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Excited states and infrared transition energies of a donor impurity in a disc-shaped GaAs quantum dot under the action of an applied magnetic field

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Abstract. We have calculated binding and transition energies of the ground and some excited states of a shallow donor impurity in a disc-shaped GaAs quantum dot (QD), under the action of a magnetic field applied in the axial direction. The binding energies were obtained using the effective-mass approximation within a variational scheme, assuming an infinite confinement potential at all surfaces. Our results were obtained for several dot radii, the impurity position along the z-direction, and as a function of the applied magnetic field. We found that some excited states are not bounded for some values of the radius of the dot and of the applied magnetic field. We have shown how the applied magnetic field split the degeneracy of some excited states. Also, we have compared our results with those found in GaAs–(Ga, Al) As quantum wells (QWs) and quantum-well wires (QWWs).

1. Introduction

The great progress in crystal growth techniques, such as molecular beam epitaxy (MBE), metal–organic chemical-vapour deposition (MOCVD) and chemical lithography have made possible the fabrication of a wide variety of semiconductor heterostructures, where the quantum mechanical nature of the electrons plays an important role [1–3]. Also, extensive theoretical and experimental investigations on optical and electronic properties, excitons and impurity levels [4–16] in QDs and QWWs have been published. The effects of applied magnetic fields on the physical properties of low dimensional systems are studied with the proposal of understanding the fascinating novel phenomena and of creating new devices or improving the performance of the existing ones. Although magnetic field effects seem to have less technological significance, they provide a far richer insight into semiconductor physics than is possible by studying electrons in electric fields. The magnetic fields have become crucial ingredients of characterization techniques used to evaluate the semiconductor physics.

In QDs there have been published numerous theoretical works on hydrogenic impurity states. Chuu *et al* [9] studied the binding energies of hydrogenic impurity states with an impurity atom located at the centre of a spherical QD. They assumed an infinite confinement potential and the impurity eigenfunctions are expressed in terms of Whittaker functions and Coulomb scattering functions. The calculated ground state energy of the impurity approaches the correct limit of the three dimensional hydrogen atom as the radius of the QD becomes very large and increases significantly as the radius goes to zero. Porras-Montenegro and Pérez-Merchancano [10] have calculated the donor binding energies in spherical QDs using a

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variational method. Li *et al* [14] calculated the donor binding energies of the ground state in a disc-shaped QD under the action of a uniform magnetic field applied parallel to the disc axis.

In this work, we calculate the binding energy and some transition energies associated with the ground and some excited states of a hydrogenic donor impurity located at the axis of a disc-shaped GaAs QD, under the action of a magnetic field applied in the axial direction. We use the effective-mass approximation within the variational approach. In section 2 we present the theory followed for this calculation. Our results and discussion are presented in section 3, and conclusions in section 4.

2. Theory

In the effective-mass approximation, the Hamiltonian of a donor impurity located at the centre of a quantum disc of GaAs of radius R and length L, with infinite confinement potential at all surfaces and in the presence of an applied magnetic field $\boldsymbol{B} = B\boldsymbol{z}$, can be written as:

$$H = \frac{1}{2m^*}\left[P - \frac{e}{c}A\right]^2 - \frac{e^2}{\varepsilon r} + V(\rho) \tag{1}$$

where the first term in equation (1) is the kinetic energy of the electron of the impurity in a magnetic field, the second term corresponds to the potential energy of the impurity and the last term is the confinement potential. Here $r = \sqrt{\rho^2 + z^2}$, z is the relative coordinate of the separation between the electron and the ion of the impurity in the axial direction of the QD, ε is the dielectric constant of the GaAs, m^* is the electron effective mass, $\boldsymbol{A}(\boldsymbol{r})$ is the vector potential of the magnetic field, and $V(\rho)$ is the confinement potential defined as

$$V(\rho) = \begin{cases} 0 & 0 \leqslant \rho \leqslant R \text{ and } |z| \leqslant L/2 \\ \infty & \rho > R \text{ and } |z| > L/2. \end{cases} \tag{2}$$

