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# Binding Energies of Impurity States in Polar Quantum Well Structures in an External Electric Field

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**Abstract:** The binding energies of donor impurity states in quantum wells in the presence of an electric field were investigated by a variational method. The impurity-center as well as the bound electron couplings with both the longitudinal optical (LO) and interface optical (IO) phonons were taken into account in the calculation. The binding energies were obtained as the functions of impurity position, well width and electric field strength. The results for GaAs/Al<sub>0.3</sub>Ga<sub>0.7</sub>As quantum wells as an example were given and discussed. It was found that the correction due to electron-phonon interaction to the impurity state binding energies and the Stark shifts is quite significant.

**Key words:** donor impurity state; electron-phonon interaction; quantum well; Stark effect

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## 1 Introduction

Impurity states play a fundamental role in transport and optical properties of layer semiconductor materials, such as heterojunctions, quantum wells *etc.* So, understanding the impurity states in quantum well structures (QWs) is an important problem in semiconductor physics. Experimental results on the binding energy of donors in QWs based on far-infrared magneto-spectroscopy and electronic Raman scattering as well as electro-reflectance spectroscopy measurements have been reported<sup>[1~6]</sup>. Some authors have investigated theoretically impurity states in quantum wells in an external field, without taking the electron-phonon (e-p) interaction into account<sup>[7~10]</sup>. These studies concluded that the electric field causes different Stark shifts for the impurity states at different positions. Further, the effects of e-p interaction on the impurity state binding energies

in QWs have also been investigated by various theoretical methods<sup>[11~14]</sup>. Different e-p effects, either enhancing or diminishing the binding energy, have been predicted by considering different phonon modes and impurity positions<sup>[11, 12]</sup>. The e-p effect on the quantum confined Stark effect of a bound polaron in a QW was studied<sup>[15]</sup>. An e-p interaction Hamiltonian deduced by Licari and Evrard<sup>[16]</sup> for a slab instead of QW was used as an approximation in their work. And the interaction between the electron and the impurity center, which screens the Coulomb potential, was omitted also. Therefore, a further investigation by using a more complicated and complete description for the electron- as well as impurity center-phonon coupling in QWs is required.

In this paper, we study the effects of the e-p interaction on the binding energies and the Stark shift of impurity states in QWs subjected to an external electric field. Different from the preceding

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work<sup>[15]</sup>, the bound electron as well as the impurity center couplings with both the longitudinal optical (LO) and interface optical (IO) phonons are considered. Donor impurity binding energies as functions of the impurity position, the well width and the electric field strength were obtained by using the LLP approach<sup>[17]</sup> with a variational calculation. The results for GaAs/Al<sub>0.3</sub>Ga<sub>0.7</sub>As, as an example, were given and discussed.

## 2 Hamiltonian

Let us consider a polar QW, for which the well material is in the range  $|z| \leq d$  and the barrier material is filled the space  $|z| > d$ . The coordinate origin is chosen at the well center. A conduction electron is bound around the donor impurity center located at  $(0, 0, z_0)$  in the QW, and a uniform electric field is perpendicular to the interfaces of the well. By adopting the effective mass and the infinite-square-well approximations, the Hamiltonian of the impurity-phonon system then can be written as

$$H = H_e + H_c + H_F + H_{LO} + H_{i-LO} + H_{IO} + H_{i-IO} \quad (1)$$

Here, the first term includes the electron kinetic energy and the well potential, and is given by

$$H_e = -\frac{\hbar^2}{2m_e} \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} - \frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial z^2} + V(z) \quad (2)$$

$$\text{with } V(z) = \begin{cases} 0 & |z| \leq d \\ \infty & |z| > d \end{cases} \quad (3)$$

where  $m_e$  is the effective mass of the electron,  $\rho = \sqrt{x^2 + y^2}$  is the radial component of the electron coordinate in the  $x$ - $y$  plane.

The second term in Eq. (1) is the Coulomb potential experienced by the electron, written as

$$H_c = -\frac{e^2}{\varepsilon_\infty \sqrt{\rho^2 + (z - z_0)^2}} \quad (4)$$

where  $\varepsilon_\infty$  is the high frequency dielectric constant of the well material.

The electric field energy of this system in the external electric field  $F$  is given by

$$H_F = |e| Fz \quad (5)$$

The fourth and fifth terms in Eq. (1) describe respectively the confined bulk-like LO phonon field and its coupling with both the electron and the impu-

rity ion, and are given by<sup>[18-21]</sup>

$$H_{LO} = \sum_{\mathbf{k}_{mp}} \hbar \omega_{L1} a_{\mathbf{k}_{mp}}^+ a_{\mathbf{k}_{mp}} \quad (6)$$

$$H_{i-LO} = \sum_{\mathbf{k}_{mp}} \{ [V_{\mathbf{k}_{mp}}(z) e^{i\mathbf{k} \cdot \boldsymbol{\rho}} - V_{\mathbf{k}_{mp}}(z_0)] a_{\mathbf{k}_{mp}} + \mathbf{h} \cdot \mathbf{c} \} \quad (7)$$

