Theory of bound polarons near interfaces of polar semiconductors

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The binding energy of the ground state of a bound polaron near an interface of a polar-polar semiconductor is obtained, using a variational method, as a function of the static electric field applied perpendicular to the interface and the impurity position. Assuming that the electron couples with both the bulk LO phonon and the interface phonons, it is shown that the total polaronic correction decreases the binding energy and depending on the system it is found that a minimum external electric field is necessary to obtain a stable, bound ground state. We have shown that the contribution of the interface phonons to the effective interaction between the electron and the impurity is repulsive. Numerical results are present for systems constituted by the heterojunctions AlAs-GaAs and GaAs-GaSb.

I. INTRODUCTION

In the past few years, the electronic and transport properties of semiconductor structures such as superlattices and multiple quantum wells have been studied both experimentally and theoretically.[1,2] The presence of impurities in these systems can be controlled experimentally and they can affect the transport mechanisms, principally at low temperatures. Several efforts to understand various properties of an electron bound to a shallow dopant impurity in polar materials have been published. In three-dimensional systems it is known that the electron–bulk-longitudinal-optical (LO) -phonon interaction plays an important role, and these studies have shown that this interaction tends to increase the binding energy and the electron effective mass.[3–5] On the other hand, in superlattices and heterojunctions the presence of interfaces changes dramatically the properties of the free polaron[6] and the bound polaron. In these systems the electron–interface-phonon interaction needs to be considered.[7]

The binding energy of an electron bound to an impurity has been calculated in several systems. In n-type Si inversion layers the binding energy was calculated as a function of the screening parameter and the external electric field.[8] In quantum wells the binding energy was calculated by several authors as a function of the layer thickness, the impurity position inside the well,[9] screening effects,[10] the finite height of the barriers at the interfaces,[11] and the polaronic effects.[12–14] Recently, Li, Zheng, and Gu[15] have investigated the properties of an electron bound to an impurity in a polar crystal slab. In their calculation the electron–surface-optical (SO) phonon interactions were considered, but the interaction of the impurity with SO and LO phonons were neglected. As has been shown by Platzman[3] and by Nettel[4] for the analogous case of the three-dimensional bound polaron, this interaction plays an important role in screening the Coulomb interaction and consequently changes the binding energy by a considerable amount.

In the present work we report the calculation of polaronic effects on the binding energy of an electron bound to a positive isolated hydrogenic impurity near a polar-polar interface, by taking into account the coupling between electrons and interface phonons and LO phonons, the electronic polarizability, and also the possible anisotropic electron effective mass. We have calculated the contribution of the interface phonons to the effective interaction between the electron and the impurity. The influence of an external static electric field, applied perpendicular to the interface, on the binding energy is also investigated. Since the heterojunctions of interest are constituted by weakly polar semiconductors, we will apply a generalization of the variational method proposed by Lee, Low, and Pines[16] which is known to be valid for this range of the electron-phonon coupling constant.

The theory is applied to heterojunctions: AlAs-GaAs and GaAs-GaSb. In the case of the heterojunction AlAs-GaAs, we discuss two different situations: (1) the impurity is localized inside the GaAs and the electron is confined at the X point of the conduction band of AlAs; (2) the impurity is localized inside the AlAs and the electron is confined at the Γ point of the conduction band of GaAs. When the electron is at the X point of the conduction band of AlAs there is a high anisotropy on the electron effective mass such that the longitudinal mass ($m_{\perp}$) is about six times larger than the transversal mass ($m_{\parallel}$), however when the electron is at the Γ point of the GaAs the electron effective mass is isotropic.[17] For the heterojunction GaAs-GaSb, we consider the situation in which the electron is confined in GaAs and the impurity is localized inside GaSb. As it is to be expected the

electron–LO-phonon interaction increases the binding energy. On the other hand, we have observed that the inclusion of the interactions of the electron and the impurity with the interface phonons in the calculation decreases the binding energy of the ground state. This result is interesting because it shows that the total polaronic correction to the binding energy can be positive and consequently decreases the stability of the electron-impurity system. As we will see, this result is due to the fact that the impurity induces interface charges with the same sign of the electron charge which tends to maintain the electron far from the interface. The presence of the static external electric field applied perpendicular to the interface increases the binding energy and the polaronic corrections since the electron is closer to the interface.