The vector potential is written as $\boldsymbol{A}(\boldsymbol{r}) = \frac{1}{2}(\boldsymbol{B} \times \boldsymbol{r})$, with $B = B\boldsymbol{z}$. In cylindrical coordinates the components of the vector potential are

$$A_\rho = A_z = 0 \qquad A_\varphi = \tfrac{1}{2}(B\rho). \tag{3}$$

The Hamiltonian of the system can be written in cylindrical coordinates and effective Rydbergs as

$$H = -\nabla^2 - \mathrm{i}\gamma\left(\frac{\partial}{\partial\varphi}\right) + \frac{\gamma^2\rho^2}{4} - \frac{2}{r} + V(\rho) \tag{4}$$

where we have used the atomic units of length $a^* = \varepsilon\hbar^2/(m^*e^2)$ and energy $R^* = e^2/(2\varepsilon a^*)$. In equation (4), $\gamma = e\hbar B/(2m^*cR^*)$ is the measure of the electron energy in the first Landau level ($n = 0$), due to the action of the magnetic field. For GaAs [10–14] $m^* = 0.065$, $\varepsilon = 12.58$, $a^* \cong 100$ Å and $R^* = 5.83$ meV.

Due to the inclusion of the impurity potential in the Hamiltonian, equation (1), the Schrödinger equation can not be analytically solved. Following Brown and Spector [17], we assume suitable variational wave functions, for the different impurity states, as the product of the hydrogenic part and the appropriate confluent hypergeometric function. The latter is the radial part of the wave function of the electron in the disc-shaped cylindrical quantum dot with infinite potential confinement in the presence of a magnetic field, that is

$$\Psi_{nlm}(r) = \begin{cases} N_{nlm}\,{}_1F_1(a_{01}, 1, \xi)\cos\left(\frac{\pi z}{L}\right)\Gamma_{nlm}(r, \{\lambda_{nl}, \beta_{nl}\}) & 0 \leqslant \rho \leqslant r \text{ and } |z| \leqslant L/2 \\ 0 & \rho > R \text{ and } |z| > L/2. \end{cases} \tag{5}$$

In equations (5), N_{nlm} are the normalization constants, ${}_1F_1(a_{01}, 1, \xi)$ is the confluent hypergeometric function, with $\xi = eB\rho^2/(2\hbar c)$, a_{01} is the eigenvalue of the ground state without the impurity, which is calculated numerically from the boundary condition for $\rho = R$,

$$ {}_1F_1(a_{01}, 1, \xi_R) = 0 \tag{6} $$

where $\xi_R = \gamma R^2/2a^{*2}$ and Γ_{nlm} are the hydrogenic wave functions, corresponding to nlm states, as proposed by Latgé *et al* [18]. The λ_{nl}, β_{nl} are variational parameters used by Chaudhury and Bajaj [19] that vary according to λ_{nl} in such a way that the orthogonalization is preserved.

Following Greene and Bajaj [20] we calculate the binding energy of a given state Ψ_{nlm} by means of

$$ \begin{aligned} E_{b,nlm} &= E_{10} - \langle H(R, B, L)\rangle \\ E_{10} &= \gamma(1 - 2a_{01}) + \left(\frac{a^*\pi}{L}\right)^2. \end{aligned} \tag{7} $$

The binding energy $E_{b,nlm}$, is a positive quantity. E_{10} is the ground-state energy of the system in the absence of the Coulomb term. The expected value of the Hamiltonian (4) is the sum of the expected values of the 'relative' kinetic $\langle T\rangle$, potential $\langle V\rangle$, diamagnetic $\langle D\rangle$ and paramagnetic $\langle P\rangle$ energies, that is

$$ \langle H(R, B, L)\rangle = \langle T\rangle + \langle V\rangle + \langle D\rangle + \langle P\rangle. \tag{8} $$

The meaning of the first term of the expected value of the Hamiltonian (4), taken alone, with the gauge defined by (3), correspond to the 'relative' kinetic energy $\langle T\rangle = P_R^2/2m^*$, where P_R is the mechanical momentum of the electron with respect to the 'Larmor frame' rotating about $\boldsymbol{B}$ with angular velocity $w_L = eB/2m^*$.

