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Exciton binding energy in type-II heterojunctions

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The binding energy of the ground-state exciton in type-II heterojunctions in the presence of a static external electric field is calculated using a variational method. The anisotropy of the electron and hole effective mass and the carriers' polarizability are considered. Polaron effects due to the coupling between exciton and LO phonons and interface phonons are included, and it is shown that these effects are important. The calculation was performed by using a generalization of the Lee-Low-Pines method, which is known to be valid for small and intermediate exciton-phonon coupling. We applied this theory to the system AlAs/GaAs, where the electron and hole are spatially separated, with the electron at the X point of the conduction band of AlAs and the hole at the Γ point of the valence band of GaAs. In this system it is observed that, due to the polaron effects, a minimum external electric field, E_0, applied perpendicular to the interface, is necessary to obtain a stable ground state for the exciton.

I. INTRODUCTION

Excitons in semiconductor superlattices and quantum wells have received considerable attention in the past few years.[1,2] Their optical and electrical properties can be used in several device applications.[3–5] Most studies have been done in type-I structures, where the electron and hole are confined spatially in the same material. In this case it was observed that the exciton binding energy increases when the confinement of the electron and hole is increased. When the electron and hole are confined in different constituent materials (making the superlattice a type-II structure), the binding energy decreases substantially relative to the value of the two-dimensional exciton. This effect was observed by Bastard *et al.*[6] studying excitons in InAs-GaSb quantum wells. On the other hand, Duggan and Ralph,[7] studying excitons in GaAs-AlAs quantum wells, found binding energies of magnitude comparable to those found for 1s heavy-hole excitons in this system when the configuration is type I. This enhancement was explained in terms of the larger longitudinal electron mass at the X minimum of AlAs relative to that of the Γ minimum of GaAs.

The effects of an optical phonon on an electron confined in a heterostructure have been studied both experimentally and theoretically.[8–11] In this system, the polar effects are due to electron–LO-phonon and electron–interface-phonon interactions. It is observed that the interface contributions increase when the electron confinement increases.[8–12] The effects of polarons on a composite particle, such as an exciton, are expected to be different from those on an electron.[13,14] For excitons, in addition to the self-energy and effective-mass renormalization, there is a Coulomb interaction and a new force occurs due to the interaction of the hole and electron with the lattice. This force is repulsive in the exciton case but is attractive if we consider two particles with charges of the same sign.[15]

When a static electric field is applied perpendicular to the interface, the exciton binding energy changes considerably. In type-I structures, since the electron and hole are in the same material, the presence of the electric field lowers the binding energy because the field spatially separates the electron and hole charge distributions. In type-II structures, an opposite effect can be observed.[6,16]

Recently, Matsuura[13] has calculated the polaron effects on excitons confined in type-I quantum wells. However, he has taken into account only the interaction of the electron (hole) and LO bulk phonons and has assumed that the barrier only yields the electronic potential barrier, neglecting the differences in dielectric constants and phonon energies between the well part and the barrier part. The results obtained reveal that, when the polaronic effects are included in the calculation, the exciton binding energy as a function of the well width remains between the exciton binding energy, calculated without polaron effects, with the Coulomb interaction screened by ϵ_0 and ϵ_∞.

The purpose of the present paper is to calculate the binding energy of the ground state of an exciton in a type-II heterojunction. Since these heterojunctions have polar materials as constituents, we will consider the interaction between the exciton and the optical phonons. Because of the presence of the interface, the exciton also couples with the interfacial phonons, and due to the difference of dielectric constants the effects of the carriers' polarizability are considered. In order to obtain the binding energy of the exciton we will use a generalization of the variational method proposed by Lee, Low, and Pines,[17] which is known to be valid up to intermediate exciton-phonon coupling. We applied this theory to study the exciton binding energy in an AlAs/GaAs heterojunction. In this system, we assume that the electron is at point X of the conduction band of AlAs and the hole is at point Γ of the valence band of GaAs. Following Duggan and Ralph,[7] we consider that the lowest X minima in the AlAs are those whose longitudinal mass is perpendicular to the plane of the interface.[18] We have observed that due to the polaronic effects there is a minimum electric field necessary for the existence of a stable ground state of the exciton. The effect of the electric field is to confine the electron and hole close to interface, such that, when the average distance between both is smaller than a critical value, a bound state occurs.

This paper is organized as follows. In Sec. II we define the model Hamiltonian of the exciton, which includes the electron and hole anisotropic mass, the interaction between an electron (hole) and an LO phonon and an electron (hole) and interface phonons, and the effects of the carriers' polarizability. In Sec. III we present the variational method used to obtain the ground-state energy of the exciton. Finally, numerical calculations and concluding remarks are presented in Sec. IV.

