Binding Energy and Photoionization Cross-Section in GaAs Quantum Well-Wires and Quantum Dots: Magnetic Field and Hydrostatic Pressure Effects

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Using a variational procedure for a hydrogenic donor-impurity we have investigated the influence of an axial magnetic field and hydrostatic pressure in the binding energy and the impurity-related photoionization cross-section in 1D and 0D GaAs low dimensional systems. Our results are given as a function of the radius, the impurity position, the polarization of the photon, the applied magnetic field, the normalized photon energy, and the hydrostatic pressure. In order to describe the Γ-X mixing in the $Ga_{1-x}Al_xAs$ layer, we use a phenomenological procedure to describe the variation of the potential barrier that confines the carriers in the GaAs layer. Our results agree with previous theoretical investigations in the limit of atmospheric pressure. We found that the binding energy and the photoionization cross-section depend on the size of the structures, the potential well height, the hydrostatic pressure, and the magnetic field.

Keywords: Magnetic field and hydrostatic pressure; Hydrogenic donor-impurity; 1D and 0D GaAs

I. INTRODUCTION

High hydrostatic pressure is a thermodynamic variable for the solid state that can provide important information to enable the understanding of the electronic properties on heterostructures. This is a powerful tool to investigate and control the electronic-related optical properties of semiconductor material. The main pressure effects on the III-V semiconductors is to increase the band gap [1], the increasing of the electron effective mass in the Γ -valley of the Brillouin zone [2], and the decrease of the static dielectric constant [3]. For the $GaAs - Ga_{1-x}Al_xAs$ heterostructures, an increasing in the electron effective-mass results in a decreasing of the electron quantized energy, whereas for the electron-impurity systems a decreasing of the dielectric constant results in the increasing of the impurity binding energy.

In the last two decades many works related with the magnetic fields effects on the properties of the electron-impurity systems have been reported in $GaAs - Ga_{1-x}Al_xAs$ quantum-well wires (QWWs) and quantum dots (QDs) [4–6]. The effects of hydrostatic pressure on such systems, and in particular on the photoionization (PI) cross-section, show that the PI depends strongly on the symmetry of the potential that confines the carriers, of the energy of the incident photon, and of the impurity distribution inside the heterostructure [7].

In this work, the hydrostatic-pressure and applied magnetic field dependence of the shallow-donor impurity related binding energy and PI cross-section in cylindrical $GaAs - (Ga,Al)As$ QDs and QWWs are calculated using a variational procedure within the effective-mass approximation. Results are calculated for different radius of the structure, applied magnetic field, hydrostatic pressure, and the energy of the incident photon. The work is organized as follows: in section II we present the theoretical framework, in section III we give our results and discussion, and finally in section IV we present our conclusions.

II. THEORETICAL FRAMEWORK

The Hamiltonian for a donor impurity in a cylindrical-shaped $GaAs - (Ga,Al)As$ QWW under the effect of an axial applied magnetic field and hydrostatic pressure (P) is given by

$$H = -\nabla . \left(\frac{m_w^*}{m_{w,b}^*} \nabla \right) - i\gamma \frac{m_w^*}{m_{w,b}^*} \frac{\partial}{\partial \varphi} + \frac{m_{w,b}^*}{4\, m_w^*} \gamma^2 \rho^2 + V(\rho, P) - \frac{\varepsilon_w^*}{\varepsilon_{w,b}^*} \frac{2}{r} , \qquad (1)$$

where $r = \sqrt{\rho^2 + z^2}$ is the impurity-carrier distance, $m_{w,b}^*$ is the electron effective mass [2], $\varepsilon_{w,b}^*$ is the static dielectric constant [3], and $V(\rho,P)$ is the potential barrier that confines the carriers inside the QWW heterostructure [8]. The equation (1) has been written in length and energy effective units defined as $a^* = \hbar^2 \varepsilon / (m_w^* e^2)$ and $R^* = e^2/(2\varepsilon_w a^*)$, respectively. The magnetic field dependent term γ is given by $\gamma = e\hbar B/(2\, m_w^*\, c\, R^*)$

For the QD case, the fourth therm in eq. (1) should be replaced by the z and ρ dependent potential $V(\rho,z,P)$. Our calculations for the QWW case (with radius R) includes both the infinite and finite potential model, in which case the variational wave functions are respectively given by [4, 5]

$$\Psi(\rho,P) = N \begin{cases} {}_1F_1(a_{01},1;\xi)\; g(r) & \text{if } \rho \le R, \\ 0 & \text{if } \rho > R. \end{cases} \qquad (2)$$

and

$$\Psi(\rho,P) = N \begin{cases} {}_1F_1(a_{01},1;\xi)\; g(r) & \text{if } \rho \le R, \\ A\, U(a_{01}^{'},1;\xi)\; g(r) & \text{if } \rho > R. \end{cases} \qquad (3)$$

For the cylindrical-shaped QD (with radius R and length L) we only consider the infinite well model. The corresponding variational wave function is taken as [5]

$$\Psi(\rho) = N \begin{cases} {}_1F_1(a_{01}, 1; \xi)\ \cos(\frac{\pi z}{L})\ g(r) & \text{if } \rho \leq R; \\ 0 & \text{if } \rho > R. \end{cases} \quad (4)$$

In Eqs (2) and (3) $g(r) = \exp[-(\xi/2 + \lambda r)]$, $\xi = \gamma^2\rho^2/2$, ${}_1F_1(x,m,y)$ is the usual confluent hypergeometric function, and $U(x,m,y)$ the so-called Kummer function. The constants a_{01} and a'_{01} are obtained from the continuity of the wave function and its derivate at the interfaces.

