magnitude of the electron-phonon interaction coefficients. The common thing is that in the finite quantum well model the polaron energy is less than in the infinite quantum well model of either structure. In spite of that, in the case of the infinite quantum well, half-space phonons are not taken into account. Strong spatial confinement of the charge leads to a considerable growth of the effective electron-phonon interaction and to larger growth of polaron binding energy. That is why curve 7 is located lower than curve 4 in the graphs.



(a) (b)

Figure 1. (a) The polaron energy for a AlAs/GaAs/AlAs crystal. 1,5 show the energy with account of confined phonons for the FQW and IQW respectively, 2,6 indicate the energy with account of interface phonons for the FQW and IQW correspondingly, 3 is the energy with account of half-space phonons of FQW, 4,7 show the polaron energy with account of all phonon branches respectively for the FQW and IQW. (b) The polaron energy for a PbS/PbTe/PbS crystal with $L = 25$ Å. The notation of curves is analogous to (a).

It is interesting to consider the result concerning the contribution of separate phonon branches to the polaron energy. It is seen that at small widths of QW the contribution of confined phonons and half-space phonons is similar. The contribution of surface phonons is fundamental. The analysis shows that the enhancement of L is accompanied by the rise of contribution of confined phonons, while the role of phonon branches decreases.

It is known that a quantity such as quasiparticle density of states is used in calculating optical and kinetic coefficients. Having the polaron dispersion law, one can determine the polaron density of states as a function of energy and compare it with a corresponding function for electron. For quasi-two-dimensional electron gas with a quadratic dispersion law, the density of states for each level does not depend on energy and is determined by the expression

$$g_{\mathrm{e}}\left(E\right) = S\frac{1}{4\pi^3}\frac{m_{\mathrm{e}}}{\hbar^2}\,.$$

In the case of polarons, as one can see from the presented results, the dispersion law in the region $k < k_f$ becomes more complicated. That is why the density of states has to be presented as follows:

$$g_{\mathrm{pol}}\left(E\right) = \frac{S}{4\pi^3}k\left(E\right)\frac{\mathrm{d}\left(k\left(E\right)\right)}{\mathrm{d}E}\,.$$

The results of calculations of the density of states as a function of energy are presented in figures 2,3. From figure 2, which shows a contribution of various phonon branches to the density of states, one can see that $g\left(E\right)$ is mainly determined by interface phonons. Meanwhile the weight of confined and half-space phonons is fairly small. The analysis of function $g\left(E\right)$ for an excited level shows that concerning the weight of the oscillation branches the picture is qualitatively similar to that of the ground state. However, in a quantitative sense the density of states of an excited level is considerably less than that of the ground state (figure 3).

As to the dependence $g = g\left(E\right)$ the density of states practically does not depend on energy in the region of low energies for either polaron state, as well as for electron states. But in the region of the polaron energy approaching the phonon energy a fairly abrupt increase of the density of states is obtained.

The above mentioned graphic dependences rest on the adiabatic approximation within the framework of which the charge motion in the direction perpendicular to the separation boundaries was considered rather fast, whereas in the other two it was considered slow. We can substantiate this approximation using the variational technique based on the expressions (31) and (32).

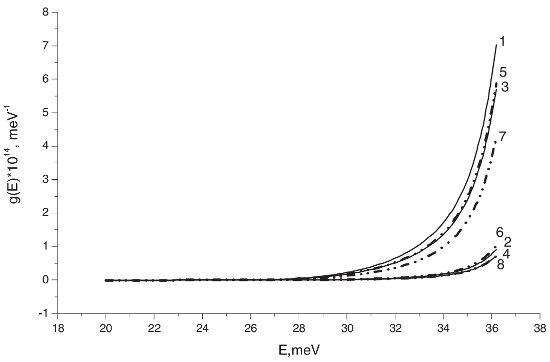


Figure 2. $g(E)$ of the polaron ground state of the AlAs/GaAs/AlAs heterosystem for the QW with $L = 25$ Å (curves 1,2,3,4) and $L = 35$ Å (curves 5,6,7,8) in the case of FQW. 1,5 take into account all phonon modes, 2,6 indicate the contribution of confined phonons, 3,7 take into account interface phonons, 4,8 show the contribution of half-space phonons.

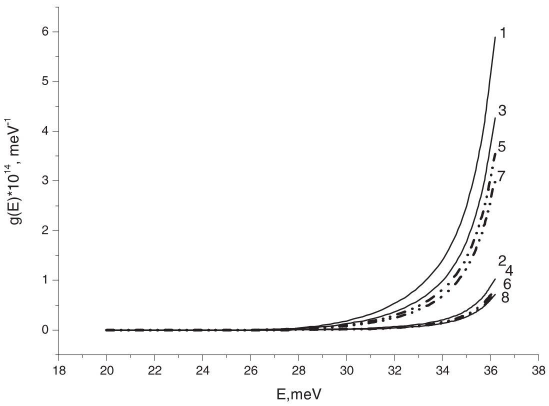


Figure 3. The polaron density of states of the AlAs/GaAs/AlAs heterosystem with $L = 35$ Å in the case of FQW for the ground state (curves 1,2,3,4) and excited state (curves 5,6,7,8). The notation of curves corresponds to the branches analogous to those in figure 2.