II. THE MODEL HAMILTONIAN

The system considered in this paper is composed of a junction of two polar semiconductors with the interface placed at $z=0$ and characterized by the wave-vector-independent lattice dielectric function $\epsilon_1(\omega)$ and $\epsilon_2(\omega)$ as shown in Fig. 1. Since we are assuming that this structure is type II, the electron and hole are spatially separated and we will consider that the electron is in material 1 ($z<0$) and the hole is in material 2 ($z>0$). Anisotropy of both the hole and electron effective mass is considered. The well-known relations $\epsilon_1(\omega_\lambda)+\epsilon_2(\omega_\lambda)=0$, $\epsilon_1(\omega_{\mathrm{LO}1})=0$, and $\epsilon_2(\omega_{\mathrm{LO}2})=0$ were used to obtain the interface phonon frequencies ω_λ and the bulk LOn phonon frequencies ($n=1,2$), respectively. The Hamiltonian of the system can be written as

$$H=H_e+H_h+H_{\mathrm{ph}}+H_{e\text{-}h}+H_{e,h\text{-ph}}\ , \tag{2.1}$$

with

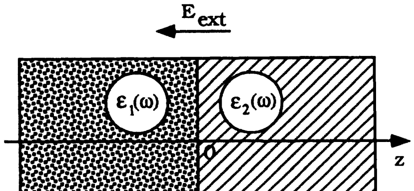

FIG. 1. Model considered in the present paper. We consider the electron inside material 1 ($z<0$) and the hole inside material 2 ($z>0$), interacting with both interface and bulk LO phonons. The anisotropy of the electron and hole effective masses is taken into account.

$$H_e=E_{\mathrm{gap}}+\frac{P_{ze}^2}{2m_{e\perp}}-eE_{\mathrm{ext}}z_e+V(z_e)+\frac{e^2}{4|z_e|\epsilon_{\infty 1}}\frac{(\epsilon_{\infty 1}-\epsilon_{\infty 2})}{(\epsilon_{\infty 1}+\epsilon_{\infty 2})} \tag{2.2}$$

and

$$H_h=\frac{P_{zh}^2}{2m_{h\perp}}+\left[\frac{\epsilon_{01}}{\epsilon_{02}}\right]eE_{\mathrm{ext}}z_h+V(z_h)+\frac{e^2}{4z_h\epsilon_{\infty 2}}\frac{(\epsilon_{\infty 2}-\epsilon_{\infty 1})}{(\epsilon_{\infty 1}+\epsilon_{\infty 2})}\ , \tag{2.3}$$

where E_{gap} is the effective gap between the valence and conduction band and E_{ext} is an external static electric field applied perpendicular to the interface, which will confine the electron-hole system close to the interface. Due to the difference between the dielectric constant, the static field will not be the same in both materials but can be related through the continuity of the displacement vector at the interface. The electron and hole effective masses perpendicular to the interface are $m_{e\perp}$ and $m_{h\perp}$, respectively. The potential $V(z_i)$ ($i=e,h$) represents the barrier at the interface for both the electron and the hole, which will be considered infinity for $z_e>0$ ($z_h<0$) for the electron (hole) and zero for $z_e<0$ ($z_h>0$). The last terms in Eqs. (2.2) and (2.3) correspond to the electron-polarizability interaction and hole-polarizability interaction, and $\epsilon_{\infty 1},\epsilon_{\infty 2}$ are the optical dielectric constants of materials 1 and 2, respectively. The Hamiltonian of the phonons H_{ph} in Eq. (2.1) is given by

$$H_{\mathrm{ph}}=\sum_{\mathbf{Q}}\sum_{\lambda}\hbar\omega_\lambda b_{\mathbf{Q}\lambda}^\dagger b_{\mathbf{Q}\lambda}+\sum_{\mathbf{q}}\hbar\omega_{\mathrm{LO}1}a_{\mathbf{q}}^\dagger a_{\mathbf{q}}+\sum_{\mathbf{q}}\hbar\omega_{\mathrm{LO}2}c_{\mathbf{q}}^\dagger c_{\mathbf{q}}\ , \tag{2.4}$$

where $a_{\mathbf{q}}$ ($c_{\mathbf{q}}$) is the annihilation operator of bulk LO phonons of material 1 (2), with wave vector $\mathbf{q}=(\mathbf{Q},q_z)$ and frequency $\omega_{\mathrm{LO}1}$ ($\omega_{\mathrm{LO}2}$), and $b_{\mathbf{Q}\lambda}$ is the annihilation operator of the interface excitation with wave vector $\mathbf{Q}$ and frequency ω_λ. The Hamiltonian describing the interaction between the electron and the hole can be written as

$$H_{e\text{-}h}=\frac{P^2}{2M_\parallel}+\frac{p^2}{2\mu}-\frac{e^2}{\epsilon_{\mathrm{eff}}[\rho^2+(z_e-z_h)^2]^{1/2}}\ , \tag{2.5}$$

where $\mathbf{P}$ is the momentum of the center of mass of the exciton parallel to the interface and $\mathbf{p}$ is the momentum associated with the relative motion, the total mass parallel to the interface is $M_\parallel=m_{e\parallel}+m_{h\parallel}$, the reduced mass is $\mu^{-1}=m_{e\parallel}^{-1}+m_{h\parallel}^{-1}$, and the last term in Eq. (2.5) is the Coulomb interaction screened by the effective dielectric constant $\epsilon_{\mathrm{eff}}=(\epsilon_{\infty 1}+\epsilon_{\infty 2})/2$.