This paper is organized as follows. In Sec. II the model Hamiltonian for the electron-impurity interaction is defined taking into account the anisotropy of the electron effective mass, the electron-LO-phonon and electron (impurity) –interface-phonon interactions, and the effects of the electronic polarizability. In Sec. III we present the variational method and set up a variational wave function to obtain the binding energy of the ground state. Finally, we present in Sec. IV the numerical calculations and concluding remarks.

II. THE MODEL HAMILTONIAN

We consider a system constituted by a junction of two semi-infinite polar semiconductors with the interface placed at $z=0$ and characterized by the wave vector independent lattice dielectric functions $\epsilon_1(\omega)$ for $z>0$ and $\epsilon_2(\omega)$ for $z<0$, respectively. Using an infinite-potential-barrier model, we will assume that the impurity will be placed at z_0 ($z_0 \leq 0$) and the electron is inside of the material 1 ($z \geq 0$), as shown in Fig. 1. The electron effective mass has transversal component $m_{\parallel}$ and longitudinal component $m_{\perp}$. To obtain the interface phonons frequencies ω_λ and the bulk LO phonons frequencies $\omega_{\mathrm{LO}i}$ ($i=1,2$) we have used the well-known relations $\epsilon_1(\omega_\lambda)+\epsilon_2(\omega_\lambda)=0$ and $\epsilon_i(\omega_{\mathrm{LO}i})=0$, respectively. The Hamiltonian of the system can be written as

$$H = H_e + H_{\mathrm{ph}} + H_{\mathrm{int}} \tag{2.1}$$

with

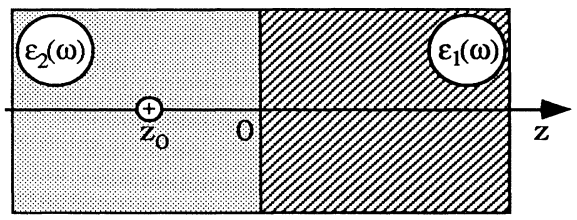

FIG. 1. System considered in the present paper. The electron is confined in material 1 and a positive hydrogenic impurity is placed at z_0. We consider the electron interacting with both interface and bulk LO phonons and we take into account the anisotropic electron effective mass.

$$H_e = \frac{p_x^2+p_y^2}{2m_{\parallel}} + \frac{p_z^2}{2m_{\perp}} + V(z) - ezE_{\mathrm{ext}} + \frac{e^2}{4z\epsilon_{\infty 1}} \frac{(\epsilon_{\infty 1}-\epsilon_{\infty 2})}{(\epsilon_{\infty 1}+\epsilon_{\infty 2})} , \tag{2.2}$$

where the third term represents the barrier at the interface which will be taken to be equal to infinity for $z<0$ and zero for $z>0$, and E_{ext} is a static external electric field applied perpendicular to the interface. The last term corresponds to the electron interaction with the electronic part of the polarization which follows the electron adiabatically, and $\epsilon_{\infty 1}$, $\epsilon_{\infty 2}$ are the optical dielectric constants of the materials 1 and 2, respectively. The Hamiltonian of the phonons H_{ph} in Eq. (2.1) is given by

$$H_{\mathrm{ph}} = \sum_{\mathbf{q}} \hbar\omega_{\mathrm{LO}} a_{\mathbf{q}}^{\dagger} a_{\mathbf{q}} + \sum_{\lambda} \sum_{\mathbf{Q}} \hbar\omega_\lambda b_{\mathbf{Q}\lambda}^{\dagger} b_{\mathbf{Q}\lambda} , \tag{2.3}$$