The allowed transition energies are given by

$$ E_T(nlm \to n'l'm') = |E_{b,nlm}(R, B, L) - E_{b,n'l'm'}(R, B, L)| \tag{9} $$

and the selection rules used for the allowed transitions are [21]:

$$ \begin{aligned} \Delta l &= l - l' = \pm 1 \\ \Delta m &= m - m' = 0, \pm 1. \end{aligned} \tag{10} $$

The competition between the magnetic and the geometric confinements can be visualized by means of the relation between the cyclotronic radius $r_c = \sqrt{1/\gamma}$ and the radius of the disc R, $r_c/R = \sqrt{1/R^2\gamma}$. For $r_c = R$ we have the limit for the transition from the geometric to the magnetic confinement regime. If $\gamma > 1/R^2$ the magnetic confinement governs the geometric one and vice versa.

3. Results and discussions

In figure 1(a) we plot the binding energy of the 1s-like state as a function of the disc radius for two lengths of the disc ($L = 1\ a^*$ and $L = 10\ a^*$) and for different values of the applied magnetic field. We reproduce the results obtained by Li *et al* [14]. For small values of the disc radius, $R < a^*$, the binding energy increases significantly, in a different way for the two lengths of disc given above. As it is seen, in this situation the binding energy is relatively insensitive to the magnetic field, because the diamagnetic energy tends to zero and the 'relative' kinetic energy of the electron increases drastically surpassing the attractive potential energy of the impurity. In this range of the disc radius and for any value of the magnetic field the geometric confinement governs the magnetic one. The binding energy for all the radii and magnetic fields is higher in the disc of length 1 a^* than in the one with 10 a^* length, because the electron is confined in a smaller volume. The donor binding energies in the quantum disc are higher than those found in QWs and QWWs of comparable dimensions. For values of the disc radius, $R > 2\ a^*$, the binding energy increases with the magnetic field for all lengths of the disc.