The last term in Eq. (2.1) is the Hamiltonian for the electron (hole) and phonon interaction. In this problem the electron and hole are spatially separated. Since we have neglected the penetration of the electron (hole) in material 2 (1), the electron (hole) will only couple with the LO phonons of material 1 (2) and with the interface modes. With these assumptions, the Hamiltonian for the exciton-phonon interaction can be written as[8]

$$H_{e,h\text{-ph}}=H_{e\text{-LO1}}+H_{h\text{-LO2}}+H_{e,h\text{-I}} , \tag{2.6}$$

where

$$H_{e\text{-LO1}}=\sum_{\mathbf{q}}\Gamma_e(q)e^{iQ\cdot R_c}e^{i\beta_h \mathbf{Q}\cdot\rho}\sin q_z z_e(a_{\mathbf{q}}+a^{\dagger}_{-\mathbf{q}}) , \tag{2.7}$$

$$H_{h\text{-LO2}}=\sum_{\mathbf{q}}\Gamma_h(q)e^{i\mathbf{Q}\cdot\mathbf{R}_c}e^{i\beta_e \mathbf{Q}\cdot\rho}\sin q_z z_h(c_{\mathbf{q}}+c^{\dagger}_{-\mathbf{q}}) , \tag{2.8}$$

and

$$H_{e,h\text{-I}}=\sum_{\lambda}\sum_{\mathbf{Q}}\gamma_\lambda(Q)e^{i\mathbf{Q}\cdot\mathbf{R}_c}(e^{i\beta_h\mathbf{Q}\cdot\rho}e^{Qz_e}-e^{-i\beta_e\mathbf{Q}\cdot\rho}e^{-Qz_h})\times(b_{\mathbf{Q}\lambda}+b^{\dagger}_{-\mathbf{Q}\lambda}) , \tag{2.9}$$

where $\beta_e=m_{e\parallel}/M_\parallel$, $\beta_h=m_{h\parallel}/M_\parallel$, and $\mathbf{R}_c=\beta_e\mathbf{R}_e+\beta_h\mathbf{R}_h$ is the exciton in the plane center of mass. The Fourier coefficients of the electron– and hole–bulk-LO-phonon interaction are given by

$$\Gamma_e(q)=-i\frac{\hbar\omega_{\text{LO1}}}{q}\left[\frac{4\pi}{\Omega}\left[\frac{1}{\epsilon_{\infty 1}}-\frac{1}{\epsilon_{01}}\right]\frac{e^2}{\hbar\omega_{\text{LO1}}}\right]^{1/2} \tag{2.10}$$

and

$$\Gamma_h(q)=i\frac{\hbar\omega_{\text{LO2}}}{q}\left[\frac{4\pi}{\Omega}\left[\frac{1}{\epsilon_{\infty 2}}-\frac{1}{\epsilon_{02}}\right]\frac{e^2}{\hbar\omega_{\text{LO2}}}\right]^{1/2} , \tag{2.11}$$

respectively, where ϵ_{0i} $(i=1,2)$ is the static dielectric constant of the material 1 or 2 and Ω is the volume. The Fourier coefficient of the exciton–interface-phonon interaction, $\gamma_\lambda(Q)$, can be written as

$$\gamma_\lambda(Q)=\frac{\hbar\omega_\lambda}{\sqrt{Q}}\left[\frac{2\pi}{A}\alpha_\lambda r_{p\lambda}\right]^{1/2} , \tag{2.12}$$

where A is the area of the interface and we have defined, by analogy with the bulk-polaron problem, the traditional dimensionless exciton–interface-phonon coupling constant α_λ:

$$\alpha_\lambda=\frac{e^2}{\hbar\omega_\lambda r_{p\lambda}}\left[\frac{\omega_\lambda^2}{\omega_{p1}^2}\Theta_1(\omega_\lambda)[\epsilon_1(\omega_\lambda)-1]^2+\frac{\omega_\lambda^2}{\omega_{p2}^2}\Theta_2(\omega_\lambda)[\epsilon_2(\omega_\lambda)-1]^2\right]^{-1} \tag{2.13}$$

and the interface exciton-polaron radius

$$r_{p\lambda}=\left[\frac{\hbar}{2\mu\omega_\lambda}\right]^{1/2} . \tag{2.14}$$

In Eq. (2.13) 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

$$\epsilon_n(\omega)=\epsilon_{\infty n}\frac{\omega_{\text{LO}n}^2-\omega^2}{\omega_{\text{TO}n}^2-\omega^2} , \tag{2.15}$$

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

$$\omega_{pn}=\left[\frac{9\epsilon_{\infty n}}{(\epsilon_{\infty n}+2)^2}(\omega_{\text{LO}n}^2-\omega_{\text{TO}n}^2)\right]^{1/2} \tag{2.16}$$

and the function $\Theta_n(\omega)$ defined as

$$\Theta_n(\omega)=\left[1+\frac{\epsilon_{0n}}{3\epsilon_{\infty n}}\frac{(\epsilon_{\infty n}-1)(\epsilon_{\infty n}+2)}{(\epsilon_{0n}-\epsilon_{\infty n})}\frac{(\omega_{0n}^2-\omega^2)}{\omega_{\text{LO}n}^2}\right]^2 , \tag{2.17}$$

with

$$\omega_{0n}=\left[\omega_{\text{LO}n}^2-\frac{2}{\epsilon_{\infty n}+2}(\omega_{\text{LO}n}^2-\omega_{\text{TO}n}^2)\right]^{1/2} . \tag{2.18}$$

Although the exciton-phonon interaction in this system, Eq. (2.6), is usually weak, we will use a generalization of the Lee-Low-Pines method[17] which is well known to be valid even when the strength of the coupling is in the intermediate regime.

