Effects of longitudinal optical phonons on the binding energy of the impurity and the exciton in quantum well

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The polaron effect on the binding energy of a hydrogenic impurity and a Wannier exciton in a semiconductor quantum well is calculated by a variational approach. We have found that the correction due to the bulk-like LO-phonon effects is quite larger than that due to the confined LO-phonon effects and that these effects have a different behaviour .

PACS number(s): 63.22.+n, 73.38.+i, 73.20.Dx

I. INTRODUCTION

The study of the properties of the exciton and the impurity in a quantum well structure consisting of the alternate layers of two different semiconductors with controllable thickness and relatively sharp interfaces has been attracting much attention both from experimental[1-5], and theoretical[6-11] physicists.

The study of shallow impurity in quantum well structure goes through the calculation of the binding energy and the wave function in the fundamental state. The first approach to the problem is to consider a quantum well where the potential barriers are infinite, the binding energy increases when the well thickness is reduced [6] . For some height to finite barriers, the binding energy reaches a maximum[7,8].

Owing to a reduction in symmetry along the axis of growth of a quantum well structure and the presence of energy band discontinuity, the degeneracy of the valence band is removed, leading to the formation of two exciton systems, namely, the heavy-hole exciton and the light-hole exciton.

In the study of the properties of superlattices and quantum well systems based on polar and semi-polar semiconductors, the charge carrier Longitudinal Optical. (LO) phonon interaction is imposed. The effect of this interaction on the exciton and the impurity binding energies in a quantum well structure is important [12,13]. Otherwise, experimental studies have been carried out [14] in order to characterize the phonon nature in GaAs/ $Ga_{1-x}Al_xAs$ superlattices and quantum wells as function of composition x, and it has been shown that for $x \leq 0.2$, LO phonons are propagating and behave in a bulk-like manner. However, for $x \geq 0.4$ and for a barrier thickness $L_B > 20\ A^0$, the LO phonons are confined.

In this paper we are dealing with the effect of electron-bulk-like LO phonon coupling on the binding energy of the shallow impurity located at the center of GaAs/ $Ga_{1-x}Al_xAs$ quantum well. In addition, we have been interested in the effects of charge carrier-phonon interactions on the binding energy of Wannier excitons in quantum well structures, where the character of the LO phonon in GaAs/$Ga_{1-x}Al_xAs$ quantum wells depends on the fraction of Al.

II. THE MODEL

A. The bulk-like LO phonon mode effect on the impurity

In the approximation of the effective mass, the Hamiltonian of the shallow impurity located in the center of quantum well of thickness L is writing using units appropriate to a polaron calculation where the lengths are in units of $l_0 = (\frac{\hbar}{2m_e\omega_0})^{1/2}$ and the energies in the units of $\hbar\omega_0$:

$$H = H_0 + \sum_k a_k^+ a_k + \sum_k (V_k \exp(ik.r)\, a_k + H.C) \qquad (1)$$

Where

$$H_0 = -\nabla_r^2 - \frac{\beta}{r} + V(z) \qquad (2)$$

with $V(z) = V_e$, for $z > L/2$; $V(z) = 0$ otherwise and V_e is the barrier height. The value of V_e is 85 % of the total band gap discontinuity ΔE_g [15]

$$V_k = \sqrt{\frac{4\pi\alpha}{\Omega}\frac{1}{|k|}} \qquad (3)$$

Ω being the volume and

$$\alpha = \frac{1}{2}(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0})\frac{e^2}{\hbar\omega_0 l_0} \qquad (4)$$

$$\beta = \frac{e^2}{\hbar\varepsilon_\infty}(\frac{2m_e}{\hbar\omega_0})^{1/2} \qquad (5)$$

m_e , ε_∞ and ε_0 are the electronic effective mass , the optic dielectric constant and the static dielectric constant , respectively.

Operators a_k^+ and a_k, respectively, create and annihilate the LO-phonon of wave vector $\vec{k} = \vec{k}_\perp + k_z.\vec{z}$ and frequency ω_0.