The donor impurity binding energy is obtained from the usual definition

$$E_b = E_0 - \frac{\langle\Psi|H|\Psi\rangle_{\min\lambda}}{\langle\Psi|\Psi\rangle} \quad (5)$$

where E_0 is the eigenvalue of the Hamiltonian in eq. (1) without the impurity potential term, and the expected value of the Hamiltonian is minimized with respect to the variational parameter λ.

In the effective mass and dipole approximations, the impurity-related PI cross-section is proportional to the matrix element of the dipole moment between the initial impurity state and the final confined, but non-impurity, state, and summing up all final states [7], i.e.,

$$\sigma(\hbar\omega) \approx \hbar\omega \sum_f |\langle\Psi_f|r|\Psi_i\rangle|^2\ \delta(E_f - E_i - \hbar\omega). \quad (6)$$

Details of the calculations will be published elsewhere.

III. RESULTS AND DISCUSSION

In Fig. 1 we present our results for the binding energy for an on-axis-located donor-impurity in a cylindrical *GaAsGa*$_{1-x}$*Al*$_x$*As* QWW as a function of the radius of the wire. As expected, in the small radius regime within the infinite potential model the binding energy diverges, whereas for the finite model the binding energy growths up to a maximun and then decreases to the 3D hydrogenic limit in the *Ga*$_{1-x}$*Al*$_x$*As* region. Additionally, in the limit for large radii all the presented results goes to the 3D limit in the *GaAs* region under the presence of an applied magnetic field. When comparing Figs. 1(a) and 1(b) we observe that the main influence of the hydrostatic pressure (associated with the linear decreasing of the dielectric constant, the linear increasing of the electron effective-mass, and the close linear diminishing of the radius of the structure) is seen for the low regime of the radius of the structure in which case the potential barriers expels the wave function towards the position where the impurity is located.

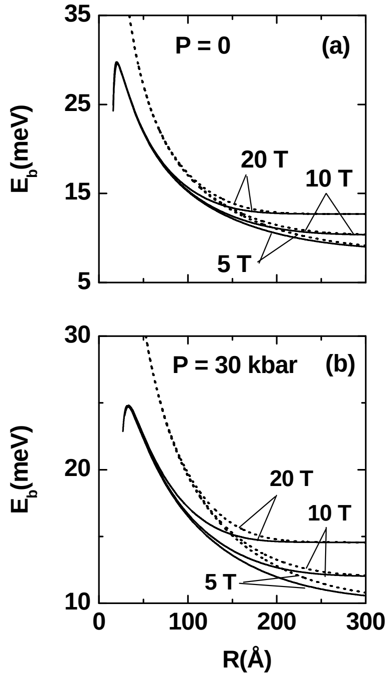

Fig. 1. Binding energy for on-axis-located donor-impurity in a cylindrical *GaAsGa*$_{1-x}$*Al*$_x$*As* QWW as a function of the radius of the wire. Results are presented for the finite as well as for the infinite confinement potential model (solid and dotted lines, respectively). Several values of the magnetic field and hydrostatic pressure are considered.

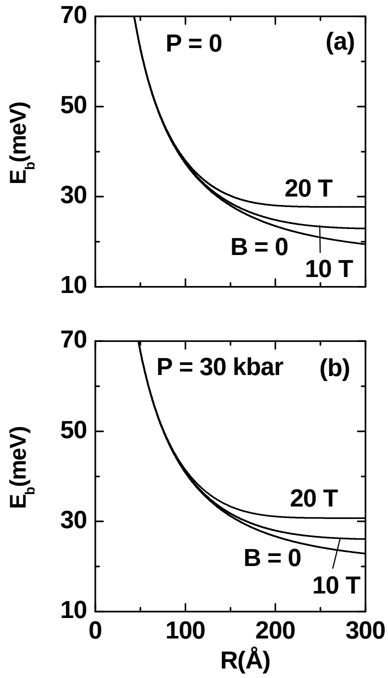

Fig. 2. Binding energy for on-axis-located donor-impurity in a cylindrical-shaped *GaAs*-vacuum QD as a function of the dot radius. The results are for $L = 50\AA$ and several values of the magnetic field and hydrostatic pressure have been considered.