III. THE VARIATIONAL MODEL

In this section we will apply a generalization of the well-known Lee-Low-Pines method[17] in order to obtain the ground-state energy of an exciton in a type-II heterojunction. We begin by introducing a canonical transformation S that removes the in-plane center-of-mass coordinate $\mathbf{R}_c$ of the exciton from the Hamiltonian H defined in Eq. (2.1),

$$S=\exp\left[i\mathbf{K}\cdot\mathbf{R}_c-i\sum_{\mathbf{Q},\lambda}\mathbf{Q}\cdot\mathbf{R}_c b^{\dagger}_{\mathbf{Q},\lambda}b_{\mathbf{Q},\lambda}-i\sum_{\mathbf{q}}\mathbf{q}\cdot\mathbf{R}_c a^{\dagger}_{\mathbf{q}}a_{\mathbf{q}}-i\sum_{\mathbf{q}}\mathbf{q}\cdot\mathbf{R}_c c^{\dagger}_{\mathbf{q}}c_{\mathbf{q}}\right] , \tag{3.1}$$

where $\mathbf{K}$ is the wave vector associated with the center of mass of the exciton-phonon system parallel to the interface. In order to eliminate the phonon coordinates, we will use the following transformation:

$$U=\exp\left[\sum_{\mathbf{Q},\lambda}(f_{\mathbf{Q},\lambda}b_{\mathbf{Q},\lambda}-f^{*}_{\mathbf{Q},\lambda}b^{\dagger}_{\mathbf{Q},\lambda})\right]\exp\left[\sum_{\mathbf{q}}[g_{\mathbf{q}}a_{\mathbf{q}}\exp(iq_z z_e\tau^e)-g^{*}_{\mathbf{q}}a^{\dagger}_{\mathbf{q}}\exp(-iq_z z_e\tau^e)]\right]\times\exp\left[\sum_{\mathbf{q}}[h_{\mathbf{q}}c_{\mathbf{q}}\exp(iq_z z_h\tau^h)-h^{*}_{\mathbf{q}}c^{\dagger}_{\mathbf{q}}\exp(-iq_z z_h\tau^h)]\right] , \tag{3.2}$$

where $f_{\mathbf{Q}\lambda}$, $g_{\mathbf{q}}$, and $h_{\mathbf{q}}$ are variational functions that will be determined by the requirement that the total energy of the system be minimum, and τ^e and τ^h are defined by

$$\tau^i=\left[\frac{m_{iz}}{M_z}\right]^{1/2} , \tag{3.3}$$

with $i=e,h$ and $M_z=m_{ez}+m_{hz}$. In Eq. (3.2) we have generalized the Lee-Low-Pines transformation including the factors τ^e and τ^h, which are necessary to recover the correct limits in the following cases: (1) m_e or m_h, the electron or hole total mass, equal to zero (polaron problem);[8] (2) $m_h \to \infty$ (bound-polaron problem).[19]

To obtain the ground-state energy, we assume the following ansatz to the wave function for the coupled exciton-phonon system:

$$\psi=\phi_e(z_e)\phi_h(z_h)\xi(\rho)|0\rangle \ , \tag{3.4}$$

where

$$\phi_e(z_e)=\left[\frac{\delta_e}{2}\right]^{1/2} z_e e^{\delta_e z_e/2} \ , \tag{3.4a}$$

$$\phi_h(z_h)=\left[\frac{\delta_h}{2}\right]^{1/2} z_h e^{-\delta_h z_h/2} \ , \tag{3.4b}$$

$$\xi(\rho)=\frac{\sigma}{\sqrt{2\pi}}e^{-\sigma\rho/2} \ , \tag{3.4c}$$

where $|0\rangle$ is the phonon vacuum state, ϕ_e and ϕ_h are the wave functions of the electron and hole perpendicular to the interface, ξ describes the relative motion of the electron and hole parallel to the interface, and δ_e, δ_h, and σ are variational parameters determined by minimizing the total energy of the system.

The total energy of the exciton-phonon system is obtained computing the expectation value $E=\langle\psi|\mathcal{H}|\psi\rangle$, where the transformed Hamiltonian is given by $\mathcal{H}=USHS^{-1}U^{-1}$. The variational functions $f_{Q\lambda}$, $g_{\mathbf{q}}$, and $h_{\mathbf{q}}$ are determined by performing the minimization of the total energy of the system with respect to $f_{Q\lambda}$, $g_{\mathbf{q}}$, and $h_{\mathbf{q}}$, that is,

$$\frac{\delta E}{\delta f_{\mathbf{Q},\lambda}}=\frac{\delta E}{\delta h_{\mathbf{q}}}=\frac{\delta E}{\delta g_{\mathbf{q}}}=0 \ . \tag{3.5}$$