For the sake of convenience, we first carry out the canonical transformation developed by Lee, Low and Pines[16]

$$U_1 = \exp\left[-i\sum_k a_k^+ a_k k_\perp.\rho\right] \tag{6}$$

$$U_2 = \exp\left[\sum_k (f_k a_k^+ - f_k^* a_k)\right] \tag{7}$$

where f_k and f^*_k are the variational parameters determined by minimizing the total energy subsequently and $\rho = (x,y)$. After some straight forward algebra, we directly get the transformed Hamiltonian .

$$H^* = U_2^{-1} U_1^{-1} H U_1 U_2 \tag{8}$$

In the low-temperature limit, few phonons will be excited and then no real phonons are proposed to be present in the phonon ground state. Hence, in our study we take $|0\rangle$ as the wave function of the phonon system. We set :

$$Q = \langle 0|H^*|0\rangle = H_0 + \sum_k |f_k|^2 + \left[\sum_k k_\perp |f_k|^2\right]^2 + \sum_k k_\perp^2 |f_k|^2 + 2i\sum_k |f_k|^2 k_\perp.\nabla_\rho + \sum_k \left(V_k \exp(ik_z.z) f_k + V_k^* \exp(-ik_z.z) f_k^*\right) \tag{9}$$

in the above expression, by symmetry , one must have

$$\sum_k k_\perp |f_k|^2 = 0 \tag{10}$$

we take the variation minimum of Q as the effective Hamiltonian of the electron -phonon system:

$$H_{eff} = H_0 - \frac{\pi\alpha}{2} + \frac{\pi\alpha}{8}\nabla_\rho^2 \tag{11}$$

The corresponding eigenenergy is given by

$$E = \langle\psi|H_0|\psi\rangle - \frac{\pi\alpha}{2} + \frac{\pi\alpha}{8}\langle\psi|\nabla_\rho^2|\psi\rangle \tag{12}$$

where is the trial wave function taken to be of non separable form[17]

B. The exciton

We develop a formalism corresponding to LO phonon-exciton interaction with respect to the phonon nature. Firstly, we will consider a bulk-like character and then a confined character.

-The bulk-like LO phonon mode

The Hamiltonian of an exciton with either heavy-hole or light-hole band in a GaAs slab sandwiched between two semi-infinite layers of $Ga_{1-x}Al_xAs$, interacting with bulk-like LO phonon can be expressed within the framework of the effective mass approximation as :

$$H^{exc} = H_{cm} + H_0 + \sum_k \hbar\omega_0 a_k^+ a_k + \sum_k (V_k \exp(ik.R) S_k a_k + H.C) \tag{13}$$

where

$$H_{cm} = E_g + \frac{P_x^2 + P_y^2}{2M_\pm} \tag{14}$$

$$H_0 = \frac{p_x^2 + p_y^2}{2\mu_\pm} + \frac{p_{z_e}^2}{2m_e} + \frac{p_{z_h}^2}{2m_\pm} + V_e(z_e) + V_h(z_h) - \frac{e^2}{\varepsilon_\infty\sqrt{\rho^2 + (z_e - z_h)^2}} \tag{15}$$

E_g is the GaAs band gap. (ρ, p) and (R, P) are the in-plane projection of the electron-hole relative position momentum, and coordinate and momentum of the center of mass , respectively.

$V_i(z_i)$ is the potential well for the electron (i = e) or for the hole (i = h) , assuming square wells with well width L.

$V_h(z_h) = V_h$, $|z_h| > L/2$, $V_h(z_h) = 0$ otherwise and V_h is 15 % of ΔE_g.

$m_\pm$ ($m_{h\pm}$) is the heavy-hole (+) or light-hole (-) effective mass along the z-direction (in-plane perpendicular to the z-axis).

$$\mu_\pm = \frac{m_e m_{h\pm}}{M_\pm} \tag{16}$$

$$M_\pm = m_e + m_{h\pm} \tag{17}$$

In the last term of (13)

$$S_k = \exp[i(k_z.z_e + \frac{m_{h\pm}}{M_\pm}k_\perp.\rho)] - \exp[i(k_z.z_h - \frac{m_e}{M_\pm}k_\perp.\rho)] \tag{18}$$

$$V_k = -i\frac{\hbar\omega_0}{k}[\frac{2\pi}{\Omega}(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0})]^{1/2} \tag{19}$$

Applying the first and the second Lee Low Pines transformations for the two-dimensional system[18] and neglecting the terms involving , the virtual phonon-electron and virtual phonon-hole interactions the corresponding eigenenergy is given by :

$$E = E_g + \langle\psi|H_0|\psi\rangle - \sum_k \frac{|V_k|^2}{\hbar\omega_0 + \frac{\hbar^2 k_\perp^2}{2M_\pm}} \langle\psi|S_k|\psi\rangle\langle\psi|S_k^*|\psi\rangle \quad (20)$$

A variational approach is adopted . The trial wave function for the exciton is taken to be of the separable form [18]. This choice could be justified by the previous result [9,11], suggesting , that our results should be reliable up to a well width of about 200Å.