Our results for the binding energy for on-axis-located donor-impurity in a cylindrical *GaAs* QD as a function of the radius of the dot are presented in Fig. 2. In the figs. 2(a) and 2(b) it is seen that as the radius of the QD diminishes the binding energy grows, finally diverging for $R = 0$. This is the behavior equivalent to the QWW case. Furthermore, the effect of the magnetic field becomes more prominent for larger radii in the structure, and the system goes to the different limiting values of the magnetic field effect for the case of the hydrogenic atom in the bulk. The effect of the magnetic field for small radius is worthless since the wave function has already been sufficiently compressed for the infinite potential barriers. In addition, when comparing the figs. (a) and (b) it is observed that the effects of the pressure are bigger for larger radii. The small variations appearing in the low regime of the radius are due to the fact that the system is strongly confined because of the small value considered for the height L of the QD. In this case $L = 50\AA$ corresponds essentially to $\frac{1}{4}$ of the expected value of the carrier-impurity distance of the hydrogenic atom in the bulk.

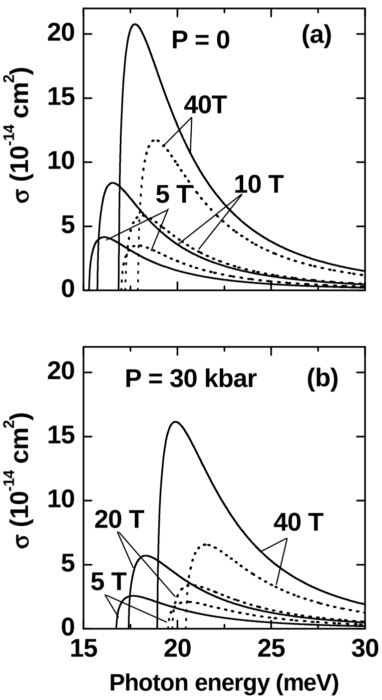

Fig. 3. PI cross-section, as a function of the photon energy, for on axis-located donor-impurity in a cylindrical $GaAsGa_{1-x}Al_xAs$ QWW as a function of the radius of the wire. Results are as in Fig. 1.

In Fig. 3. the results are for the donor-impurity-related PI cross-section in cylindrical $GaAsGa_{1-x}Al_xAs$ QWW as a function of the radius of the wire. The polarization of the incident photon is along the wire axis, and for this reason the selection rules for the matrix element of the dipole moment implies that the transition is given from the first impurity state to the fundamental state of the quantum well. The observed shift to higher energies for the infinite confinement model is essentially due to the larger energy separation between the first and the second confined states in the wire. Additionally, the blue shift of the PI peak is associated with the variation of the binding energy with the magnetic field. The same situation can be inferred with the presence of hydrostatic pressure, from comparison of the figs. 3(a) and 3(b). The spread of the peak is associated with the free motion of the carriers along the z-direction which allows a set of continuous k_z-dependent final states for the PI cross-section.

In Fig. 4. our results are as in fig. 3 but for cylindrical shaped *GaAs* QDs. Note the large blue-shift of the peak with respect to the results of the QWW. Due to the fact that the binding energy is defined as the difference of the correlated carrier-impurity system with respect to the non-correlated one, this shift can not be inferred from Fig. 1. It is associated -in fact- with the higher energy of the first confined state in the dot, with respect to those in the wire. The very narrow shape of the central peak can be attributed to the discrete set of final states of the matrix elements of the dipole moment.

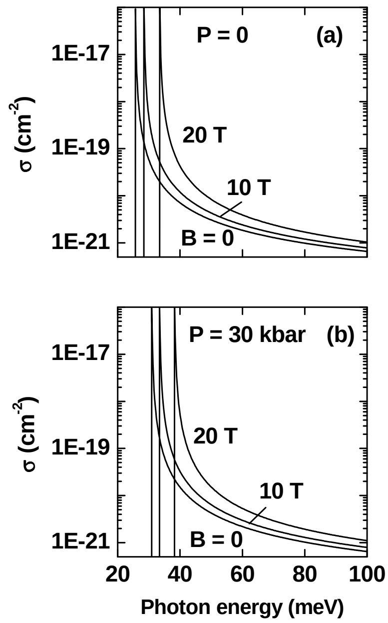

Fig. 4. PI cross-section, as a function of the photon energy, for on-axis-located donor-impurity in a cylindrical-shaped *GaAs*-vacuum QD as a function of the radius of the dot. Results are for the same data as in figure 2.

IV. CONCLUSIONS

In the scheme of the effective mass-approximation and using a variational procedure for a hydrogenic shallow-donor impurity we have investigated the influence of a strong magnetic field and hydrostatic pressure in the binding energy and the impurity-related PI cross-section in *GaAs* QWWs and QDs. We have included the pressure-dependent Γ-X mixing by using a phenomenological model of the potential barrier function that confines the carriers inside the structure. We have found that the binding energy and the PI cross-section depend on the sizes of the structures, the potential well heights, the hydrostatic pressure, and the applied magnetic field.

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