We then find that

$$g_{\mathbf{q}}=\frac{\Gamma_e(q)\langle\psi|e^{i\beta_h\mathbf{Q}\cdot\rho}e^{iq_z z_e\tau^e}\sin q_z z_e|\psi\rangle}{\hbar\omega_{\mathrm{LO1}}+\frac{\hbar^2Q^2}{2M_\parallel}+\frac{\hbar^2q_z^2}{2M_z}+\frac{\hbar^2}{M_\parallel}(\eta-1)\mathbf{K}\cdot\mathbf{Q}} \ , \tag{3.6a}$$

$$h_{\mathbf{q}}=\frac{\Gamma_h(q)\langle\psi|e^{i\beta_e\mathbf{Q}\cdot\rho}e^{-iq_z z_h\tau^h}\sin q_z z_h|\psi\rangle}{\hbar\omega_{\mathrm{LO2}}+\frac{\hbar^2Q^2}{2M_\parallel}+\frac{\hbar^2q_z^2}{2M_z}+\frac{\hbar^2}{M_\parallel}(\eta-1)\mathbf{K}\cdot\mathbf{Q}} \ , \tag{3.6b}$$

$$f_{\mathbf{Q},\lambda}=\frac{\gamma_\lambda(Q)\langle\psi|e^{i\beta_h\mathbf{Q}\cdot\rho}e^{Qz_e}-e^{i\beta_e\mathbf{Q}\cdot\rho}e^{-Qz_h}|\psi\rangle}{\hbar\omega_\lambda+\frac{\hbar^2Q^2}{2M_\parallel}+\frac{\hbar^2}{M_\parallel}(\eta-1)\mathbf{K}\cdot\mathbf{Q}} \ , \tag{3.6c}$$

where

$$\eta\mathbf{K}=\sum_{\mathbf{Q},\lambda}\mathbf{Q}|f_{\mathbf{Q},\lambda}|^2+\sum_{\mathbf{q}}\mathbf{Q}|g_{\mathbf{q}}|^2+\sum_{\mathbf{q}}\mathbf{Q}|h_{\mathbf{q}}|^2 \ . \tag{3.7}$$

By substituting Eqs. (3.6) and (3.7) back in the total energy and expanding up to second order in the wave vector $\mathbf{K}$, we obtain the following expression:

$$E(\mathbf{K})=E_{\mathrm{gap}}+E_{\mathrm{exc}}(0)+\frac{\hbar^2K^2}{2M^*} \ , \tag{3.8}$$

where M^* is the total effective mass of the exciton-phonon system parallel to the interface, the $E_{\mathrm{exc}}(0)$ is given by

$$E_{\mathrm{exc}}(0)=\left\langle\psi\left|\frac{p_{ze}^2}{2m_{ez}}+\frac{p_{zh}^2}{2m_{hz}}+\frac{p^2}{2\mu}-\frac{e^2}{\epsilon_{\mathrm{eff}}[\rho^2+(z_e-z_h)^2]^{1/2}}+eE_{\mathrm{ext}}\left[\frac{\epsilon_{01}}{\epsilon_{02}}z_h-z_e\right]\right|\psi\right\rangle$$
$$+\left\langle\phi_e\left|\frac{e^2}{4z_e\epsilon_{\infty1}}\frac{(\epsilon_{\infty1}-\epsilon_{\infty2})}{(\epsilon_{\infty1}+\epsilon_{\infty2})}\right|\phi_e\right\rangle+\left\langle\phi_h\left|\frac{e^2}{4z_h\epsilon_{\infty2}}\frac{(\epsilon_{\infty2}-\epsilon_{\infty1})}{(\epsilon_{\infty1}+\epsilon_{\infty2})}\right|\phi_h\right\rangle+\Delta E_{e\text{-LO1}}+\Delta E_{h\text{-LO2}}+\Delta E_{e,h\text{-I}} \ , \tag{3.9}$$

where

$$\Delta E_{i\text{-LO}n}=-\sum_{\mathbf{q}}\frac{|\Gamma_i(q)|^2|W_i(q_z)|^2|F_j(Q)|^2}{\hbar\omega_{\mathrm{LO}n}+\frac{\hbar^2Q^2}{2M_\parallel}+\frac{\hbar^2q_z^2}{2M_z}} \ , \tag{3.10}$$

with $n=1,2$ and $(i,j)=(e,h)$ or (h,e), and

$$\Delta E_{e,h\text{-I}}=-\sum_{\mathbf{Q},\lambda}\frac{|\gamma_\lambda(Q)|^2|G(\mathbf{Q})|^2}{\hbar\omega_\lambda+\frac{\hbar^2Q^2}{2M_\parallel}} \ , \tag{3.11}$$

with

$$W_i(q_z)=\langle\phi_i|e^{-iq_z z_i\tau^i}\sin q_z z_i|\phi_i\rangle, \quad i=e,h \tag{3.12}$$

$$F_j(Q)=\langle\xi|e^{i\beta_j\mathbf{Q}\cdot\rho}|\xi\rangle, \quad j=e,h \tag{3.13}$$

and

$$G(\mathbf{Q})=\langle\psi|e^{i\beta_h\mathbf{Q}\cdot\rho}e^{Qz_e}-e^{i\beta_e\mathbf{Q}\cdot\rho}e^{-Qz_h}|\psi\rangle \ . \tag{3.14}$$

