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The binding energy of donor impurities in GaAs quantum dots under the pressure effect

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Calculations of the binding energy of an on-center and off-center shallow hydrogenic impurity in a GaAs quantum dot under hydrostatic pressure are presented. The variational approach within the effective mass approximation is used as the framework for this calculation. The effect of the pressure is to exert an additional confinement on the impurity inside the dot; therefore the binding energy increases for any dot radius and impurity position. We also found that the binding energy depends on the location of the impurity and the pressure effects are less pronounced for impurities on the edge.

Keywords: Quantum dot; impurity; hydrostatic pressure

Nosotros presentamos calculos de la energía de enlace de impurezas hidrogenoides centradas y por fuera del centro en puntos cuánticos de GaAs bajo presión hidrostática. En este calculo nosotros usamos el método variacional dentro de la aproximación de la masa efectiva. Se encontro que el efecto de la presión es ejercer un confinamiento adicional sobre la impureza dentro del punto cuántico, por lo tanto la energía de enlace aumenta para cualquier valor del radio del punto, sin importar la posición de la impureza. También encontramos que la energía de enlace depende de la posición de la impureza dentro del punto y que los efectos de la presión son menos pronunciados cuando la impureza esta en el borde del punto.

Descriptores: Puntos cuánticos; impurezas; presión hidrostática

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1. Introduction

In the last few decades, there has been considerable interest in the study of the physics underlying various properties of low-dimensional semiconductor systems, due to their importance for potential applications in electronic and optoelectronic devices [1–6]. A great experimental and theoretical work has also been devoted to the quantitative understanding of the physical properties of a few particles (excitons, impurities, etc...) in GaAs/Ga$_{1-x}$Al$_x$As quantum wells (QWs), quantum-well wires (QWWs) and quantum dots (QDs) [7–12].

A deep understanding of the effects of impurities on the electronic states of semiconductor heterostuctures is a fundamental issue in semiconductor physics because their presence can dramatically alter the performance of quantum devices and their optical and transport properties [13].

The binding energy of shallow donor impurities in nanoscopic systems depends on materials and geometry, size and shape, although it seems that shape has a minor influence [14, 15]. The position of the impurity also has a strong influence [16].

Exact solutions for hydrogenic donors located at the center of spherical QDs have been obtained [17–20], while variational [7–11] and perturbational calculations [12] have been carried out for on- and off-centered impurities. In particular, Pérez-Merchancano *et al.* [9] and Zhu *et al.* [11] made the first studies about the confinement effects on the impurity states (donor and acceptor) in quantum dots. They calculated binding energies for the ground and excited states as a function of dot size and the impurity position. The more real zero dimensional quantum heterostructure (cubic dot) was studied by Ribeiro and Latgé [14]. They found that the values of donor binding energies for cubic and spherical quantum dots are very close, provided the dots have similar volumes.

Different experimental techniques permit the fabrication of quantum dots. Using the masked implantation enhanced intermixing technique, and the dry etching technique with subsequent overgrowth, Schweizer *et al.* [21] have produced rectangular transversal section GaAs-(Ga,Al)As quantum well wires and quantum dots. A spherical colloidal nanocrystal of CdTe has also been made [22].

In the last few years, the hydrostatic pressure effect on the band structure of bulk material and low dimensional systems has been considered both theoretically and experimentally. Photoluminescence studies of self-organized InAlAs/AlGaAs quantum dots under pressure were carried out by Phillips *et al.* [23]. The effect of hydrostatic pressure on the optical transitions in self-assembled InAs/GaAs quantum dots was studied by Duque *et al.* [24]. Oyoko *et al.* [25] studied donor impurities in a parallelepiped-shaped GaAs-(Ga,Al)As quantum dot and they found that the donor binding energy increases with increasing uniaxial stress and decreasing sizes of the quantum dot. On the other hand, donor impurities in a spherical quantum dot with parabolic confinement potential under hydrostatic pressure were considered by Gerardin Jayam and Navaneethakrishnan [26] and they found that the hydrostatic pressure increases the donor ionization energy so that the variation is larger for a smaller dot.