where $a_{\mathbf{q}}$ is the annihilation operator of the bulk LO phonons of material 1 with wave vector $\mathbf{q}=(\mathbf{Q},q_z)$ and the energy $\hbar\omega_{\mathrm{LO}}$, and $b_{\mathbf{Q}\lambda}$ is the annihilation operator of the interface excitation with wave vector $\mathbf{Q}$, the in-plane projection of $\mathbf{q}$ with energy $\hbar\omega_\lambda$. In Eq. (2.3), we have considered only the bulk LO phonons of material 1 since we are using the infinite-potential-barrier model and consequently the electron does not couple with the bulk LO phonons of material 2. The interaction between the impurity and bulk LO phonons of material 2 was not considered due to the fact that it does not contribute to the binding energy of the bound polaron.

The Hamiltonian H_{int} in Eq. (2.1) is given by

$$H_{\mathrm{int}} = \frac{e^2}{\epsilon_{\mathrm{eff}}[\rho^2+(z-z_0)^2]^{1/2}} + H_B + H_I , \tag{2.4}$$

where $\epsilon_{\mathrm{eff}}=(\epsilon_{\infty 1}+\epsilon_{\infty 2})/2$ and

$$H_B = \sum_{\mathbf{q}} \Gamma(\mathbf{q}) e^{i\mathbf{Q}\cdot\rho} \sin(q_z z)(a_{\mathbf{q}}+a_{\mathbf{q}}^{+}) \tag{2.5}$$

is the electron–bulk-LO-phonon interaction and

$$H_I = \sum_{\lambda} \sum_{\mathbf{Q}} \gamma_\lambda(\mathbf{Q})(e^{i\mathbf{Q}\cdot\rho}e^{-Qz} - e^{Qz_0})(b_{\mathbf{Q}\lambda}+b_{-\mathbf{Q}\lambda}^{+}) , \tag{2.6}$$

is the electron (impurity) –interface-phonon interaction. The Fourier coefficients for the interactions described in Eqs. (2.5) and (2.6) are

$$\Gamma(\mathbf{q}) = -i\frac{\hbar\omega_{\mathrm{LO}}}{q} \left[\frac{4\pi}{\Omega} \left[\frac{1}{\epsilon_{\infty 1}} - \frac{1}{\epsilon_{01}} \right] \frac{e^2}{\hbar\omega_{\mathrm{LO}}} \right]^{1/2} \tag{2.7}$$

and

$$\gamma_\lambda(Q) = \frac{\hbar\omega_\lambda}{\sqrt{Q}} \left[\frac{2\pi}{A} \alpha_\lambda r_{p\lambda} \right]^{1/2} , \tag{2.8}$$

respectively,[6] where Ω is the volume of material 1, A is the area of the interface, ϵ_{01} is the static dielectric constant of material 1, and by analogy with the bulk polaron problem we have defined the traditional dimensionless electron–interface-phonon coupling α_λ and the interface polaron radius as

$$\alpha_\lambda=\frac{e^2}{\hbar\omega_\lambda r_{p\lambda}}\left[\frac{\omega_\lambda^2}{\omega_{pl}^2}\theta_1(\omega_\lambda)[\epsilon_1(\omega_\lambda)-1]^2+\frac{\omega_\lambda^2}{\omega_{p2}^2}\theta_2(\omega_\lambda)[\epsilon_2(\omega_\lambda)-1]^2\right]^{-1}, \quad (2.9)$$

$$r_{p\lambda}=\left[\frac{\hbar}{2m_\parallel\omega_\lambda}\right]^{1/2}, \quad (2.10)$$

respectively. In Eq. (2.9) the dielectric function of both media is considered in the simplest case of diatomic crystals where we have only one set of infrared-active modes,

$$\epsilon_n(\omega)=\epsilon_{\infty n}\frac{\omega_{\mathrm{LO}n}^2-\omega^2}{\omega_{\mathrm{TO}n}^2-\omega^2}, \quad (2.11)$$