Substituting the variational wave function Eq. (3.4) in Eq. (3.9) and performing a straightforward calculation, we obtain

$$E_{\rm exc}(0)=\frac{\hbar^2}{8}\left[\frac{\delta_e^2}{m_{ez}}+\frac{\delta_h^2}{m_{hz}}+\frac{\sigma^2}{\mu}\right]-\frac{e^2}{\epsilon_{\rm eff}}\int_0^\infty dQ\left[\frac{\delta_e}{\delta_e+Q}\right]^3\left[\frac{\delta_h}{\delta_h+Q}\right]^3\left[\frac{\sigma^2}{\sigma^2+Q^2}\right]^{3/2}$$
$$+3eE_{\rm ext}\left[\frac{\epsilon_{01}}{\epsilon_{02}}\frac{1}{\delta_h}-\frac{1}{\delta_e}\right]+\Delta E_{\rm pol}+\Delta E_{e\text{-LO}1}+\Delta E_{h\text{-LO}2}+\Delta E_{e,h\text{-I}}\ , \tag{3.15}$$

where

$$\Delta E_{\rm pol}=\frac{e^2}{8}\frac{(\epsilon_{\infty 1}-\epsilon_{\infty 2})}{(\epsilon_{\infty 1}+\epsilon_{\infty 2})}\left[\frac{\delta_e}{\epsilon_{\infty 1}}-\frac{\delta_h}{\epsilon_{\infty 2}}\right]\ , \tag{3.16}$$

$$\Delta E_{i\text{-LO}1}=-\frac{e^2}{8}\left[\frac{1}{\epsilon_{0i}}-\frac{1}{\epsilon_{\infty i}}\right]\int_0^\infty dQ\frac{Y_i(r_{pi}Q)}{[1+(\beta_j/\sigma)^2 r_{pn}Q]^3}\ , \tag{3.17}$$

with $(i,j)=(e,h)$ or (h,e), $r_{pn}=(\hbar/2M_z\omega_{{\rm LO}n})^{1/2}$, $n=1$ (2) for the electron (hole), and

$$\Delta E_{e,h\text{-I}}=\sum_\lambda \alpha_\lambda r_{p\lambda}\hbar\omega_\lambda\int_0^\infty dQ\frac{1}{1+(r_{p\lambda}Q)^2}\left[\left[\frac{\delta_e}{\delta_e+Q}\right]^3\frac{1}{[1+(\beta_h Q/\sigma)^2]^{3/2}}-\left[\frac{\delta_h}{\delta_h+Q}\right]^3\frac{1}{[1+(\beta_e Q/\sigma)^2]^{3/2}}\right]^2 \tag{3.18}$$

and

$$Y_i(Q)=T_{1i}(Q,\chi_\pm^i)+T_{2i}(Q,\chi_\pm^i)-T_{1i}(Q,\vartheta_\pm^i)-T_{2i}(Q,\vartheta_\pm^i)\ , \tag{3.19}$$

where $\chi_\pm^i=\sqrt{Q}\,(1\pm\tau^i)$, $\vartheta_\pm^i=[1+(M_z/M_\parallel)Q]^{1/2}(1\pm\tau^i)$, and

$$T_{1i}(a,b_\pm)=\frac{1}{\sqrt{a}}\frac{1}{1+a\left[\dfrac{M_z}{M_\parallel}-1\right]}$$
$$\times\left\{\left[1+\frac{b_-}{\delta_i}\right]^{-3}\left[1+\frac{9b_-}{8\delta_i}+\frac{3}{8}\left[\frac{b_-}{\delta_i}\right]^2\right]+\left[1+\frac{b_+}{\delta_i}\right]^{-3}\left[1+\frac{9b_+}{8\delta_i}+\frac{3}{8}\left[\frac{b_+}{\delta_i}\right]^2\right]\right\}, \tag{3.19a}$$

$$T_{2i}(a,b_\pm)=\frac{-2}{\sqrt{a}}\left\{\left[1+a\left[\frac{M_z}{M_\parallel}-1\right]\right]\left[1+\frac{b_+}{\delta_i}\right]^3\left[1+\frac{b_-}{\delta_i}\right]^3\right\}^{-1}, \tag{3.19b}$$

with $i=e,h$.

The binding energy of the exciton is obtained calculating the difference between the energies of the system without and with Coulomb interaction. In order to calculate the energies of the free electron and the free hole, we have used the same procedure as in Ref. 8, that is, for each electric field we minimized Eq. (3.6) of Ref. 8 to obtain $(E_e)_{\rm min}$ and $(E_h)_{\rm min}$, respectively. The energy of the exciton is obtained by minimizing $E_{\rm exc}(0)$, Eq. (3.15), with respect to the variational parameters δ_e, δ_h, and σ. Thus, the binding energy of the exciton will be given by

$$E_B=(E_e)_{\rm min}+(E_h)_{\rm min}-[E_{\rm exc}(0)]_{\rm min}\ . \tag{3.20}$$

The minimization of Eq. (3.20) can only be evaluated numerically and the results of this calculation will be presented in Sec. IV.

IV. NUMERICAL RESULTS AND CONCLUSIONS

In this section we present the numerical results of the binding energy of the exciton as a function of the external electric field. We have chosen the heterojunction AlAs/GaAs to illustrate the numerical results. We assume that the electron is at the X point of the conduction band of AlAs (material 1) and the hole is at the Γ point of the valence band of GaAs (material 2). The physical parameters relevant to the calculation are listed in Table I.[20] In Fig. 2 we plot the binding energy of the exciton with and without polaron corrections. When we neglect the carrier-phonon interaction and the polarizability terms in Eq. (3.20), it is observed that the exciton is stable even for zero external electric field. Under this circumstance, the binding energy was studied considering two different situations: (1) the Coulomb interaction was screened by $\epsilon_{\rm eff}=(\epsilon_{\infty 1}+\epsilon_{\infty 2})/2$; (2) the Coulomb interaction was screened by $\epsilon_{\rm eff}=(\epsilon_{01}+\epsilon_{02})/2$.

