Polaron effect on the binding energy of a hydrogenic impurity in GaAs-$Ga_{1-x}Al_xAs$ superlattice

L. Tayebi [1,*], M. Fliyou [2], Y. Boughaleb[1] and L.Bouziaene [3]

[1]Faculté des Sciences Ben M' Sik, Département de Physique, L.P.M.C,BP.7955, Casablanca, Morocco.
[2]Ecole Normale Supérieure, E.N.S, B.P 2400, Marrakech, Morocco.
[3]Laboratoire de Physique des Semiconducteurs et des Composants pour l'Electronique, Faculté des Sciences de Monastir, Avenue de L'Environnement, Tunisie.
[*] tayebi_lakhdar@yahoo.fr

The effect of the bulk Longitudinal-Optical (LO) phonon on the binding energy is investigated for a shallow donor impurity in a superlattice in the effective mass approximation by using the variational approach. The results are obtained as a function of parameters which characterize the superlattice and the position of the impurity center. The results show that the bulk Longitudinal-Optical (LO) phonon effect decreases by displacing the impurity from the center to the well boundary.

Keywords: *Low dimensional system, impurity, binding energy, polaronic effct.*

I. INTRODUCTION

With recent advances in epitaxial crystal-growth techniques such as molecular-beam epitaxy (MBE) and metal-organic chemical vapor deposition (MOCVD), it has become possible to grow systems of alternate layers of either two different materials (heterostructures) or of the same material with different doping properties, having controlled thickness and sharp interfaces. These relatively new one-dimensional periodic structures, with dimensions which can approach the atomic spacings of the constituent materials of which they are composed, are referred to as superlattices. Among the most extensively of alternate layers of GaAs and $Ga_{1-x}Al_xAs$. Depending on the Al content in $Ga_{1-x}Al_xAs$, its band gap can be made considerably larger than that of GaAs, thus leading to discontinuities of the conduction- and valence-band edges at the interfaces between GaAs and $Ga_{1-x}Al_xAs$. For Al concentration less than about 40% ($x \leq 4$), $Ga_{1-x}Al_xAs$ has a direct band gap at the Γ point [1]. The conduction- and the valence-band discontinuities at the interfaces have been suggested to be about 85 and 15%, respectively, of the direct-band-gap difference between the two semiconductors [2]. This leads to the formation of quantum wells in the GaAs layers.

Over past years, a large number of works [3-14] have been carried out to investigate the electronic, the optical and the transport properties of an electron confined in a quasi-two dimensional semiconductor structures. Bastard [15] reported the first calculation for binding energies of hydrogenic impurities in quantum wells (QW's) with an infinite potential in the barriers. Several groups [16,17] have extended the works of Bastard to calculate the low-lying energy levels of a donor in the finite high barrier QW. The first attempt to use more than a single quantum well was done by Chaudhuri [18], who used three quantum wells in this variational calculation of the ground-state energy of a donor electron with respect to the lowest subband level. This work will be generalized by Lane and Greene [19], to the case of superlattices for a calculation of the binding energies for the ground state energy (1s-like) and low-lying exited states ($2p_{\pm}$-like) energy of a hydrogenic donor associated with the first subband level.

The above studies have been considered without taking into account the polaronic effect. The polaronic process has become a main research subject in those systems due to the key role played by the optical phonons on the scatting of charge carriers. This process is important for the understanding of the experimental observation of semiconductor optical spectra. Several works have been carried out to evaluate the contribution of the coupling between charge carriers and phonons [20-36] to the impurities and excitons states in low dimensional structures. In the superlattices and quantum well systems based on polar and semi-polar semiconductors, the interaction of an electron weakly bound to a hydrogenic impurity with the longitudinal optical phonon of the host semiconductor is then imposed and this yields to an increasing of the binding energy. Shi et al [20] presented a theoretical investigation of the transitions energies for shallow donor impurities in a GaAs-$Ga_{1-x}Al_xAs$ superlattice in the presence of a magnetic field applied along the growth axis. They have shown that the energy levels depend strongly on the magnetic-field strength, the well width, and the donor position. The magnetopolaron effect on

these donor energies was studied within second-order perturbation theory in which a formal summation over all electron states is performed. The effect of band nonparabolicity is also included to correctly explain magneto-optic experimental results at high magnetic fields.