In the present paper, we show results of the binding energy of off-center shallow donor impurities confined in spherical quantum dots under hydrostatic pressure. We consider infinite well confinement potential and we use the variational method within the effective mass approximation.

2. The Model

We consider a spherical quantum dot of GaAs under the hydrostatic pressure influence assuming the presence of shallow impurities and the effective mass aproximation. Then the Hamiltonian is given by

$$H = \frac{\mathbf{P}^2}{2m^*(P)} - \frac{e^2}{\varepsilon(P)|\mathbf{r}-\mathbf{r}_0|} + V(r), \tag{1}$$

where $m^*(P)$ and $\varepsilon(P)$ are the effective mass of an electron and the static dielectric constant respectively, as a function of the hydrostatic pressure. In the Hamiltonian (1) $\mathbf{r}_0$ denotes the impurity position and $V(r)$ is the confinement potential which is zero for $r < R$ and infinite for $r > R$, $R = R(P)$ being the radius of the dot, which also depends on the hydrostatic pressure.

The eigenfunction of the Hamiltonian in the absence of the impurity for the ground state ($n = 1$ and $l = 0$) is

$$\psi_{10}(\mathbf{r}) = \frac{\sin(\zeta_{10} r)}{(2\pi R)^{1/2} r}, \tag{2}$$

where $\mathbf{r}$ is (r, θ, ϕ). In order to satisfy the boundary conditions $\psi_{10}(r = R) = 0$, the energies corresponding to Eqs. (1) and (2) are

$$E_{10} = \frac{\hbar}{2m^*(P)}\zeta_{10}^2 \quad \text{with} \quad \zeta_{10} = \frac{\pi}{R(P)}. \tag{3}$$

Equation (2) is the wave function of a particle confined in an infinite spherical potential well. Inclusion of the impurity potential makes it necessary to use a variational approach to approximate the wave functions and eigenvalues implied by the Hamiltonian. Taking into account the spherical confinement geometry and the hydrogenic impurity potential, we use the trial wave function

$$\psi(\mathbf{r}) = \begin{cases} N\dfrac{\sin(\zeta_{10} r)}{r} e^{-\lambda|\mathbf{r}-\mathbf{r}_0|}, & r \leq R(P) \\ 0, & r \geq R(P) \end{cases} \tag{4}$$

for the ground-state wave function, where N is the normalization constant of the wave function and λ is the variational parameter obtained by minimizing the binding energy. The binding energy $E_b(R, r_0, P)$ of the hydrogenic impurity is defined as the ground-state energy of the system without the impurity present, minus the impurity being ground-state energy $\xi(R, r_0, P)$, *i.e.*,

$$E_b(R, r_0, P) = \frac{\hbar}{2m(P)}\zeta_{10}^2 - \xi(R, r_0, P), \tag{5}$$

with $\xi(R, r_0, P) = \langle T\rangle + \langle U\rangle$, where $\langle T\rangle$ and $\langle V\rangle$ are given by

$$\begin{aligned}\langle T\rangle = -\frac{\pi N^2\hbar^2}{m}\int_0^R\int_0^\pi r\,dr\,d\theta \sin\theta\, e^{-2\lambda|\mathbf{r}-\mathbf{r}_0|} \\ \times\left\{-\frac{2\lambda\zeta_{10}\cos(\zeta_{10} r)}{|\mathbf{r}-\mathbf{r}_0|} + \frac{2\lambda k_{10}\cos\theta\cos(\zeta_{10} r)}{r|\mathbf{r}-\mathbf{r}_0|}\right. \\ \left. +(\lambda^2-\zeta_{10}^2)\frac{\sin(\zeta_{10} r)}{r} - \frac{2\lambda r_0\cos\theta\sin(\zeta_{10} r)}{r^2|\mathbf{r}-\mathbf{r}_0|}\right\}\end{aligned} \tag{6}$$