with $\omega_{\mathrm{TO}n}$ as the transverse optical frequency of the material n ($n=1,2$), and the ion plasma frequency is given by

$$\omega_{pn}=\left[\frac{9\epsilon_{\infty n}}{(\epsilon_{\infty n}+2)^2}(\omega_{\mathrm{LO}n}^2-\omega_{\mathrm{TO}n}^2)\right]^{1/2}, \quad (2.12)$$

and the function $\theta_n(\omega)$ is defined as

$$\theta_n(\omega)=\left[1+\frac{\epsilon_{on}}{3\epsilon_{\infty n}}\frac{(\epsilon_{\infty n}-1)(\epsilon_{\infty n}+2)}{(\epsilon_{on}-\epsilon_{\infty n})}\frac{(\omega_{on}^2-\omega^2)}{\omega_{\mathrm{LO}n}^2}\right]^2, \quad (2.13)$$

with

$$\omega_{on}=\left[\omega_{\mathrm{LO}n}^2-\frac{2}{\epsilon_{\infty n}+2}(\omega_{\mathrm{LO}n}^2-\omega_{\mathrm{TO}n}^2)\right]^{1/2}. \quad (2.14)$$

III. THE VARIATIONAL METHOD

Since the materials of interest are weakly polar, such that the electron-phonon interaction is in the weak-coupling regime, we will use a generalization of the Lee, Low, and Pines method[16] in order to obtain the ground-state energy of the bound polaron near an interface of a polar-polar semiconductor. This method has been used extensively and is very well established in the literature such that we will not present all calculations in detail. Thus, the variation technique developed by Lee, Low, and Pines,[16] is generalized considering the following ansatz to the wave function of the bound polaron:

$$\psi=\Phi(z)\varphi(\rho)U|0\rangle, \quad (3.1)$$

where $\Phi(z)$ is the electron wave function in the z direction, $\varphi(\rho)$ describes the electron wave function parallel to the interface, $|0\rangle$ is the phonon vacuum state, and the canonical transformation U is given by

$$U=\exp\left[\sum_{\lambda,Q}(f_{Q\lambda}b_{Q\lambda}-f_{Q\lambda}^*b_{Q\lambda}^\dagger)\right]\times\exp\left[\sum_q(g_qa_q-g_q^*a_q^\dagger)\right], \quad (3.2)$$

where $f_{Q\lambda}$ and g_q are variational functions to be determined requiring that the energy of the system be minimum. The total energy of the bound interface polaron is obtained computing the expectation value $\langle\psi|H|\psi\rangle$, which gives

$$E=\left\langle\varphi\left|\frac{p_x^2+p_y^2}{2m_\parallel}\right|\varphi\right\rangle+\left\langle\Phi\left|\frac{p_z^2}{2m_\perp}\right|\phi\right\rangle-\frac{e^2}{\epsilon_{\mathrm{eff}}}\int_0^\infty dQe^{Qz_0}M(Q)G(Q)-\langle\Phi|ezE_{\mathrm{ext}}|\Phi\rangle+\frac{(\epsilon_{\infty1}-\epsilon_{\infty2})}{(\epsilon_{\infty1}+\epsilon_{\infty2})}\frac{e^2}{4\epsilon_{\infty1}}\langle\Phi|z^{-1}|\Phi\rangle+\Delta E_B+\Delta E_I, \quad (3.3)$$

where the contributions from the electron–bulk-LO-phonon interaction and the electron (impurity) –interface-phonon interaction are given by

$$\Delta E_B=-\frac{e^2}{2}\left[\frac{1}{\epsilon_{\infty1}}-\frac{1}{\epsilon_{o1}}\right]\int_0^\infty dQ\,M^2(Q)[F(Q)-G^2(Q)] \quad (3.4)$$