with

$$V_{\mathbf{k}_{mp}}(z) = \frac{iB}{(k^2 + k_m^2)^{1/2}} \text{csn}(k_m z) \quad (7.1)$$

$$B = \sqrt{2} \left( \frac{4\pi\alpha_1}{\Omega} \right)^{1/2} \left( \frac{\hbar}{2m_e \omega_{L1}} \right)^{1/4} \hbar \omega_{L1} \quad (7.2)$$

$$k_m = \frac{m\pi}{2d} \quad (7.3)$$

$$\Omega = S2d \quad (7.4)$$

$$\text{csn}(k_m z) = \begin{cases} \cos(k_m z), & m = 1, 3, 5, \dots \\ \sin(k_m z), & m = 2, 4, 6, \dots \end{cases} \quad (7.5)$$

where  $a_{\mathbf{k}_{mp}}^+$  ( $a_{\mathbf{k}_{mp}}$ ) is the creation (annihilation) operator for the LO phonon confined in the well material with frequency  $\omega_{L1}$ , wave vector  $(\mathbf{k}, k_m)$  and parity  $p$ . For the even (odd) parity,  $p$  is positive (negative) and  $m$  odd (even). The wave vector  $k_m$  is limited by the Brillouin-zone boundary, that is,  $m\pi/2d \leq \pi/d$  ( $d$  is the lattice constant of the well material).

$$\alpha_1 = \left( \frac{1}{\varepsilon_{\infty 1}} - \frac{1}{\varepsilon_{01}} \right) \left( \frac{m_e e^4}{2\hbar^3 \omega_{L1}} \right)^{1/2} \quad (7.6)$$

is the Fröhlich electron-LO-phonon coupling constant.  $\varepsilon_{\infty 1}$  and  $\varepsilon_{01}$  are respectively the high-frequency and static dielectric constants of the well material.  $\Omega$  is the volume and  $S$  is the interface area.

The last but one term stands for the IO-phonon field energy:

$$H_{IO} = \sum_{\mathbf{k}_{\sigma p}} \hbar \omega_{\sigma p} a_{\mathbf{k}_{\sigma p}}^+ a_{\mathbf{k}_{\sigma p}} \quad (8)$$

with

$$\omega_{\pm p}^2 = \frac{B_p(k) \pm \{ B_p^2(k) - 4A_p(k)C_p(k) \}^{1/2}}{2A_p(k)} \quad (8.1)$$

$$A_p(k) = a_1^p + a_2^p \quad (8.2)$$

$$B_p(k) = a_1^p (\omega_{L1}^2 + \omega_{T2}^2) + a_2^p (\omega_{L2}^2 + \omega_{T1}^2) \quad (8.3)$$

$$C_p(k) = a_1^p \omega_{L1}^2 \omega_{T2}^2 + a_2^p \omega_{L2}^2 \omega_{T1}^2 \quad (8.4)$$

$$a_1^\pm = (1 \mp e^{-2kd}) \varepsilon_{\infty 1} \quad (8.5)$$

$$a_2^\pm = (1 \pm e^{-2kd}) \varepsilon_{\infty 2} \quad (8.6)$$

where putting  $\sigma, p = +, -$  give four branches of IO phonon modes, respectively.

The last term is the IO-phonon interactions with both the bound-electron and the impurity-center:

$$H_{i-IO} = \sum_{k\sigma p} \{ [W_{k\sigma p}(z) e^{ik \cdot \rho} - W_{k\sigma p}(z_0)] a_{k\sigma p} + h \cdot c \} \quad (9)$$

where

$$W_{k\sigma+}(z) = -iD_{\sigma+}(kd) \left[ \frac{2\pi\hbar e^2}{Sk\omega_{\sigma+}} \right]^{1/2} \frac{\cosh(kz)}{\cosh(kd)} \quad (9.1)$$

$$W_{k\sigma-}(z) = -iD_{\sigma-}(kd) \left[ \frac{2\pi\hbar e^2}{Sk\omega_{\sigma-}} \right]^{1/2} \frac{\sinh(kz)}{\sinh(kd)} \quad (9.2)$$

$$D_{\sigma+}(kd) = [2\xi_{1\sigma+}^2 \tanh(kd) + 2\xi_{2\sigma+}^2]^{-1/2} \quad (9.3)$$

$$D_{\sigma-}(kd) = [2\xi_{1\sigma-}^2 \coth(kd) + 2\xi_{2\sigma-}^2]^{-1/2} \quad (9.4)$$

$$\xi_{\lambda\sigma p} = \frac{(\varepsilon_{\lambda\sigma p} - \varepsilon_{\infty\lambda})}{\omega_{T\lambda}(\varepsilon_{0\lambda} - \varepsilon_{\infty\lambda})^{1/2}} \quad (\lambda = 1, 2) \quad (9.5)$$