For the phonons used, we have worked with the bulk-like phonon approximation instead of the confined-phonon modes, since this approximation was recently nicely demonstrated by several experiments [37, 38].

In the present paper, the ground state of a polaron bound to a hydrogenike donor impurity is investigated by considering the effect of bulk Longitudinal-Optical (LO) phonon. A modified Lee, Low, and Pines intermediate coupling method [39] is adopted to deal with the interaction between the phonon and the electron. In our calculations, we have assumed the static dielectric constant to be the same in GaAs and $Ga_{1-x}Al_xAs$, since Green and Bajaj [10] have shown that the difference between calculations with and without taking into consideration the contribution arising from the differences in the dielectric constants is very small.

In section 2, we present the theory of calculation of the binding energy in a superlattice system taking into consideration the interaction between the electron and the bulk phonon by means of a Lee-Low-Pines transformation. The last section represents the discussion of the numerical results and a brief conclusion is given in the same section.

II. MODEL

Within the framework of an effective mass approximation, the total Hamiltonian for a single conduction band electron coupled to a Coulombic impurity and interacting with the Longitudinal-Optical (LO) phonons is written in units of energy $\hbar\omega_0$ (polaron energy) and length $\ell_0 = (\hbar / 2m\omega_0)^{1/2}$ (polaron radius):

$$H = H_e + H_{ph} + H_{int} \qquad (1)$$

Where H_e is the electronic part which describes a hydrogenic impurity atom placed in a superlettice is:

$$H_e = -\nabla_r^2 + V(z) - \frac{\beta}{r} \qquad (2)$$

The potential is modeled by a square-well potential:

$$V(z) = \begin{cases} 0, & -L_w/2 + nl \le z \le L_w/2 + nl \\ V_0, & L_w/2 + nl \le z \le -L_w/2 + (n+1)l \end{cases} \qquad (3)$$

With L_w the well width, L_b the barrier width, $l = L_w + L_b$ the periodicity, and $n = 0, \pm 1, \pm 2, \ldots$, an integer.

For a GaAs-$Al_xGa_{1-x}As$ interface, the barrier height V_0 is taken to be 85% of the total energy-band-gap difference between the two semiconductors: $\Delta E_g = 1.155x + 0.37x^2$ eV [1].

The position of the electron is denoted by $r = (r_\perp^2 + (z - z_i)^2)^{1/2}$ where $r_\perp = (x^2 + y^2)^{1/2}$ being the distance in the x-y plane, and z_i is the position of the impurity along the growth direction.
The parameter β is defined as:

$$\beta = \frac{e^2}{\hbar\varepsilon_\infty}\left(\frac{2m_e^*(z)}{\hbar\omega_0}\right)^{1/2} \qquad (4)$$

where ε_∞ is the optic dielectric constant.
In the absence of electron-phonon interaction ε_∞ is replaced by ε_0.
the quantity $m_e^*(z)$ is the electron effective mass, which is different in the two somiconductors:

$$m_e^*(z) = \begin{cases} m_w^* = 0.067\, m_0 \text{ in well} \\ m_b^* = (0.067 + 0.083x)\, m_0 \text{ in barrier} \end{cases} \qquad (5)$$

where m_0 is the free electron mass and x is the Aluminum concentration.

H_{ph} is the LO-phonon Hamiltonian which is given by:

$$H_{ph} = \sum_k a_k^+ a_k \qquad (6)$$

where a_k^+ (a_k) is the creation (annihilation) operator of a LO phonon with wave vector $\vec{k} = \vec{k}_\perp + k_z\vec{z}$ and frequency ω_0.
Evidently, we have to address why the free phonon Hamiltonian is averaged with respect to the electron wave function.

Our motivation is based on the fact that we are going to apply our model to calculate polaron effect. That is, our effective phonons will be only in a cloud around the electron, and the properties of this cloud depend on the electron position. So in our model the effective phonons replace numerous phonon modes whose frequencies depend on the coordinate z of the electron.