and

$$\Delta E_I=-\sum_\lambda\alpha_\lambda\hbar\omega_\lambda r_{p\lambda}\int_0^\infty dQ[M(Q)G(Q)-e^{-Qz_0}]^2, \quad (3.5)$$

with

$$M(Q)=\langle\varphi|e^{iQ\cdot\rho}|\varphi\rangle, \quad (3.6)$$

$$G(Q)=\langle\Phi|e^{-Qz}|\Phi\rangle, \quad (3.7)$$

and

$$F(Q)=\int_0^\infty dz'\Phi^2(z')\int_0^\infty dz\,\Phi^2(z)e^{-Q|z-z'|}. \quad (3.8)$$

The ground-state energy of the interface bound polaron will be obtained using the following variational wave functions:

$$\Phi(z)=\left[\frac{\delta}{2}\right]^3ze^{-\delta z/2} \quad (3.9)$$

and

$$\varphi(\rho)=\left[\frac{\sigma}{2\pi}\right]^{1/2}e^{-\sigma\rho/2}, \quad (3.10)$$

where δ and σ are variational parameters determined minimizing the total energy of the system. The binding energy of the bound interface polaron is obtained, as usual, by taking the difference of the minimum total energy of the system with and without the impurity. The numerical results of this theory will be presented in the next section.

IV. RESULTS AND DISCUSSION

As an application of this theory we will use the systems constituted by the heterojunctions AlAs-GaAs and GaSb-GaAs. In order to calculate the binding energy of the ground state of the interface bound polaron we have

TABLE I. The parameters used in the calculations: the frequencies of the bulk LO phonons (in meV), dielectric constants (static and optical), and effective mass for electron in units of free-electron mass (Refs. 7 and 18).

	ω_{LO}	ϵ_0	ϵ_∞	$m_\parallel/m_0$	$m_\perp/m_0$
GaAs	36.25	12.83	10.9	0.067	0.067
AlAs	50.09	10.06	8.16	0.19	1.1
GaSb	29.80	15.69	14.44		

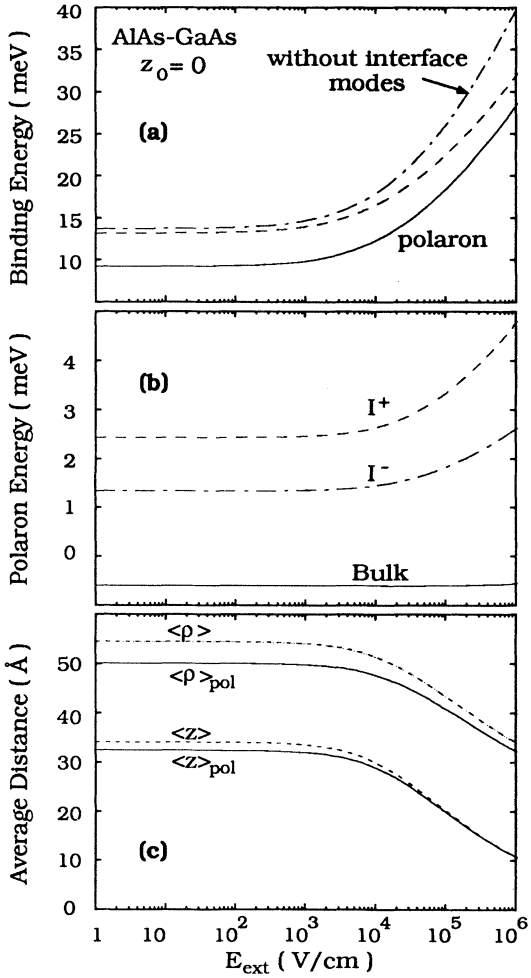

FIG. 2. The ground-state binding energy of the bound polaron near the interface of the heterojunction AlAs-GaAs is plotted in (a) as a function of the external electric field. The impurity is placed at the interface and the electron is confined in AlAs. The solid line (—)is the result of the present theory, the dashed line (---) is the binding energy when we neglect the presence of phonons, and the dashed–dotted line (-·-) is the result of the binding energy where we have neglected only the electron–interface-phonons interaction. In (b) we show the polaronic contributions to the binding energy due to the electron interaction modes (I^+ and I^-) and the bulk LO phonons as a function of the electric field. In (c) we plotted the average distance to the interface $\langle z \rangle$ and the in-plane average radius $\langle \rho \rangle$, with and without polaron effects, as a function of the electric field.

used the parameters listed in Table I. The binding energy was obtained as a function of the electric field applied perpendicular to the interface and the impurity position.