When the polaron corrections and the polarizability due to the presence of the interface are taken into account, the binding energy of the exciton presents a very different behavior, as shown in Fig. 2, that is (1) a minimum external electric field E_0 ($\approx$20 kV/cm), applied perpendicular to the interface, is required in order to obtain a stable ground state for the exciton; (2) the binding energy is reduced significantly when compared to

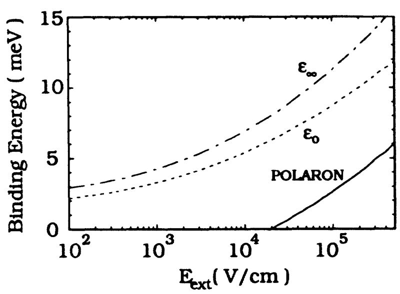

FIG. 2. Exciton binding energy as a function of the external electric field. The trace line (— — —) and the trace-dot line (—·—·—·) represent the results without polaron corrections and the polarizability effects. We have shown the results with the Coulomb term screened by $\epsilon_{eff}=\epsilon_\infty=(\epsilon_{\infty 1}+\epsilon_{\infty 2})/2$ and $\epsilon_{eff}=\epsilon_0=(\epsilon_{01}+\epsilon_{02})/2$, where there is a stable ground state for the exciton even with zero electric field. The solid line represents the results with polaron corrections and polarizability effects. It is necessary to have a minimum electric field applied perpendicular to the interface in order to obtain a stable ground state.

the simple calculation described above. In order to understand qualitatively these results, we present in Fig. 3 an energy diagram for the system without and with the polaron effects. As can be seen schematically in Fig. 3(a), for electric fields smaller than the critical electric field E_0, the energy shift due to the inclusion of the polaron effects, for the lowest ionized exciton state ($E_1=E_e^{\text{free}}+E_h^{\text{free}}$) is much larger than that for the exciton ground state (E_2), such that the lowest ionized state

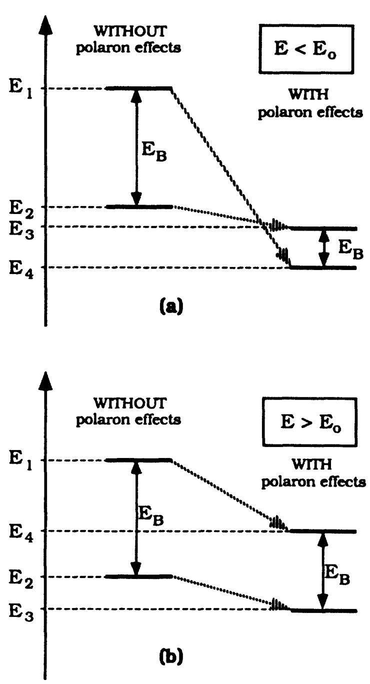

FIG. 3. Energy diagram with and without polaron effects for the ground state of the exciton as a function of the external electric field.

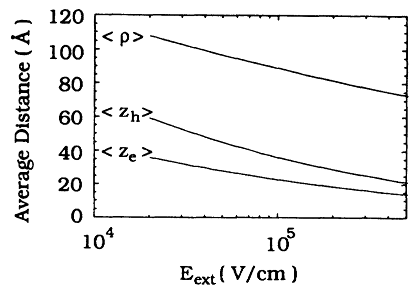

FIG. 4. Average distance of the electron and hole to the interface and the average of the in-plane radius of the exciton as a function of the external electric field.

E_1 is shifted to E_4 and the exciton ground state E_2 is shifted to E_3. Under this condition, E_4 is smaller than E_3 and the electron-hole system has no bound state. When the external electric field is increased over the critical value, Fig. 3(b), the energy shift ($\Delta E^{\text{free}}=E_1-E_4$) for the lowest ionized exciton state is still larger than the energy shift ($\Delta E^{\text{bound}}=E_2-E_3$) for the ground state, but the difference between the final energies (E_4-E_3) of these states is positive, such that the system electron hole is bound. Because the energy shift due to the polaron effects is larger for the free electron and free hole than for the exciton ground state, the binding energy is reduced.

In Fig. 4 we present the average distances of the electron and hole to the interface and the average in-plane radius of the exciton as a function of the external electric field. As we can observe, the confinement of the electron and hole in the z direction is smaller than 40 and 60 Å, respectively. The electron confinement is bigger than the hole basically for two reasons. First, because the image potential due to the polarizability is attractive for the electron and repulsive for the hole, and second, because the electron longitudinal effective mass at the X point of the conduction band of AlAs is almost three times the hole longitudinal effective mass at the Γ point of the valence band of GaAs.

The polaronic corrections to the exciton binding energy as a function of the external electric field are present in Fig. 5. The main contribution comes from the

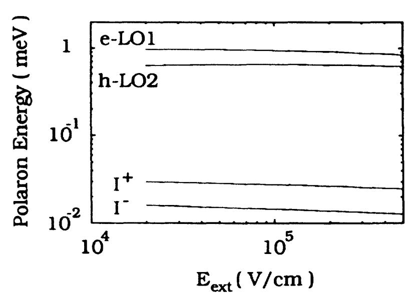

FIG. 5. Absolute values of the polaron corrections to the ground-state energy of the exciton as a function of the external electric field. The contribution of the electron–LO-bulk-phonon and the hole–LO2-bulk-phonon interaction is shown. The contribution of the two interface modes (+) and (−) is also plotted.