$$\varepsilon_{\lambda\sigma p} = \varepsilon_{\infty\lambda} \frac{\omega_{L\lambda}^2 - \omega_{\sigma p}^2}{\omega_{T\lambda}^2 - \omega_{\sigma p}^2} \quad (\lambda = 1, 2) \quad (9.6)$$

in which  $a_{k\sigma p}^+$  ( $a_{k\sigma p}$ ) is the creation (annihilation) operator for the IO phonon with frequency  $\omega_{\sigma p}$  and wave vector  $\mathbf{k}$ ,  $\omega_{L1}$  ( $\omega_{L2}$ ) and  $\omega_{T1}$  ( $\omega_{T2}$ ) are the well (barrier) material LO phonon frequency and TO phonon frequency, respectively.  $\varepsilon_{\infty 2}$  ( $\varepsilon_{02}$ ) is the high-frequency (static) dielectric constant of the barrier material. In writing the Hamiltonians (7) and (9), the impurity ion is assumed to be rest and contributes the terms of  $V_{kmp}(z_0)$  and  $W_{k\sigma p}(z_0)$  respectively to the interactions of LO- and IO-phonon fields with the donor-impurity, by extending the treatment used by Platzman for bulk bound polarons to QWs<sup>[20, 21]</sup>.

### 3 Variational Procedure

For ease to solve the Hamiltonian (1) we firstly eliminate the term related to the impurity-phonon coupling by performing a previous canonical transformation<sup>[20]</sup>

$$U_0 = \exp \left\{ \sum_{kmp} (a_{kmp}^+ + a_{kmp}) V_{kmp}^*(z_0) / \hbar\omega_{L1} + \sum_{k\sigma p} (a_{k\sigma p}^+ + a_{k\sigma p}) W_{k\sigma p}^*(z_0) / \hbar\omega_{\sigma p} \right\} \quad (10)$$

The transformed Hamiltonian is given by

$$\begin{aligned} H^* &= U_0^{-1} H U_0 = \\ &= -\frac{\hbar^2}{2m_e} \frac{1}{\rho} \frac{\partial}{\partial \rho} \frac{\partial}{\partial \rho} - \frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial z^2} + V(z) + \\ &= |e| Fz - \frac{e^2}{\varepsilon_{\infty} \sqrt{\rho^2 + (z - z_0)^2}} + \sum_{kmp} \hbar\omega_{L1} a_{kmp}^+ a_{kmp} + \\ &= \sum_{k\sigma p} \hbar\omega_{\sigma p} a_{k\sigma p}^+ a_{k\sigma p} + \sum_{kmp} \{ V_{kmp}(z) e^{ik \cdot \rho} a_{kmp} + h \cdot c \} + \\ &= \sum_{k\sigma p} \{ W_{k\sigma p}(z) e^{ik \cdot \rho} a_{k\sigma p} + h \cdot c \} - \\ &= \sum_{kmp} \left( \frac{V_{kmp}(z) V_{kmp}(z_0) e^{ik \cdot \rho}}{\hbar\omega_{L1}} + h \cdot c \right) - \\ &= \sum_{k\sigma p} \left( \frac{W_{k\sigma p}(z) W_{k\sigma p}(z_0) e^{ik \cdot \rho}}{\hbar\omega_{\sigma p}} + h \cdot c \right) \quad (11) \end{aligned}$$

For convenience here we have dropped the infinite constant self-energy term of the positive point charge  $\left( -\sum_{kmp} |V_{kmp}(z_0)|^2 / \hbar\omega_{L1} \text{ and } -\sum_{k\sigma p} |W_{k\sigma p}(z_0)|^2 / \hbar\omega_{\sigma p} \right)$ , which is equivalent to adjusting the baseline of the energy. And then we use two LLP-like unitary transformations<sup>[17]</sup> to simplify the calculation

$$U_1 = \exp \left[ \left( -i \sum_{kmp} a_{kmp}^+ a_{kmp} \mathbf{k} \cdot \boldsymbol{\rho} \right) + \left( -i \sum_{k\sigma p} a_{k\sigma p}^+ a_{k\sigma p} \mathbf{k} \cdot \boldsymbol{\rho} \right) \right] \quad (12)$$

$$U_2 = \exp \left[ \sum_{kmp} \left( a_{kmp}^+ f_1 - a_{kmp} f_1^* \right) + \sum_{k\sigma p} \left( a_{k\sigma p}^+ f_2 - a_{k\sigma p} f_2^* \right) \right] \quad (13)$$