In Fig. 2 the results for a hydrogenic impurity placed at the interface and the electron confined in the X point of the conduction band of AlAs are presented. The binding energy of the ground state is plotted as a function of the electric field in Fig. 2(a), with and without the polaronic corrections. Also plotted is the binding energy of the bound polaron considering just the bulk LO phonon and neglecting the interface phonons contribution. The

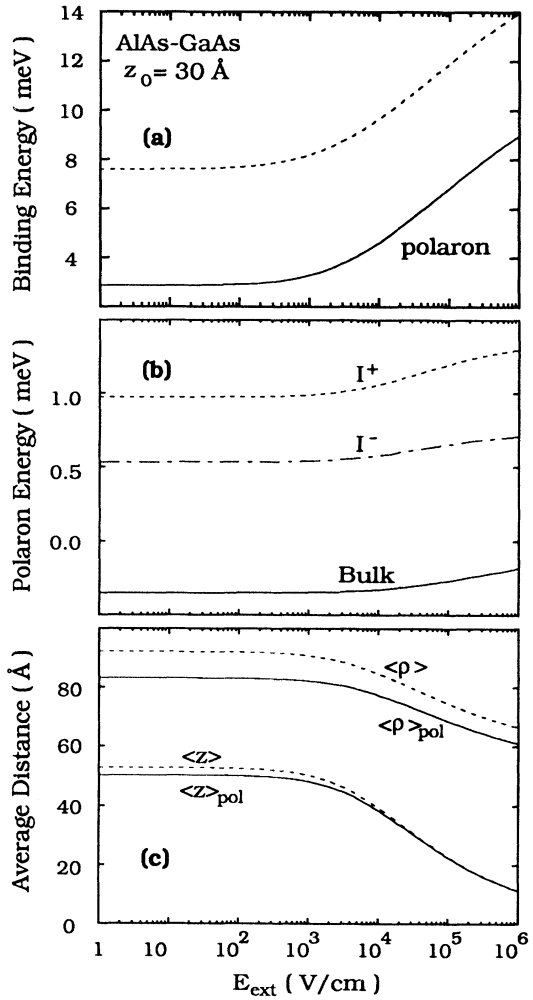

FIG. 3. The ground-state binding energy of the bound polaron near the interface of the heterojunction AlAs-GaAs is plotted in (a) as a function of the external electric field. The impurity is placed 30 Å from the interface inside GaAs and the electron is confined in AlAs. The solid line (—) is the result of the present theory and the dashed line (---) is the binding energy when we neglect the presence of phonons. In (b) we show the polaronic contributions to the binding energy due to the electron interaction with the interface modes (I^+ and I^-) and the bulk LO phonons as a function of the electric field. In (c) we plotted the average distance to the interface $\langle z \rangle$ and the in-plane average radius $\langle \rho \rangle$, with and without polaron effects, as a function of the electric field.