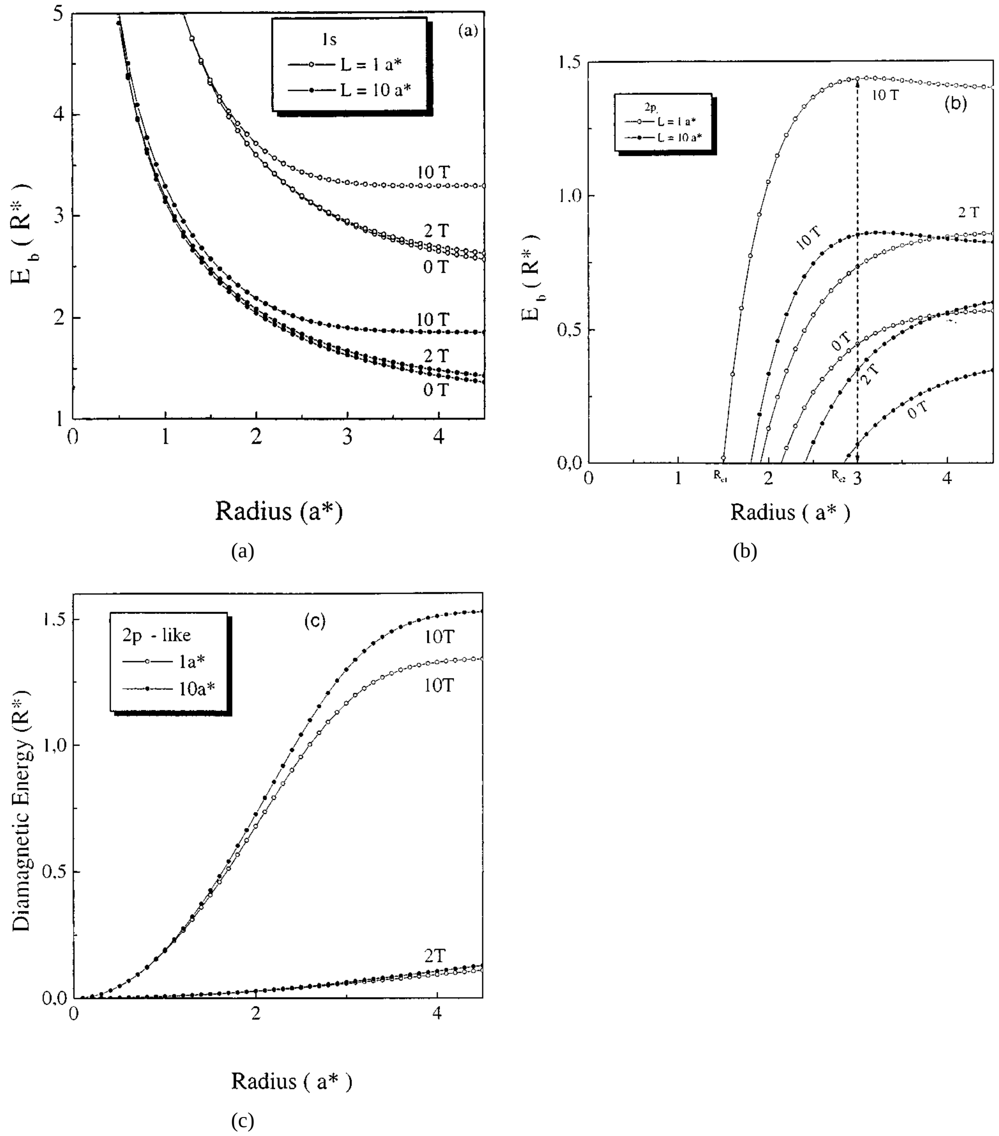

Figure 1. Binding energies of the 1s-like (a) and $2p_-$-like states (b) and diamagnetic energy of the $2p_-$-like state (c) of an on-centre donor impurity in a disc-shaped GaAs QD as a function of the radius, for discs of lengths $L = 1\ a^*$ (open circles) and $L = 10\ a^*$ (full circles), and for different values of the applied magnetic field.

The binding energy of the 2p-like state is presented in figure 1(b) as a function of the disc radius and for different values of the applied magnetic field and two disc lengths ($L = 1\ a^*$ and $L = 10\ a^*$). It is observed that the binding energy increases with the magnetic field, and it is seen that there are two characteristic radii $R_{c1}(B)$ (beyond this radius the states are bounded) and $R_{c2}(B)$ (the radius for which the binding energy reaches its maximum value). Both characteristic radii diminish with increasing $\boldsymbol{B}$ and their values lie in the range of strong and intermediate geometrical confinement. For QD radii, $R_{c1}(B) < R < R_{c2}(B)$, the binding energy increases with R and the slope of the curve becomes larger when the magnetic field is augmented. The existence of the critical radius R_{c1} is due to the strong confinement of the wave function in the radial direction and therefore the corresponding energy is higher than the first ionization level within the structure (the first Landau level). There is a maximum value of the binding energy for this state for $B = 10$ T, in both quantum discs, because while the diamagnetic energy increases, as shown in figure 1(c), the 'relative' kinetic energy diminishes with the radius in the range $1.5 < R < 3.5$. Here also, the donor binding energies are higher than in the corresponding QWs and QWWs structures. Although the $2p_+$-like state is not presented, we found that this state is bounded in a disc with length of 1 a^* and the binding energy decreases with the magnetic field, becoming unbounded for large values of the magnetic field. For the disc lengths we are considering, the $3p_-$-and the $3p_+$-like states are unbounded for all values of the applied magnetic field.

In figure 2(a) we plot the binding energy versus the magnetic field, for the 1s-, $2p_-$-, $2p_+$-, $3p_-$-like states, in disc-shaped GaAs QDs with radius of 4 a^* and lengths $L = 1\ a^*$ and $L = 10\ a^*$, respectively. For all these states, the binding energies corresponding to the disc of length 1 a^* are higher than in that with 10 a^* length. The binding energy of the 1s-, and $2p_-$-like states increases with the magnetic field. The energy of the $2p_+$-like state diminishes with the magnetic field up to 1.8 T ($L = 10\ a^*$) and 3.2 T ($L = 1\ a^*$), and the $3p_-$-like state is only bounded for values of the magnetic field between 4 and 7.5 T. In figure 2(b) we plot the E_{10} and the total energy of the impurity, $\langle H\rangle$, as a function of the magnetic field, for quantum discs of lengths $L = 1\,a^*$, $L = 10\,a^*$ and $R = 4\,a^*$. The purpose of this figure is to understand the behaviour of binding energy of the states presented in figure 2(a). For the $2p_-$-like state, the total energy $\langle H\rangle$ of the impurity presents a minimum value for $B = 3.2$ T and $B = 2.5$ T, for quantum discs of lengths $L = 1\ a^*$ and $L = 10\ a^*$, respectively, because the paramagnetic energy (negative) increases faster than the other energies of the impurity. For values larger than 2.5 and 3.2 T of the magnetic field the total energy begins to increase due to the fact that the 'relative' kinetic and diamagnetic energies augment a little faster than the potential and paramagnetic energies. When the magnetic field is increased the difference between E_{10} and $\langle H\rangle$, becomes higher and the binding energy increases according with equation (7). E_{10} and $\langle H\rangle$ are presented as a function of the magnetic field for the $3p_-$-like state in the inset of figure 2(b), which allows us to understand why the binding energy is only bounded for certain values of the magnetic field.