The electron-phonon interaction in Equation (1) is given by:

$$H_{int} = \sum_k \left(V_k a_k \exp(ik.r) + V_k^* a_k^+ \exp(-ik.r)\right) \qquad (7)$$

where $V_k = \sqrt{\frac{4\pi\tau}{\Omega}}\ \frac{1}{k}$ (8)

with Ω the volume of the system and τ the electron-phonon coupling constant

$$\tau = \frac{1}{2}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}\right)\left(\frac{e^2}{\hbar\omega_0 l_0}\right) \quad (9)$$

$\varepsilon_0\,(\varepsilon_\infty)$ is the static (high) dielectric constant, in our calculation we take $\tau = 0.070$, being the value for GaAs.

In the adiabatic approximation the total trial wave function describing the electron-phonon system can be written as product of the electron wave function $|\psi\rangle$ ant the phonon wave function, and its takes the form of:

$$|\Phi\rangle = |\Psi\rangle U_2\, U_1 |0\rangle \quad (10)$$

the phonon states is assumed as a coherent like state $U_2\, U_1 |0\rangle$, where $|0\rangle$, is the vacuum phonon state and U_1 and U_2 are the modified Lee-Low-pines unitary transformation operator of the variational method, as was used previously [24, 37].

$$U_1 = \exp(-i\sum_k a_k^+ a_k \vec{k}_\perp \vec{r}_\perp) \quad (11)$$

$$U_2 = \exp(\sum_k (g_k a_k^* - g_k^* a_k)) \quad (12)$$

where g_k and g_k^* are the variational parameters determined by minimizing the total energy subsequently.

Within the adiabatic approximationthe only effect of the electron-(LO) phonon coupling is to displace the ion equilibrium positions. This displacement is performed by means of the canonical transformation. Then the expected Hamiltonian eigenvalue in such state is given by:

$$E = \langle\Psi|\langle 0|U_2^{-1}\, U_1^{-1}\, H\, U_1 U_2|0\rangle|\Psi\rangle \quad (13)$$

which can be written as

$$E = \langle\Psi|H_e + \sum_k \left[1 + k_\perp^2 - 2qk_\perp\right]|g_k|^2 + \sum_k \left[V_k g_k \exp(ik_z z)\right] + H.c|\Psi\rangle \quad (14)$$

With: $q = -i\nabla_{r\perp}$

Then from: $\frac{\partial E}{\partial g_k} = \frac{\partial E}{\partial g_k^*} = 0$ (15)

We obtain: $g_k = -\frac{V_k^* \exp(-ik_z z)}{1 + k_\perp^2 - 2k_\perp q}$ (16)

Where $qk_\perp = 0$ and $q = -i\nabla_{r\perp}$

$$E = \langle\Psi|H_e - \sum_k \frac{|V_k|^2}{1 + k_\perp^2 - 2k_\perp q}|\Psi\rangle \quad (17)$$

For a low value of q, we have:

$$E = \langle\Psi|\, H_e - \sum_k \frac{|V_k|^2}{(1 + k_\perp^2)} - \sum_k \frac{|V_k|^2}{(1 + k_\perp^2)^3} 4k_\perp^2 q^2 |\Psi\rangle \quad (18)$$

After equation (8) we have:

$$E = \langle\Psi|H_e - \frac{1}{2}\pi\tau + \frac{1}{4}\pi\tau\nabla_{r_\perp}^2|\Psi\rangle \quad (19)$$

We solve this equation by a variational method using the non-separable wave function

$$\Psi_\alpha^\pm(r) = A\Psi^\pm(z - nl)\exp(-\frac{1}{\alpha}\sqrt{r_\perp^2 + (z - z_i)^2}) \quad (20)$$

with α being a variational parameter obtained by minimizing the impurity energy, and A the normalization factor. This function form is more appropriate to describe the system in large domain.