total polaronic corrections decrease the binding energy as compared to the case in which it neglected the presence of any phonons. When only the bulk LO phonon is included in the calculation we recover the usual result that this interaction increases the binding energy. As expected, when the electric field is increased the electron will be closer to the interface, and consequently will raise the binding energy. In Fig. 2(b) we present the contribution of the polaronic energy to the binding energy of the system as a function of the electric field. As can be seen, the interface contributions, I^+ and I^-, are always positive and increase as a function of the electric field due to the fact that the electron is closer to the interface. On the other hand, the bulk LO phonon contribution is negative and tends to zero for large electric fields. It is important to note that the polaronic corrections from the interface phonons are greater than the absolute value of the contribution from the bulk LO phonons. In Fig. 2(c) we have plotted the average distance of the electron to the interface $\langle z \rangle$ and the average in-plane radius $\langle \rho \rangle$, as a function of the electric field, with and without polaron effects. As $\langle z \rangle$ as $\langle \rho \rangle$ decreases with the enhancement of the

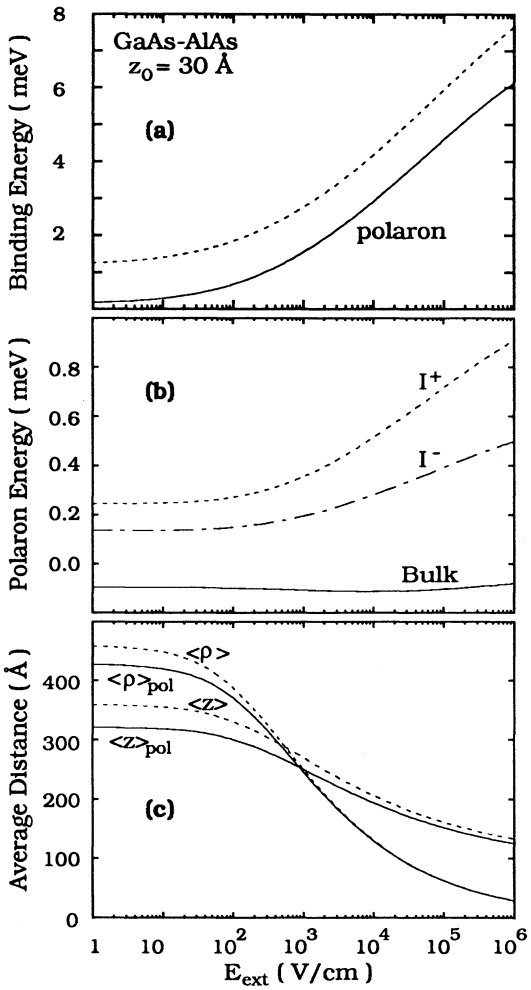

FIG. 4. The ground-state binding energy of the bound polaron near the interface of the heterojunction GaAs-AlAs is plotted in (a) as a function of the external electric field. The impurity is placed 30 Å from the interface inside AlAs and the electron is confined in GaAs. The solid line (—) is the result of the present theory and the dashed line (---) is the binding energy when we neglect the presence of phonons. In (b) we show the polaronic contributions to the binding energy due to the electron interaction with the interface modes (I^+ and I^-) and the bulk LO phonons as a function of the electric field. In (c) we plotted the average distance to the interface $\langle z \rangle$ and the in-plane average radius $\langle \rho \rangle$, with and without polaron effects, as a function of the electric field.