and

$$\langle V\rangle = -\frac{N^2 e^2}{2\varepsilon}\int_0^R dr\sin^2(\zeta_{10} r)\int_0^\pi d\theta\sin\theta\frac{e^{-2\lambda|\mathbf{r}-\mathbf{r}_0|}}{|\mathbf{r}-\mathbf{r}_0|} \tag{7}$$

respectively, with

$$N^{-2} = 2\pi\int_0^R dr\sin^2(\zeta_{10} r)\int_0^\pi d\theta\sin\theta e^{-2\lambda|\mathbf{r}-\mathbf{r}_0|}. \tag{8}$$

The application of hydrostatic pressure modifies the lattice constants, dot size, barrier height, effective masses and dielectric constants. These values are obtained in the following way: the variation of the well width with pressure is given by

$$R(P) = R_0(1 - 1.5082 \times 10^{-4}P), \tag{9}$$

where P is in kbar, R_0 is the radius value of the quantum dot when the hydrostatic pressure is equal to zero, taking into account that $(da/dP) = -2.6694 \times 10^{-4}a_0$, where a_0 is the lattice constant of GaAs [27]. The variation of dielectric constant with the pressure is given as

$$\varepsilon(P) = 13.13 - 0.0088P, \tag{10}$$

where P is in kbar. The effective mass in the well and barrier region changes to

$$m^*(P) = m^*(0)\exp(0.0078P), \tag{11}$$

where P is in kbar. The total band gap difference between GaAs and $\text{Ga}_{1-x}\text{Al}_x\text{As}$ as a function of x is given by

$$\Delta E_g(x, P) = \Delta E_g(x) + PD(x), \tag{12}$$

where

$$\Delta E_g(x) = 1.155x + 0.37x^2 \text{ in eV} \tag{13}$$

is the variation of the energy gap difference and $D(x)$ is the pressure coefficient of the band gap given by

$$D(x) = [-1.3 \times 10^{-3}x] \text{ eV/kbar}. \tag{14}$$

With these variations, the donor binding energies are obtained for different pressures, using the variational method within the effective mass approximation.

3. Results and Discussion

In Fig. 1, we present the binding energy of shallow impurities in spherical quantum dots of infinite well depth as a function of the dot radius for different values of the hydrostatic pressure, with the impurity placed in the center of the quantum dot. We observed that the binding energy decreases when the radius increases, showing that for hydrostatic pressure $P = 0$, the results are in agreement with the results of Pérez *et al.* and Zhu *et al.* [9, 11]. In a similar fashion, it is observed that for different values of the hydrostatic pressures (20 and 40 kbar), the binding energy for the quantum dots presents a similar behavior to that of pressure $P = 0$, but for radii between 100 and 1000 Å, it can be more clearly seen that these energies increase with the increase in hydrostatic pressure. It is also observed that for radii below 60 Å, the binding energy is not affected by the hydrostatic pressure; therefore we can conclude that the action of the presssure on the binding energy depends on the quantum dot radii.

The variation of the binding energy with the quantum dot radii for the shallow impurity placed in different positions under a hydrostatic pressure equal to 20 kbar is presented in Fig. 2. The binding energy decreases when the size of the dot increases for any impurity position, reflecting the lower confinement potential. Likewise, when we move the impurity from the center ($r_0/R = 0.0$) to the edge ($r_0/R = 1.0$), this energy decreases. It is important to note that the binding energy takes characteristic values of the bulk material for large values of the dot radius, independently of the impurity position, although for the radius values shown, this is not evident. On the other hand, we have observed that the binding energy, when the impurity is placed along the edge of the quantum well; does not take the same values as when is placed in the center or in the middle of the well, this is due to the potential barrier repulsion.