$f_1, f_2, f_1^*, f_2^*$  are the variational parameters. After the two unitary transformations the Hamiltonian of the system becomes

$$\begin{aligned} H^{**} &= U_2^{-1} U_1^{-1} H U_1 U_2 = \\ &= -\frac{\hbar^2}{2m_e} \frac{1}{\rho} \frac{\partial}{\partial \rho} \frac{\partial}{\partial \rho} - \frac{\hbar^2}{2m_e} \frac{\partial^2}{\partial z^2} + V(z) + |e| Fz - \\ &= \frac{e^2}{\varepsilon_{\infty} \sqrt{\rho^2 + (z - z_0)^2}} + \sum_{kmp} \left( \hbar\omega_{L1} + \frac{\hbar^2 k^2}{2m_e} \right) \cdot \\ &= (a_{kmp}^+ a_{kmp} + f_1 a_{kmp}^+ + f_1^* a_{kmp} + |f_1|^2) + \sum_{k\sigma p} \left( \hbar\omega_{\sigma p} + \frac{\hbar^2 k^2}{2m_e} \right) \cdot \end{aligned}$$

$$\begin{aligned} &= (a_{k\sigma p}^+ a_{k\sigma p} + f_2 a_{k\sigma p}^+ + f_2^* a_{k\sigma p} + |f_2|^2) + \\ &= \sum_{kmp} \{ V_{kmp}(z) a_{kmp} + V_{kmp}(z) f_1 + h \cdot c \} + \\ &= \sum_{k\sigma p} \{ W_{k\sigma p}(z) a_{k\sigma p} + W_{k\sigma p}(z) f_2 + h \cdot c \} - \\ &= \sum_{kmp} \left\{ \frac{V_{kmp}(z) V_{kmp}(z_0) e^{ik \cdot \rho}}{\hbar\omega_{L1}} + h \cdot c \right\} - \end{aligned}$$

$$\sum_{\mathbf{k}\sigma\mathbf{p}} \left\{ \frac{W_{\mathbf{k}\sigma\mathbf{p}}(z) W_{\mathbf{k}\sigma\mathbf{p}}(z_0) e^{i\mathbf{k}\cdot\mathbf{p}}}{\hbar\omega_{\sigma\mathbf{p}}} + h \cdot c \right\} -$$

$$\frac{\hbar}{m} \sum_{\mathbf{k}\sigma\mathbf{p}} \mathbf{p} \cdot \mathbf{k} (a_{\mathbf{k}\sigma\mathbf{p}}^+ a_{\mathbf{k}\sigma\mathbf{p}} + f_1 a_{\mathbf{k}\sigma\mathbf{p}}^+ + f_1^* a_{\mathbf{k}\sigma\mathbf{p}} + |f_1|^2) -$$

$$\frac{\hbar}{m} \sum_{\mathbf{k}\sigma\mathbf{p}} \mathbf{p} \cdot \mathbf{k} (a_{\mathbf{k}\sigma\mathbf{p}}^+ a_{\mathbf{k}\sigma\mathbf{p}} + f_2 a_{\mathbf{k}\sigma\mathbf{p}} + f_2^* a_{\mathbf{k}\sigma\mathbf{p}} + |f_2|^2)$$
(14)

Here we have ignored the multi-phonon processes for this kind of weak e-p coupling case. Since we are interested only in the ground state of the impurity system, and assume that momentum of the electron in  $x$ - $y$  plane is zero, the last two terms in the above equation can be assumed to be zero.

Considering the polaron being bound by the impurity center as well as confined in the QW, we choose a variational trial wave function as follows

$$|\Phi\rangle = N_0(\beta, \lambda) \phi_0(z) \cdot$$

$$\exp \left[ -\frac{\lambda}{2} \sqrt{(z - z_0)^2 + \rho^2} \right] |0\rangle \quad (15)$$

where

$$\phi_0(z) = \cos\left(\frac{\pi z}{2d}\right) \exp\left(-\frac{\beta z}{2d}\right) \quad (16)$$

$|0\rangle$  in (15) is the phonon vacuum state.  $N_0(\beta, \lambda)$  is the normalization constant of wave function (16).  $\beta$  and  $\lambda$  are both the variational parameters and will be determined by minimizing the expectation values of Hamiltonian (1).

The ground-state energy of the bound polaron then can be calculated by the following minimizing equation

$$E_g = \min_{\lambda, \beta} \langle \Phi | H^{**} | \Phi \rangle \quad (17)$$

The binding energy of the bound polaron is then given by subtracting the ground state energy from the free polaron energy  $E_{\text{free}}$

$$E_B = E_{\text{free}} - E_g \quad (18)$$

To calculate the free polaron energy, we write down the corresponding Hamiltonian by dropping the free motion of the electron in the  $x$ - $y$  plane:

$$H_{\text{free}} = -\frac{\hbar^2 d^2}{2m_e dz^2} + V(z) + H_F + H_{\text{LO}} + H_{e\text{-LO}} +$$

$$H_{\text{IO}} + H_{e\text{-IO}} \quad (19)$$

where

$$H_{e\text{-LO}} = \sum_{\mathbf{k}\sigma\mathbf{p}} \{ V_{\mathbf{k}\sigma\mathbf{p}}(z) e^{i\mathbf{k}\cdot\mathbf{p}} a_{\mathbf{k}\sigma\mathbf{p}} + h \cdot c \} \quad (19.1)$$

$$H_{e\text{-IO}} = \sum_{\mathbf{k}\sigma\mathbf{p}} \{ W_{\mathbf{k}\sigma\mathbf{p}}(z) e^{i\mathbf{k}\cdot\mathbf{p}} a_{\mathbf{k}\sigma\mathbf{p}} + h \cdot c \} \quad (19.2)$$