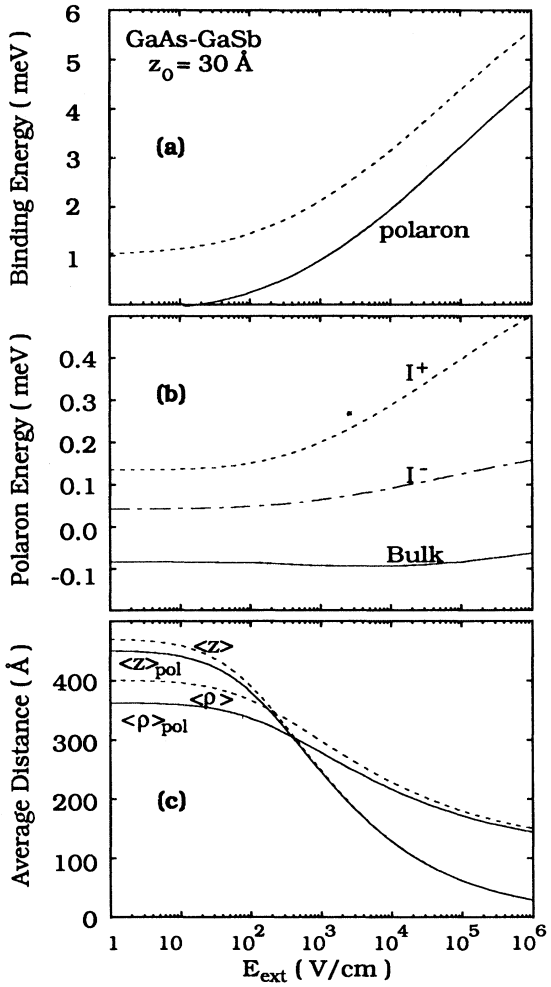

FIG. 5. The ground-state binding energy of the bound polaron near the interface of the heterojunction GaAs-GaSb is plotted in (a) as a function of the external electric field. The impurity is placed 30 Å from the interface inside GaSb and the electron is confined in GaAs. The solid line (—) is the result of the present theory, and the dashed line (---) is the binding energy when we neglect the presence of phonons. In (b) we show the polaronic contributions to the binding energy due to the electron interaction with the interface modes (I^+ and I^-) and the bulk LO phonons as a function of the electric field. In (c) we plotted the average distance to the interface $\langle z \rangle$ and the in-plane average radius $\langle \rho \rangle$, with and without polaron effects, as a function of the electric field.

electric field and the confinement of the electron is larger when the polaronic effects are taken into account. In order to understand the reduction of the binding energy due to polaronic effects, we have calculated the contribution of the interface phonons to the effective interaction between the electron and the impurity, which is given by

$$\Delta V_I(\rho,z)=\sum_{\lambda} 2\alpha_\lambda \hbar\omega_\lambda \frac{1}{[\rho^2+(z-z_0)^2]^{1/2}} \ . \tag{4.1}$$

Since the effective potential given by Eq. (4.1) is repulsive it will decrease the binding energy of the bound polaron.

In Fig. 3 we present the results for the bound polaron when the hydrogenic impurity is placed in GaAs 30 Å from the interface and the electron is confined at the X point of the conduction band of AlAs. The binding energy is reduced significantly compared to the preceding results in which the impurity was placed at the interface. Also, the polaronic corrections are decreased, as can be seen in Fig. 3(b), since the electron average distance from the interface has increased [Fig. 3(c)].

Now we will consider the case where the electron is at the Γ point of the conduction band of the GaAs, and the impurity is inside the AlAs. In Fig. 4 the results of the binding energy, polaronic corrections, and electron average distance are plotted as a function of the electric field for the impurity placed 30 Å from the interface. These results are qualitatively similar to those shown in Figs. 2 and 3. Comparing the results in Figs. 3 and 4, we have observed that the binding energy and the polaronic corrections are significantly reduced and the electron average distance is increased. This fact occurs basically due to the difference in the electron effective mass in AlAs and GaAs.

Another interesting system that we have studied is the heterojunction GaAs-GaSb. In this system the electron is confined inside GaAs, and we will consider that the impurity is placed inside of the GaSb. In Fig. 5 the results for the binding energy, polaronic corrections, and the electron average distance for an impurity placed inside the GaSb, 30 Å from the interface are presented. We have observed that the bound polaron is unstable for low electric fields. As can be seen in Fig. 5(a), there is a minimum electric field required to create a bound state. The others results are qualitatively similar to those already obtained in this paper.

In conclusion, we have shown in this paper that for a bound polaron close to the interface of polar-polar semiconductors the total polaronic correction is positive and decreases the binding energy of the ground state. Depending on the system, the reduction on the binding energy is large enough to avoid a bound state for low electric fields. Finally, in this work it has been shown that the interface modes play a fundamental role in the understanding of the properties of the ground state of a bound polaron.

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