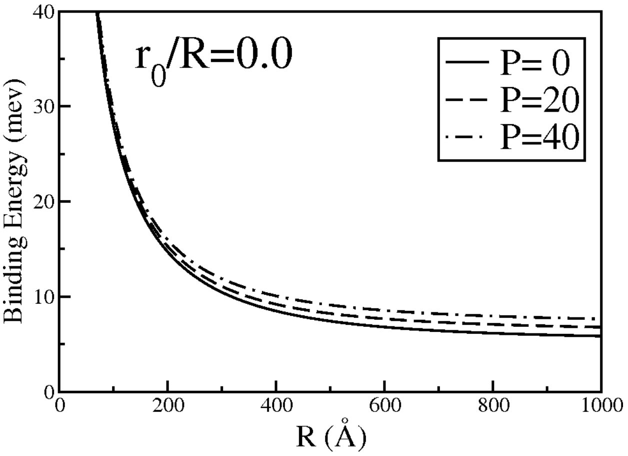

FIGURE 1. Donor binding energy as a function of the quantum dot radius for a spherical quantum dot with different hydrostatic pressures $P = 0, 20, 40$ kbar. Here the shallow impurity is placed in the center of the dot.

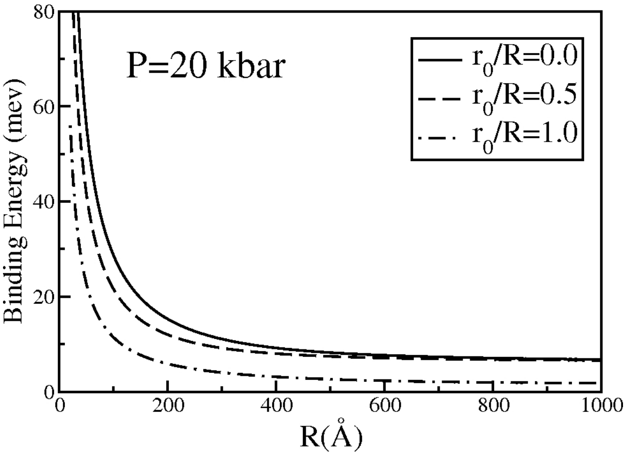

FIGURE 2. Binding energy as a function of quantum dot radii with a hydrostatic pressure $P = 20$ kbar, for different impurity positions, $r_0/R = 0.0, 0.5$ and 1.0..

For a quantum dot of radius 50 Å we show in Fig. 3, the binding energy as a function of the impurity position, when hydrostatic pressures of $P = 0$, $P = 20$ and $P = 40$ kbar are applied. Here we have observed a decrease in the binding energy when the impurity moves from the center to the edge of the quantum dot; this is in agreement with the results obtained previously [12, 16]. We also show that, depending on the position of the impurity inside the dot, the binding energy increases as a function of the hydrostatic pressure; this allows us to claim that the pressure causes a greater electronic confinement in the system. We have also observed that the binding energy variation as a function of the pressure for the shallow impurity in different positions is not homogeneous; for example, we have observed that the binding energy is less sensitive to the pressure when the impurity is near the edge.

Figure 4 shows the binding energy as a function of the donor position inside the quantum dot for an infinite potential well with different radii. The hydrostatic pressure is constant and equal to $P = 40$ kbar. The donor binding energy

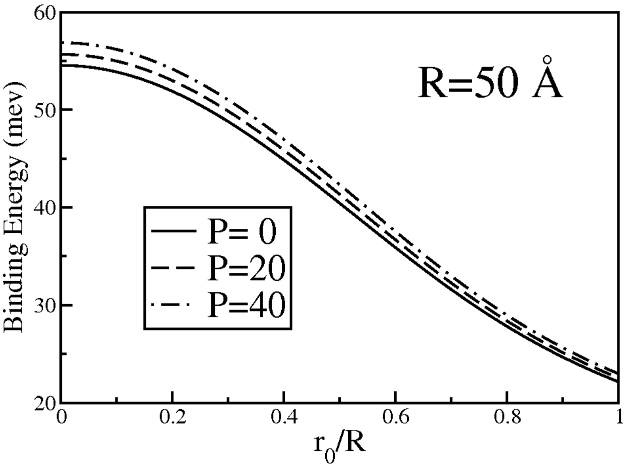

FIGURE 3. Donor binding energy as a function of impurity positions for spherical quantum dots of radius 50 Å with different hydrostatic pressures $P = 0$, 20, 40 kbar.