Using the LLP-like unitary transformations (12) and (13), the free polaron Hamiltonian is transformed into

$$H_{\text{free}}^{**} = U_2^{-1} U_1^{-1} H_{\text{free}} U_1 U_2 =$$

$$-\frac{\hbar}{2m_e} \frac{d^2}{dz^2} + V(z) + |e| Fz + \sum_{\mathbf{k}\sigma\mathbf{p}} \left( \hbar\omega_{\text{Ll}} + \frac{\hbar^2 k^2}{2m_e} \right) \cdot$$

$$a_{\mathbf{k}\sigma\mathbf{p}}^+ a_{\mathbf{k}\sigma\mathbf{p}} + \sum_{\mathbf{k}\sigma\mathbf{p}} \left( \hbar\omega_{\sigma\mathbf{p}} + \frac{\hbar^2 k^2}{2m_e} \right) a_{\mathbf{k}\sigma\mathbf{p}}^+ a_{\mathbf{k}\sigma\mathbf{p}} -$$

$$\sum_{\mathbf{k}\sigma\mathbf{p}} \frac{|V_{\mathbf{k}\sigma\mathbf{p}}(z)|^2}{\hbar\omega_{\text{Ll}} + \frac{\hbar^2 k^2}{2m_e}} - \sum_{\mathbf{k}\sigma\mathbf{p}} \frac{|W_{\mathbf{k}\sigma\mathbf{p}}(z)|^2}{\hbar\omega_{\sigma\mathbf{p}} + \frac{\hbar^2 k^2}{2m_e}} \quad (20)$$

Choosing the trial wave function

$$|f\rangle = \phi_0(z) |0\rangle \quad (21)$$

the free polaron energy can be calculated by

$$E_{\text{free}} = \min_{\beta} \langle f | H_{\text{free}}^{**} | f \rangle \quad (22)$$

Finally, the Stark shift of the binding energy of the bound polaron is then determined by

$$\Delta E_B = E_B(F) - E_B(F=0) \quad (23)$$

## 4 Numerical Results and Discussion

The calculations of the binding energies of donor impurity states with and without including electron-IO- and LO-phonon interactions for various values of the electric field are numerically performed for several III-V compound QW systems. The results for GaAs/Al<sub>0.3</sub>Ga<sub>0.7</sub>As QW, as an example, are shown in Figs. 1 ~ 3. The parameters used in the calculations are listed in Table 1.

In Fig. 1 we plot the variations of the binding energies of the impurity state located at the well-center of GaAs/Al<sub>0.3</sub>Ga<sub>0.7</sub>As QW as functions of the

**Table 1 Parameters used in the computation. Phonon energies are measured in units of meV and electronic effective mass in units of the bare electron mass**

	$\varepsilon_0$	$\varepsilon_\infty$	$\hbar\omega_{\text{LO}}$	$\hbar\omega_{\text{TO}}$	$m_e$
GaAs <sup>[22]</sup>	13.18	10.89	36.25	33.29	0.067
Al <sub>x</sub> Ga <sub>1-x</sub> As <sup>[22]</sup>	13.18 - 3.12x	10.89 - 2.73x	36.25 - 6.55x + 1.79x <sup>2</sup>	33.29 - 0.64x - 1.16x <sup>2</sup>	0.067 + 0.083x

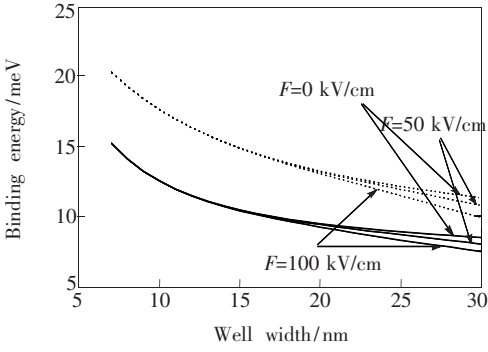


Fig. 1 Donor impurity binding energy with (solid) and without (dotted) impurity-phonon interaction as functions of the well width in GaAs/Al<sub>0.3</sub>Ga<sub>0.7</sub>As QWs for three different values of electric field:  $F = 0, 50, 100$  kV/cm. The impurity center is located at the well-center.