We choose the ground state wave function for the nth well and the nth barrier as:

$$\Psi_{sub}^\pm(z - nl) = A\frac{e^{ik_\perp r_\perp}}{\sqrt{S}}\Psi^\pm(z - nl), \quad (21)$$

where $\Psi^\pm(z - nl)$ as [40]:

$$\Psi^\pm(z - nl) = \frac{e^{\pm ink_z l}}{\sqrt{N^\pm}}\xi^\pm(z - nl) \quad (22)$$

with

$$\xi^\pm(z - nl) = \begin{cases} p^{\pm *} ch\rho(z - nl + \frac{L_w}{2}) - q^{\pm *} sh\rho(z - nl + \frac{L_w}{2}); & (a) \\ b_2 \exp ik(z - nl) + \beta^\mp \exp -ik(z - nl); & (b) \\ p^\pm ch\rho(z - nl - \frac{L_w}{2}) - q^\pm sh\rho(z - nl - \frac{L_w}{2}); & (c) \end{cases} \quad (23)$$

$$(a): -L_b/2 - L_w/2 \le z - nl \le -L_w/2$$
$$(b): -L_w/2 \le z - nl \le L_w/2$$
$$(c): L_w/2 \le z - nl \le L_w/2 + L_b/2$$

which is periodically repeated, and $\Psi^\pm(z - nl) = \Psi^\pm(z)$ where $l = L_w + L_b$ is the length of the period. The parameters k and ρ are determined by the matching conditions at the interfaces. It is assumed that both $\Psi^\pm(z)$ and $(1/m_e^*)\partial\Psi^\pm(z)/\partial z$ are continuous across the interface. We find

$k = \sqrt{2m_w^* E/\hbar^2}$, $\rho = \sqrt{2m_b^*(V_0 - E)/\hbar^2}$,

and E is the electron's energy ($E < V_0$).

The energy momentum relation is determined by transcendental equation:

$$\cos(k_z l) = \cosh(\rho L_b)\cos(k L_w) + K^- \sinh(\rho L_b)\sin(k L_w)$$

and $K^- = (1/2)(\lambda\rho/k - k/\lambda\rho)$

λ ratio between effective masses wells (m_w^*) and barriers (m_b^*): $\lambda = m_w^*/m_b^*$

$$\beta^{\pm} = (\mathrm{ch}(L_b\rho)\sin(kL_w) - K^-\mathrm{sh}(L_b\rho)\cos(kL_w)) \pm \sin(k_z l) = \beta_0 \pm \sin(k_z l)$$

$$p^{\pm} = b_2 \exp(ikL_w/2) + \beta^{\mp}\exp(-ikL_w/2)$$

$$q^{\pm} = \frac{ik}{\lambda\rho}(b_2\exp(ikL_w/2) - \beta^{\mp}\exp(-ikL_w/2))$$

$$K^{\pm} = (1/2)(\lambda\rho/k \pm k/\lambda\rho),\quad b_2 = K^+\mathrm{sh}(L_b\rho),$$

$$N^{\pm} = A'(b_2^2 + \beta^{\mp 2}) + B'\beta^{\mp},\quad \Pi^{\pm} = (2k/\lambda\rho)K^{\pm}$$

$$A' = L_w + (L_b/2)(\Pi^- + \Pi^+(\mathrm{sh}2y/2y)),$$

$$B' = 2b_2 L_b\left[\Pi^+/2 + \Pi^-(\mathrm{sh}(2L_b\rho)/4L_b\rho)\right]\cos(kL_w) + 2b_2\left[(1-\mathrm{ch}(2L_b\rho)/2\lambda\rho^2)k + 1/k\right]\sin(kL_w)$$

The binding energy E_b of the hydrogenic impurity is obtained by subtracting the minimized energy E_g from the ground-state energy E_0 without impurity potential.

The binding energy E_b^0 without phonons:

$$E_b^0 = E_0^{sub} - \min_\alpha E_g^0(\alpha) \quad (24)$$

where $$E_0^{sub} = \langle\psi_{sub}|-\nabla_r^2 + V(z)|\psi_{sub}\rangle \quad (25)$$

and $$E_g^0(\alpha) = \langle\psi_\alpha(\alpha)|-\nabla_r^2 - \frac{\beta}{r} + V(z)|\psi_\alpha(\alpha)\rangle \quad (26)$$

In the absence of electron-phonon interaction ε_∞ is replaced by ε_0 in equation the Hamiltonian He.