-The confined LO-phonon mode

The Hamiltonian of an exciton interacting with the confined longitudinal optical phonon can be written as

$$H^{exc} = H_{cm} + H_0 + \sum_{q,m,p} \hbar\omega_0\, a^+_{m,p}(q)\, a_{m,p}(q) + H_{int} \quad (21)$$

The last term in (21) represents the interaction Hamiltonian of both electron and hole with the confined LO-phonon and is given by:

$$H_{int} = \sum_q \left\{ B \exp(iq.R) \left[\sum_{m=1,3,} \left(\frac{1}{(q^2 + (\frac{m\pi}{L})^2)^{1/2}} \right) \left[\exp(i\beta_h q.\rho)\cos(\frac{m\pi z_e}{L}) - \exp(-i\beta_e q.\rho)\cos(\frac{m\pi z_h}{L}) \right] \times a_{m,+}(q) + \sum_{m=2,4,} \left(\frac{1}{(q^2 + (\frac{m\pi}{L})^2)^{1/2}} \right) \times \left[\exp(i\beta_h q.\rho)\sin(\frac{m\pi z_e}{L}) - \exp(-i\beta_e q.\rho)\sin(\frac{m\pi z_h}{L}) \right] \times a_{m,-}(q) \right] + H.C \right\} \quad (22)$$

where

$$B = -i \left[\frac{4\pi e^2}{\Omega} \hbar\omega_0 (\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_0}) \right]^{1/2} \quad (23)$$

$$\beta_e = \frac{m_e}{M_\pm} \quad \textit{and} \quad \beta_h = \frac{m_h}{M_\pm} \quad (24)$$

$a^+_{m,p}(q)$ $(a_{m,p}(q))$ is the creation (annihilation) operatorfor the LO phonon of wave vector (q, mπ/L) and parity p refers the mirror symmetry with respect to the plane z = 0, and the positive integer m refers to the discrete values of the z-component of the LO-phonon wave vector . For even parity (p takes +) , m is odd , and for odd parity (p takes -) m is even . It should be noted that the wave vector of the LO phonon is limited by the Brillouin zone boundary, namely, $m\pi/L < \pi/2a$ or $m < L/2a$ (a is the lattice constant). As for the case of the bulk-like LO phonon[18] , the transformations can have the following form :

$$T_1 = \exp\left[-i \sum_{q,m,p} a^+_{m,p}(q)\, a_{m,p}(q)\, q.R \right] \quad (25)$$

$$T_2 = \exp\left[\sum_{q,m,p} (a^+_{m,p}(q)\, g_{m,p}(q) - c.c) \right] \quad (26)$$

where $g_{m,p}(q)$ and $g^*_{m,p}(q)$ are variational parameters. Then the corresponding eigenenergy is given by:

$$E_c = E_g + \langle\psi|H_0|\psi\rangle - E_p \quad (27)$$

The polaronic exciton energy shift is given by :

$$E_p = \sum_q \left(\frac{|B|^2}{\hbar\omega_0 + \frac{\hbar^2 q^2}{2M_\pm}} \right) \left\{ \sum_{m=1,3,5}^{N_0/2} \frac{\langle\psi|S_{m,+}(q)|\psi\rangle\langle\psi|S^*_{m,+}(q)|\psi\rangle}{q^2 + \left(\frac{m\pi}{L}\right)^2} + \sum_{m=2,4,6}^{N_0/2} \frac{\langle\psi|S_{m,-}(q)|\psi\rangle\langle\psi|S^*_{m,-}(q)|\psi\rangle}{q^2 + \left(\frac{m\pi}{L}\right)^2} \right\} \quad (28)$$

where $L=N_0 a$ and

$$S_{m,+} = \exp(i\beta_h q.\rho)\cos(\frac{m\pi z_e}{L}) - \exp(-i\beta_e q.\rho)\cos(\frac{m\pi z_h}{L}) \quad (29)$$

$$S_{m,-} = \exp(i\beta_h q.\rho)\sin(\frac{m\pi z_e}{L}) - \exp(-i\beta_e q.\rho)\sin(\frac{m\pi z_h}{L}) \quad (30)$$

III. RESULTS AND DISCUSSIONS

The physical parameters, in particular the effective masses, used in our study are adopted from previous works[10,19,20] . We have used the same values of mass for semiconductors constituting the quantum well . In fact , for the range of values of x ($x \le 0.4$) the values of the physical parameters are not very different in these two semiconductors [10].