well width for  $F = 0, 50$  and  $100$  kV/cm. As expected the donor impurity binding energies increase monotonically with decreasing the well width. It is clearly seen by comparing the results for  $F = 0, 50$  and  $100$  kV/cm in Fig. 1 that the external electric field reduces the binding energies and causes a Stark shift. The electric field effect on the binding energy is rather weak for small size QWs. Only at large QW sizes, the electron wave function is significantly modified by the applied electric field, leading to smaller values of the binding energy for a donor located at the center of the well. It is well known that the electron is pushed against the direction of the applied

electric field and therefore the binding energy of the donor is weakened. It is also seen clearly that the Stark effect becomes stronger with increasing well width. Furthermore, the influence of the impurity state-phonon interaction on the Stark shift can also be found for the GaAs/Al<sub>0.3</sub>Ga<sub>0.7</sub>As QW in Fig. 1. The binding energies with phonon influence are lower than those without phonons for the whole field range from  $F = 0$  to  $100$  kV/cm. It is known that the e-p coupling screens the coulomb interaction between the donor and the bound electron, so that the impurity state binding energy is obviously reduced. The characteristics of the Stark energy shift of the impurity state on the well-width and the field obtained in this work are in agreement with Ref. [15]. However, the latter gave over weak effect for the e-p influence on the bound polaron energy, due to omitting the impurity-ion-phonon interaction.

Fig. 2 displays the variation of the donor impurity binding energies as functions of the impurity position  $z_0$ , with field intensities of 0, 100 and 200 kV/cm for the QWs of  $d = 3.5, 5.0$  and  $7.5$  nm. For the zero-field case we obtain central symmetrical curves of the binding energy around the impurity center, either with or without considering the phonon effect. The peak of the binding energy curve moves towards the  $z_0 < 0$  direction and the symmetry around the

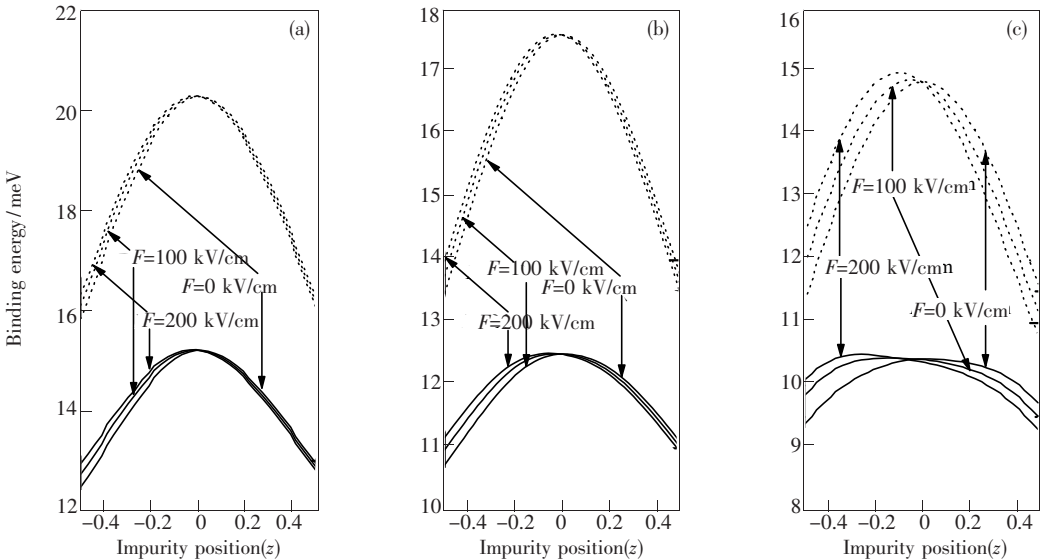


Fig. 2 Donor impurity binding energy with (solid) and without (dotted) phonons as functions of the impurity position  $z$  in the GaAs/Al<sub>0.3</sub>Ga<sub>0.7</sub>As QWs with the well width (a)  $d = 3.5$  nm, (b)  $d = 5$  nm and (c)  $d = 7.5$  nm for the electric field  $F = 0, 100, 200$  kV/cm.