TABLE I. The parameters used in the calculations: the frequencies of the bulk LO phonons, the frequencies of the interface phonons ω_{I^+} and ω_{I^-} (in meV), the dielectric constants (static and optical), and the band effective mass for the electron and the hole (in units of free-electron mass) (Ref. 20).

ω_{LO1}	ω_{LO2}	ω_{I^+}	ω_{I^-}	$\epsilon_{\infty 1}$	$\epsilon_{\infty 2}$	ϵ_{01}	ϵ_{02}
50.09	36.25	47.54	34.75	8.16	10.9	10.06	12.83
	$m_{e\perp}$		$m_{h\perp}$	$m_{e\parallel}$		$m_{h\parallel}$	
	1.1		0.34	0.19		0.18	

exciton–LO-bulk-phonon coupling. The interface-phonon contribution is very small because the interaction of electron-interface phonons has the opposite sign of the interaction between hole-interface phonons. This result can be seen from Eq. (3.18), since β_e and β_h are almost equal and δ_e and δ_h are very close for this range of the electric field. The polarizability effects are also small due to the fact that the dielectric constants of these materials have almost the same value.

In these calculations, we have retained only the diagonal terms of the Luttinger-Kohn Hamiltonian.[21] In a quantitatively better calculation, the valence-band coupling and valence–conduction-band coupling need to be considered. Since we have used a variational approach that represents an upper bound of the total energy of the system, it is possible that the electron-hole pair can have a bound state for fields smaller than E_0. Also, if the interface potential is considered finite, the wave functions of the electron and hole are allowed to penetrate in different materials. Probably, the average distance between the electron and the hole will decrease and, consequently, the binding energy of the exciton will increase.

In conclusion, we have obtained the binding energy of an exciton in a type-II heterojunction as a function of an external electric field, taking into account the anisotropy of the electron and hole effective mass, the exciton–LO-bulk-phonon interaction, the exciton–interface-phonon interaction, and the polarizability of the carriers. The inclusion of these effects changes dramatically the binding energy of the exciton. These results can be applied for any heterojunction where the electron (hole) and phonon coupling is small or moderate. Particularly for the system AlAs/GaAs, we have observed the existence of a minimum external electric field in order to obtain a stable ground state for the exciton. The same formalism can also be applied to the known problem of an electron bound to a hydrogenic impurity (bound polaron) just by taking the limit of the total hole mass to infinity ($m_h \to \infty$).

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[1] *Semiconductors and Semimetals,* edited by R. Dingle (Academic, New York, 1987), Vol. 24.
[2] K. J. Nash and D. J. Mowbray, J. Lumin. **44**, 315 (1989).
[3] D. A. B. Miller, D. S. Chemla, T. C. Damen, A. C. Gossard, W. Wiegmann, T. H. Wood, and C. A. Burrus, Appl. Phys. Lett. **45**, 13 (1984).
[4] D. A. B. Miller, D. S. Chemla, T. C. Damen, A. C. Gossard, W. Wiegmann, T. H. Wood, and C. A. Burrus, Phys. Rev. B **32**, 1043 (1985).
[5] D. S. Chemla, D. A. B. Miller, P. W. Smith, A. C. Gossard, and W. Wiegmann, IEEE J. Quantum Electron. **QE-20**, 265 (1984).
[6] G. Bastard, E. E. Mendez, L. L. Chang, and L. Esaki, Phys. Rev. B **26**, 1974 (1982).
[7] G. Duggan and H. I. Ralph, Phys. Rev. B **35**, 4152 (1987).
[8] M. H. Degani and G. A. Farias, Phys. Rev. B **41**, 3572 (1990).
[9] M. A. Brummell, R. J. Nicholas, M. A. Hopkins, J. J. Harris, and C. T. Foxon, Phys. Rev. Lett. **58**, 77 (1987).
[10] M.-H. Meynadier, E. Finkman, M. D. Sturge, J. M. Worlock, and M. C. Tamargo, Phys. Rev. B **35**, 2517 (1987).
[11] S. Das Sarma and B. A. Mason, Ann. Phys. (N.Y.) **163**, 78 (1985).
[12] M. H. Degani and O. Hipólito, Surf. Sci. **196**, 459 (1988); Superlatt. Microstruct. **5**, 141 (1989).
[13] M. Matsuura, Phys. Rev. B **37**, 6977 (1988).
[14] M. H. Degani and O. Hipólito, Phys. Rev. B **35**, 9345 (1987).
[15] H. Haken, in *Advances in Solid State Physics,* edited by A. P. Grosse (Vieweg, Braunschweig, 1986), Vol. 26, p. 55.
[16] M. Matsuura and Y. Shinozuka, Phys. Rev. B **38**, 9830 (1988).
[17] T. D. Lee, F. E. Low, and D. Pines, Phys. Rev. **90**, 297 (1953).
[18] B. Rheinländer, A. Neumann, P. Fisher, and G. Kühn, Phys. Status Solidi B **49**, K167 (1972).
[19] M. H. Degani and O. Hipólito, Phys. Rev. B **33**, 4090 (1986).
[20] S. Adachi, J. Appl. Phys. **58(3)**, 1 (1985).
[21] J. M. Luttinger and W. Kohn, Phys. Rev. **97**, 869 (1955).