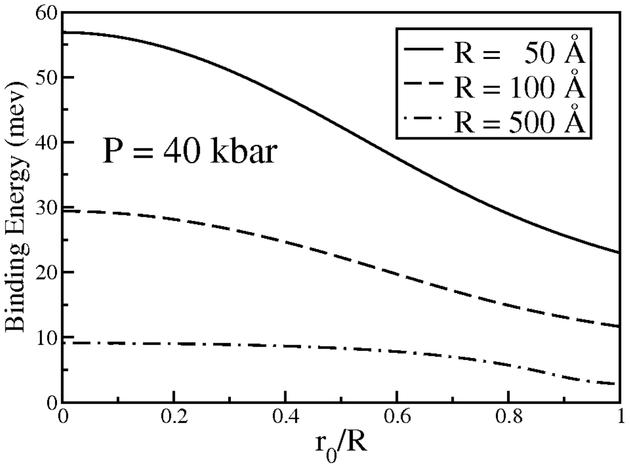

FIGURE 4. Binding energy for spherical quantum dots with a hydrostatic pressure $P = 40$ kbar as a function of impurity positions. Here different radii were considered $R = 50, 100, 500$ Å.

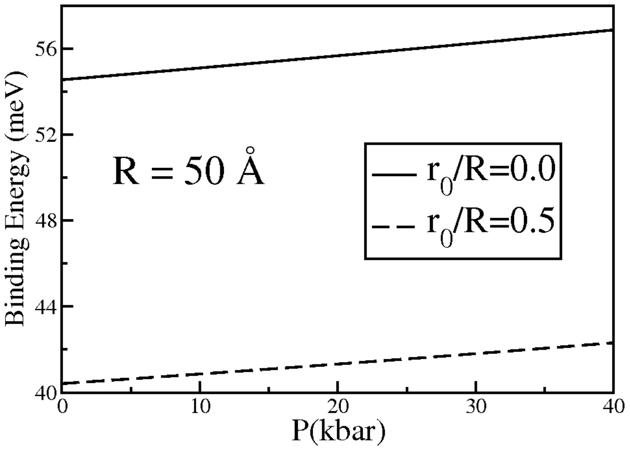

FIGURE 5. Donor binding energy as a function of hydrostatic pressure P for different positions of shallow impurities $r_0/R = 0, 0.5$

decreases as the donor position increases, reaching a minimum when the donor position is equal to the radius of the quantum dot. It can further be noted from the figure that the variation in the binding energy with the impurity position is more pronounced for smaller dots. This observation is in agreement with the results reported in [12, 16] without pressure and [25] with pressure.

The variation of the binding energy with pressure is shown in Fig. 5. Here we consider a quantum dot of radius $R = 50$ Å and two different impurity positions $r_0/R = 0$ (on-center) and $r_0/R = 0.5$ (on-middle). The binding energy shows a nearly linear increase with the pressure. Note that the slope of the curve depends on the impurity position and the smaller value is found on the edge. This curve tells us that a system that operates under hydrostatic pressure may be used to syntonize the output of optoelectronic devices without modifying the physical size of the quantum dot. We have not considered pressures beyond 40 kbar, as there is a direct to indirect bandgap transition for GaAs at about 40 kbar [28].

4. Conclusions

In summary, we have reported the study of the effects of hydrostatic pressure on spherical quantum dots of the GaAs. We have used the effective-mass approximation and variational method in which the trial function takes into account the variational parameter λ. We have calculated the binding energy as a function of the radius of the quantum dot for various values of hydrostatic pressure, different positions of the impurity in the quantum dot. We found that the binding energy increases with the hydrostatic pressure for any position of the impurity. The hydrostatic pressure effects are less pronounced for impurities on the edge. The slope of the curve of binding energy versus pressure depends on the impurity position.

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