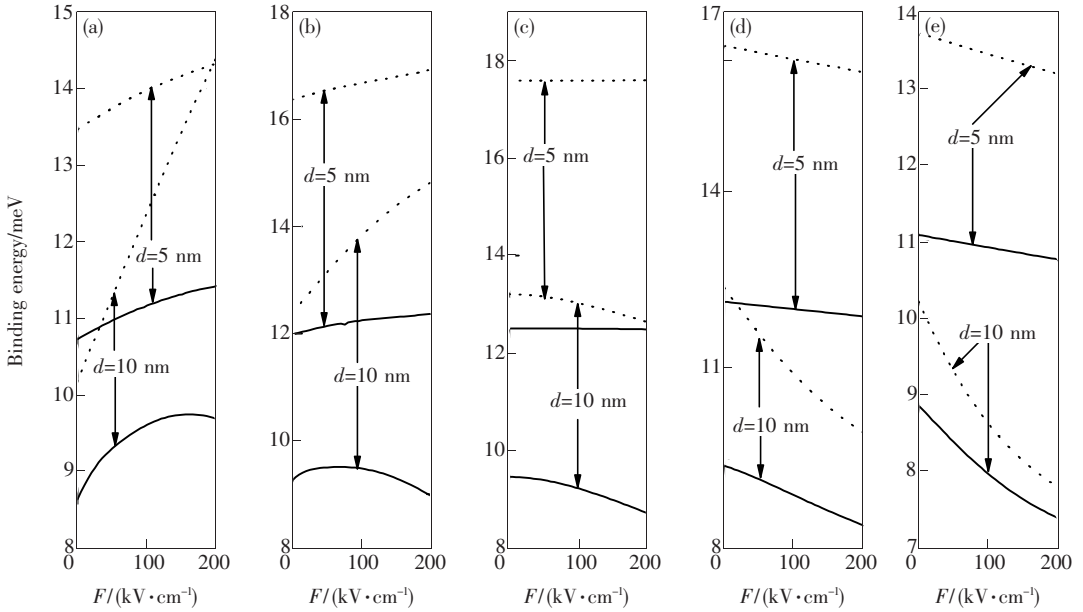


Fig. 3 Impurity binding energies with (solid) and without (dotted) phonons as functions of the applied electric field for GaAs/ $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$  QWs with the well width  $d=5$  and  $10$  nm for different QWs of the donor impurity (a)  $z=-d$ ; (b)  $z=-d/2$ ; (c)  $z=0$ ; (d)  $z=d/2$ ; (e)  $z=d$ .

$z_0 = 0$  position disappears when  $F \neq 0$ , since the electron is pulled against the electric field with increasing the field intensity. At the same time, the binding energies become more sensitive to the electric field when the impurity center deviates from the center of the well. On the other hand, the binding energy increases and the Stark shift decreases for all impurity positions with decreasing well width, due to an increase of the quantum confinement effect. It is also found from the figures that the electric field enhances the donor impurity binding energy, when the impurity center is positioned on the left of the binding energy curve peak. In contrast, it decreases when the impurity is positioned at the right side of the peak. As was mentioned above the donor impurity state binding energy with phonon effect is lower than that without phonon field. It is worthwhile to note that the e-p interaction has a stronger effect on the binding energies of polarons when the impurity centers are located near the well center.

For the sake of demonstrating the electric field effect, we also illustrate the dependence of the donor impurity binding energy as a function of the applied electric field for different donor impurity positions in the GaAs/ $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$  QWs with several well widths,

as shown in Fig. 3.

One can see from the figures that the binding energies of donor impurity states vary with the electric field strength significantly for the wide well case. Whereas the curves are almost flat for narrow wells, especially, when the impurity center is located at the well center, because the electron and the impurity ion can not be pulled apart very far due to the confinement by two closed spaced barriers. Moreover, the characteristics of the variations of the binding energies with the field are different for various locations of the impurity center. Since the electric field pulls the electron towards  $-z$ -direction in the QW against the field (along to  $z$ -direction), the binding energies decrease with increasing the electric field for the donor located at the center and  $z > 0$  positions, where the probability of finding the electron is reduced. On the other hand, the binding energies increase significantly with the electric field for the donor located at the left edge ( $z = -d$ ) in the well. Another interesting feature seen from Fig. 3 is that the slopes of the curves for the binding energies without phonon effect are steeper than those with phonon contribution for this system. This is due to the fact that the e-p interaction introduces a depolar-

rized field and reduces the macroscopic electric field, so that the Stark effect is weakened.

## 5 Conclusion

In conclusion, by taking electron-phonon interaction into account, the numerical results of the binding energies of donor impurity state in the GaAs/AlGaAs QW are obtained as the functions of well thickness, impurity position and applied electric field. The results show that the electron-phonon interaction reduces the donor binding energy and the Stark effect. The binding energy as well as Stark effect is sensitive to both the well width and the impurity position in QW. The binding energy may either enhance or diminish with increasing field strength.

This behavior depends on the well width and the impurity position in the quantum well. It is also shown that the electron-phonon interaction causes so significant correction to the impurity state binding energies that the Stark effect cannot be neglected.

It is pointed out that the image potential caused by the polarization of the valence electrons is ignored in our calculations, because the attention is focused on the phonon contributions to the binding energy. Previous authors have also concluded that the total image potential effect on the impurity binding energy is much weak by taking both the impurity ion and bound electron image potentials into account in this kind of QWs<sup>[23]</sup>.