The binding energy E_b^{ph} with phonons:

$$E_b^{ph} = E_{ph}^{sub} - \min_\alpha E_g^{ph}(\alpha) \quad (27)$$

where

$$E_{ph}^{sub} = \langle\psi_{sub}|-\nabla_r^2 + V(z) - \frac{\pi}{2}\tau + \frac{\pi}{4}\tau\nabla_{r_\perp}^2|\psi_{sub}\rangle \quad (28)$$

since we have $\nabla_{r_\perp}^2|\psi_{sub}\rangle = 0$ then:

$$E_{ph}^{sub} = \langle\psi_{sub}|-\nabla_r^2 + V(z) - \frac{\pi}{2}\tau|\psi_{sub}\rangle \quad (29)$$

where the subband energy is corrected by taking into account the effect of the bulk LO-phonon in the first subband state. And

$$E_g^{ph} = \langle\psi_\alpha(r)|-\nabla_r^2 + V(z) - \frac{\beta}{r} - \frac{\pi}{2}\tau + \frac{\pi}{4}\tau\nabla_{r_\perp}^2|\psi_\alpha(r)\rangle \quad (30)$$

III. RESULTS AND DISCUSSIONS

We have calculated the effect of the electron-bulk phonon interaction on the binding energy for both on-center and off-center impurities located in a period of the superlattice. For numerical computations, we have chosen the GaAs-$Ga_{1-x}Al_xAs$ as a superlattice, since this system is the well known and almost all the properties are known. The parameters pertaining to the system are: $\varepsilon_0 = 12.83$, $\varepsilon_\infty = 10.9$ and $\hbar\omega_0 = 36.7$ meV.

Figure1 shows the variations of the ground-state binding energy of a hydrogenic impurity placed at the center of the well of the superlattice as a function of well width L_w for a fixed value of barrier L_b= 50 A, and a potential V_0= 100 meV corresponding to the Aluminum concentration $x = 0.1$. Curve a (b) corresponds to the case with (without) electron-bulk phonon interaction. For both cases curves (a) and (b), the binding energy as a function of the well width for a fixed value in a superlattice presents the same behavior as it is exhibited in the case of an isolated quantum well, i.e., when the well width diminishes, the binding energy increases monotonically until it reaches a maximum value, and then falls off sharply to a characteristic value of bulk $Ga_{1-x}Al_xAs$ at $L_w = 0$. This decrease originates from the penetration of the wave function in the material barrier. The same figure reveals that the difference between curves (a) and (b), respectively, with and without phonons increases as the size of the well decreases. This is due to the fact that as the well thickness is reduced, the electron wave function becomes more localized, this localization leads in turn to an increasing of the importance of the electron-phonon interaction.

In order to give a clear picture of the role of polaronic effects on the binding energy of the impurity, we define the variation energy due to the phonon as the difference between the binding energy in the presence and absence of the phonons $\Delta E_b = E_b^{ph} - E_b^0$.

Curve c illustrates the correction to the binding energy due to the electron-bulk (LO) phonon interaction.

It is clear to see that for a given value of the Al concentration x, the polaron correction is more pronounced for narrower wells of superlattice where the binding energy reaches a maximum. For larger wells, the effect of the barrier height on the binding energy correction is negligible because of a small electronic confinement. For L_b= 50 A our results of the binding energy we have obtained as a function of well width are in accordance with those obtained by [24] in the case of Quantum well structure.

In figure 2, we display the donor binding energy as a function of the donor position z_i for a superlattice characterized by L_w= 200 A and L_b= 50 A for value of V_0 = 100 meV corresponding to the Aluminum concentration $x = 0.1$, .