A. Impurity

In the case of the infinite-well approximation ($V_e \to \infty$), the binding energy increases monotonically as the well thickness (L) is reduced and varied between the effective Rydberg 3D and 2D . The polaronic correction to the ground-state binding energy due to the bulk-like LO phonon mode also increases as L is reduced . Such a

feature clearly arises from the fact that, with decreasing L , the electron is forced to orbit in two dimensions and the wave function is squeezed on to the Coulomb center, resulting in stronger binding and hence an enhancement in the polaron effect . The result of the correction varies between that of 2D an 3D, and the per cent shifts owing to the most significant correction (depending on the non-separate parameters α , β and L) varies such as 2% from $L = 10\ A^0$ to 1.3 % for $L=150A^0$. Our results are in the accordance with those obtained in ref. [21]

It must be noted that the supposition of the infinite well's potential does describe the reality of the very narrow wells ($L \leq 30\ A^0$), as the energy of the subband becomes comparable to the real potential of the barrier height .

In the case of the finite barrier potential , the binding energy presents a maximum depending on L and Al fraction (x) . The contribution of the electron-phonon interaction increases as the thickness L is reduced, up to a value which corresponds to the maximum of the binding energy [22] . In fact , the binding energy becomes larger, the localization of the electron becomes pronounced and this in turn increases the importance of the electron-phonon coupling . In addition, the correction increases as the fraction x of aluminium varies from 0.1 to 0.4 (i.e. the barrier height increases) . We note that the bulk-like LO phonon approximation is rather valid for $x = 0.1$ than for $x = 0.4$ [14] .

In the case of the confined LO-phonon mode[23] , the polaronic effect increases .This behaviour is different to the results of the bulk-like phonon mode approximation . The confined LO-phonon effects are very weak when the quantum well is thin . In fact, there is a competition between the effects of the confined LO-phonon and the interface phonon[24]. Thus , the electron is squeezed to the interface as the well width decreases , increasing the contribution of interface phonons to the electron-phonon interaction[25,26] and reducing that of the confined LO-phonon .

Comparing the effects of the confined LO-phonon on impurity in quantum well and quantum well wire (QWW)[27], we can note that the correction is more important in the case of QWW . In fact, an enhancement of the confinement degree increases the binding energy, leading to an enhancement of the contribution of confined LO-phonon.

B. Exciton

For Al fraction $x = 0.2$, the phonon mode considered is bulk-like[14] . For a specific quantum well width , the polaronic contribution to the exciton binding energy for the light hole is more important than that for the heavy hole , due to the light-hole electron reduced mass (μ_-) being heavier than the heavy-hole electron reduced mass (μ_+) . The variation of the binding energy as a function of the well width is the same as that obtained in previous work [10] , presenting a maximum for a specific well width. For $x = 0.35$, the contribution of charge carriers-phonon interactions are more important than for the case $x = 0.2$. In fact, the confinement increases when x increases, involving an enhancement of the exciton binding energy and consequently an enhancement of the polaronic contribution .

For $x = 0.4$, we have assumed that the phonons are confined [14]. One can note that their effects are very weak However , the correction due to phonon-exciton interaction on the binding energy of the light-hole exciton is more important than that of the heavy-hole exciton [18] .

Comparing the effects of the LO phonon on the exciton binding energy within the approximation of the bulk-like phonon mode , the contribution of the confined phonon effect is very weak and has a different behaviour because it increases as the well width increases . In addition , we can note that the polaronic effect is more important in the case of the quantum well wire (quasi-one dimension) than that in the case of the quantum well (quasi-two dimension) [28,30] . In fact, the binding energy increases as the confined degree increases .

We can note that the results of the several theoretical works, using other methods[12] such as the perturbative variational approach [29] overestimate the phonon effect . It is interesting to note that our theoretical results for both light and heavy-hole exciton are in qualitative agreement with recent experimental data[2,4,5]..

IV. SUMMARY

In this work, we have studied the LO-phonon effects on the exciton and the impurity binding energies in a quantum well structure . The results show clearly that the bulk-like phonon effects are more important than the confined phonon effects . The electron bulk-like LO phonon interaction increases as the impurity binding energy increases .We have found that the polaronic effects on the binding energy of the light-hole exciton are larger than those of the heavy-hole exciton.

ACKNOWLEDGMENTS

This work was supported by the PARS grant n°: physique 03

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