## References:

- [ 1 ] Jarosik N C, McCombe B D, Shanabrook B V, *et al.* Binding of shallow donor impurities in quantum-wells structures [J]. *Phys. Rev. Lett.*, 1985, **54**(12):1283-1286.
- [ 2 ] McCombe B D, Jiang Z X, Hawrylak P. Spectroscopy of neutral and charged donors in semiconductor quantum wells: Many body effects [J]. *Phys. Stat. Sol. (b)*, 1998, **210**(2):587-597.
- [ 3 ] Shanabrook B V, Comas J, Perry T A, *et al.* Raman scattering from electrons bound to shallow donors in GaAs-Al<sub>x</sub>Ga<sub>1-x</sub>As quantum-well structures [J]. *Phys. Rev. B*, 1984, **29**(12):7096-7098.
- [ 4 ] Lemos V, Ritter T, Weinstein B A. Anomalies in the pressure response of the Raman modes in (211)-oriented In<sub>x</sub>Ga<sub>1-x</sub>As/GaAs strained-layer superlattices [J]. *Appl. Phys. Lett.*, 1992, **61**(12):1417-1419.
- [ 5 ] Spagnolo V, Scamarcio G, Colombelli R, *et al.* Evidence of electronic confinement in pseudomorphic Si/GaAs superlattices [J]. *Phys. Rev. B*, 1998, **57**(24):R15100-R15103.
- [ 6 ] Klipstein P C, Tapster P R, Apsley N, *et al.* Electroreflectance spectroscopy from quantum well structures in an electric field [J]. *J. Phys. C: Solid State Phys.*, 1986, **19**(6):857-871.
- [ 7 ] Kasapoglu E, Sari H, Sokmen I. Binding energies of shallow donor impurities in different shaped quantum wells under an applied electric field [J]. *Physica B*, 2003, **339**(1):17-22.
- [ 8 ] Matos-Abiague A, Berakdar J. Femtosecond control of electronic motion in semiconductor double quantum wells [J]. *Phys. Rev. B*, 2004, **69**(15):155304-1-3.
- [ 9 ] Chen H, Li X D, Zhou S X. Stark shift of hydrogenic impurity states in a quantum well [J]. *Phys. Rev. B*, 1991, **44**(12):6220-6223.
- [ 10 ] López-Gondar J, d'Albuquerque e Castro J, Oliveira L E. Electric-field effects on shallow impurity states in GaAs-(Ga,Al)As quantum wells [J]. *Phys. Rev. B*, 1990, **42**(11):7069-7077.
- [ 11 ] Shen Z J, Yuan X Z, Shen G T, *et al.* Effect of electron-surface-optical-phonon interaction on the impurity-state energies in a semiconductor quantum well [J]. *Phys. Rev. B*, 1994, **49**(16):11035-11039.
- [ 12 ] Sil S, Chatterjee A. Ground and excited states of a bound polaron in a purely two-dimensional quantum well [J]. *J. Phys.: Cond. Mat.*, 1991, **3**(47):9401-9416.
- [ 13 ] Apostolova T, Huang D H, Cardimona D A. Photon-absorption-induced intersubband optical-phonon scattering of electrons in quantum wells [J]. *Phys. Rev. B*, 2003, **67**(20):205323-1-3.
- [ 14 ] Bibik A I, Gerlach L B, Smondyrev M A. Large polaron in an asymmetrical rectangular quantum well [J]. *Phys. Stat. Sol. (b)*, 2003, **237**(1):186-193.

- [15] Li Y C, Gu S W. Electron-phonon effects on Stark shifts of a bound polaron in a quantum well [J]. *Phys. Rev. B*, 1992, **45**(20):12102-12105.
- [16] Licari J C, Evrard R. Electron-phonon interaction in a dielectric slab; Effect of the electronic polarizability [J]. *Phys. Rev. B*, 1977, **15**(4):2254-2264.
- [17] Lee T D, Low F, Pines D. The motion of slow electrons in a polar crystal [J]. *Phys. Rev.*, 1953, **90**:297-302.
- [18] Liang X X. The interaction of interface optical phonons with an electron in an asymmetric quantum well [J]. *J. Phys. : Condensed Matter*, 1992, **4**(49):9769-9778.
- [19] Zheng R S, Ban S L, Liang X X. Effect of interface and bulk optical phonons on polarons in a quantum well [J]. *Phys. Rev. B*, 1994, **49**(3):1796-1801.
- [20] Platzman P M. Ground-state energy of bound polarons [J]. *Phys. Rev.*, 1962, **125**(6):1961-1965.
- [21] Bouhassoune M, Charrou R, Fliyou M, *et al.* Binding energy of shallow impurities in a polar quantum well wire [J]. *Physica B*, 2001, **304**(1-4):389-397.
- [22] Adachi S. GaAs, AlAs, and  $\text{Al}_x\text{Ga}_{1-x}\text{As}$ : Material parameters for use in research and device applications [J]. *J. Appl. Phys.*, 1985, **58**(3):R1-R29.
- [23] Deng Z Y, Lai T R, Guo J K, *et al.* Electronic and shallow donor impurity states in GaAs- $\text{Ga}_{1-x}\text{Al}_x\text{As}$  quantum-well wires; Effects of dielectric mismatch [J]. *J. Appl. Phys.*, 1994, **75**(11):7389-7393.

## 外电场下极性量子阱中杂质态结合能

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**摘要:** 我们用变分方法研究了外电场下量子阱中的杂质态结合能, 计算中既考虑了电子-声子相互作用又考虑了杂质中心-声子相互作用。我们以 GaAs/ $\text{Al}_{0.3}\text{Ga}_{0.7}\text{As}$  量子阱为例, 讨论了结合能随杂质位置、阱宽和电场强度的变化规律。得到了电子-声子相互作用对杂质态结合能和斯塔克效应的修正是相当明显的。

**关键词:** 施主杂质态; 电子-声子相互作用; 量子阱; 斯塔克效应

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