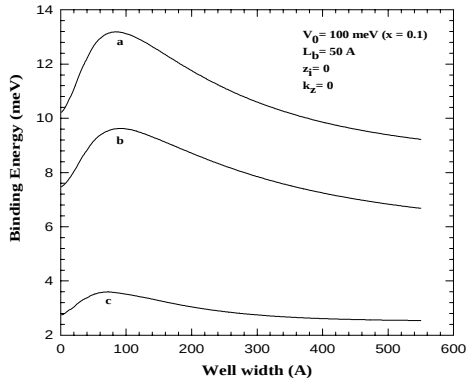

Fig. 1: Donor binding energy as a function of the well width L_w, for a GaAs-$Ga_{1-x}Al_xAs$ superlattice with a fixed barrier L_b = 50 A and barrier height V_0 = 100 meV, corresponding to the Aluminum concentration x = 0.1, the curve a (b) corresponds to the case with (without) electron -bulk phonon coupling. Curve c Shift of the binding energy due to electron –Bulk (LO) phonon interaction

As we can note from this figure, for donor position z_i = 0, as the Al concentration increases, the barrier height of the potential increases, this leads to a more localized wave function in the ground state of the impurity and as a consequence, the importance of the electron-phonon interaction increases. The above description leads in turn to an increasing of the binding energy.

The curve a (b) corresponds to the case with (without) electron-bulk phonon interactions, the figure reveals that the polaronic Shift becomes more and more pronounced as the impurity moves from the edge of the well to the center and it is maximum at $z_i = 0$, this originates from the decreasing of the Coulomb potential with the impurity position, which leads to a pronounced localization of the wave function at the center of the well and hence to an increasing polaronic effect.

The results show clear evidence of the dependence of the binding energy on the impurity position and the effects of the bulk LO-phonon. This work well be important for a detailed study of the impurity-related optical properties in superlattice.

The width for optical transitions from (to) the first valence band to (from) the impurity state is related closely to the width of optical absorption (emission) spectra. Also, at low (high) energies, the spectral density consists of narrows (larges) peaks coming from the contribution of impurities near the edge (impurities located on the center) in relation with homogeneous width due to the phonon.

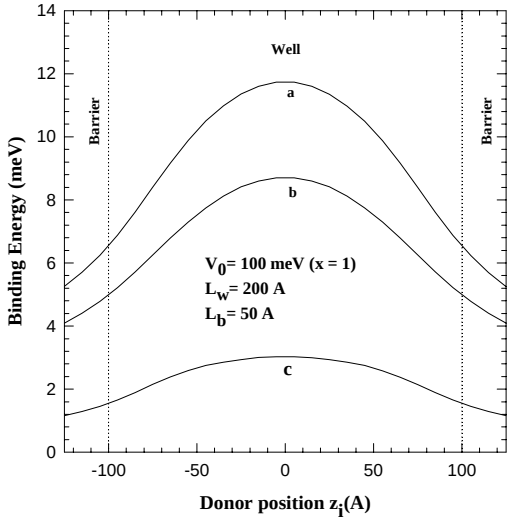

Fig. 2: Variation of the binding energy as a function of the impurity position z_i for a GaAs-$Ga_{1-x}Al_xAs$ superlattice of the well width L_w = 200 A, barrier size L_b = 50 A, and barrier height V_0 = 100 meV. The curve a (b) corresponds to the case with (without) electron -Bulk (LO) phonons interaction. Curve c correction the binding energy due to electron –Bulk phonon interaction.

Corrections to the binding energy due to the electron-bulk (LO) phonon interactions are presented by curve c as a function of the impurity position z_i along the grow axis in a period of the superlattice ($l = L_w + L_b$).

IV. CONCLUSION

In conclusion, we have studied the polaron effect on the hydrogenic impurity in the GaAs-$Ga_{1-x}Al_xAs$ superlattice system. The results show that the correction due to the bulk-phonon LO on the binding energies is higher for small wells than for large wells and depend strongly on the impurity position. It is found that the shifts of binding energy due to electron-phonon couplings are quite important for the on-center ($z_i = 0$) than for the ($z_i \neq 0$) impurities. This fact is very important for a correct description of impurity-related absorption and photoluminescence experiments.

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