Figure 4 presents polaron dispersion laws at $L = 25$ Å in the case of finite QW with account of all phonon branches for the AlAs/GaAs/AlAs heterosystem. It is seen that within the framework of variational calculations, the particle energy is predictedly smaller than that in the adiabatic approximation. However, due to the small value of L, the adiabatic approximation is fairly good (at $k = 0$ the error is 10%).

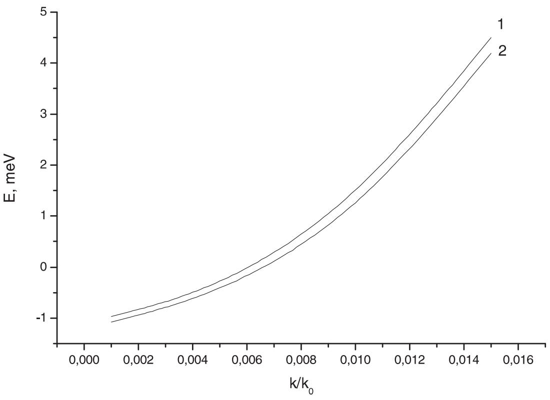


Figure 4. 1 shows the polaron energy for the AlAs/GaAs/AlAs heterostructure at the transition layer width $L = 25$ Å calculated using the LLP method in the case of FQW, 2 indicates this without the adiabatic approach.

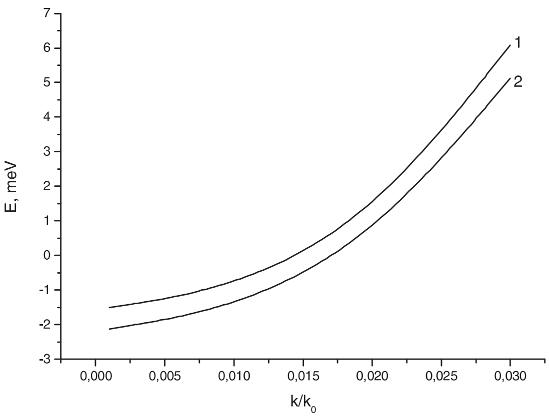


Figure 5. 1 shows the polaron energy for the PbS/PbTe/PbS heterostructure at the transition layer width $L = 25$ Å, calculated using the LLP method in the case of FQW, 2 indicates this without the adiabatic approach.

Similar dependences with the use of the two calculation techniques for PbS/PbTe/PbS are presented in figure 5. It is seen that in either approach, the function $E = E(k)$ is practically the same. However, within variational calculations, the polaron energy is essentially smaller. This shows that due to large electron-phonon interaction, the motion in the direction perpendicular to the separation boundaries can be considered fast. However, the error makes up 30% .

Therefore, the polaron energy spectrum of quasi-two-dimentional heterosystem (AlAs/GaAs/AlAs and PbS/PbTe/PbS) is studied in this paper as a function of the wave vector. The electron interaction with confined, interface and half-space phonons is taken into account. Using the Li-Lou-Pines variational method, a comparative analysis of a polaron energy spectrum in the heterostructures with finite and infinite breakdown of energy bands at the interface is made. Based on the performed calculations, the dependence of polaron density of states in the region of energies less than the phonon energy is defined. The weight of every phonon branch in the density of states is determined. The calculations of the polaron energy spectrum are made based on the adiabatic approximation and Ritz variational technique. The comparative analysis for two AlAs/GaAs/AlAs and PbS/PbTe/PbS heterostructures is performed. It is shown that for the first structure at small α, the adiabatic approximation can be used with a high degree of accuracy, whereas for the PbS/PbTe/PbS structure it can be applied with certain precautions.

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Густина поляронних станів плоскої квантової ями типу AlAs/GaAs/AlAs і PbTe/PbS/PbTe

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На основі адіабатичного наближення та варіаційного методу Рітца досліджено енергетичний спектр полярона квазідвовимірної гетеросистеми AlAs/GaAs/AlAs та PbTe/PbS/PbTe в залежності від хвильового вектора. Враховано взаємодію електрона як з обмеженими, так і з поверхневими та напівобмеженими фононами. Використовуючи варіаційний метод Лі-Лоу-Пайнса, зроблено порівняльний аналіз енергетичного спектру полярона у гетероструктурах із скінченним та нескінченним розривом енергетичних зон на межі поділу. Досліджено залежність густини станів поляронів від енергії в області енергій, менших за енергію фононів. Визначено внесок у густину станів кожної з фононних віток. Проведено порівняльний аналіз для двох гетероструктур AlAs/GaAs/AlAs та PbTe/PbS/PbTe.

Ключові слова: *полярон, гетероструктура, квантова яма, густина станів*

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