Figure 3 shows the binding energy as a function of the impurity position along the z-direction, for the 1s-like and $2p_-$-like states, for disc of radius 4.5 a^* and 1 a^* in length. For the two mentioned states, and for any position of the impurity along the z-axis, the binding energy increases with the magnetic field and it has a maximum at $z_i = 0$, and decreases as the impurity moves from the centre to the edge of the well. This is due to the repulsive barrier potential which pushes the electronic charge distribution away from the donor, thereby leading to a reduced Coulomb attraction between the electron and the ion impurity.

In figure 4 we display our theoretical results for donor transitions between the 1s-like and the $2p_\pm$-, $3p_\pm$-like states as a function of the magnetic field in disc-shaped GaAs QDs with 4 a^* radius and with $L = 1\ a^*$, $L = 10\ a^*$, respectively. We compare our theoretical results with experimental data by McCombe *et al* [22]. We observe that the transition energies in the QD with $L = 1\ a^*$ are higher than those corresponding to the QD with $L = 10\ a^*$. For the two QDs, the transition energies between the 1s-like and the $2p_+$- $3p_+$-like states increase with the magnetic field. Otherwise, the transition energy between the 1s-like and the $3p_-$-like

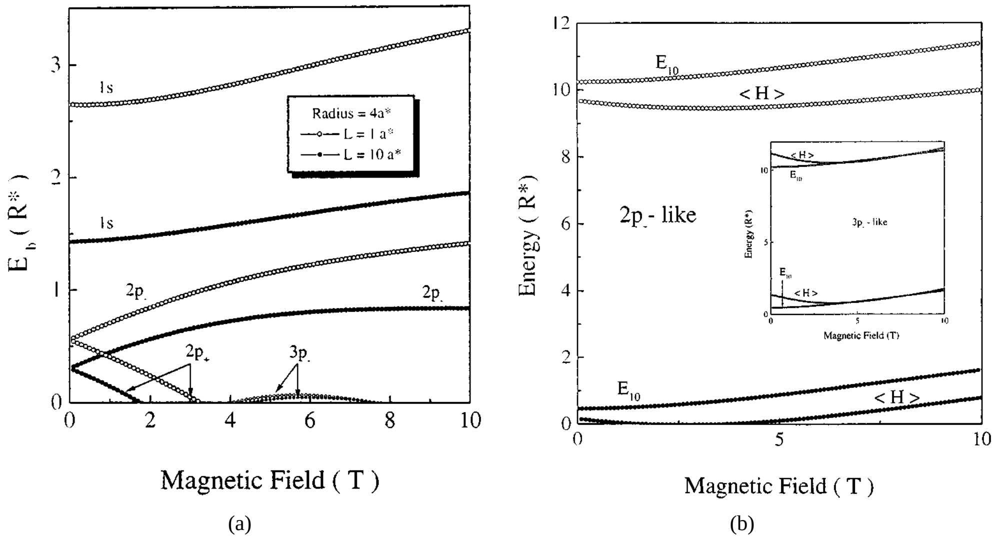

Figure 2. Binding energies of the ground and some excited states (a) and E_{10} and $\langle H \rangle$ (b) of an on-centre donor impurity in a disc-shaped GaAs QDs with $R = 4\,a^*$, and lengths $L = 1\,a^*$ (open circles) and $L = 10\,a^*$ (full circles), as a function of the applied magnetic field.

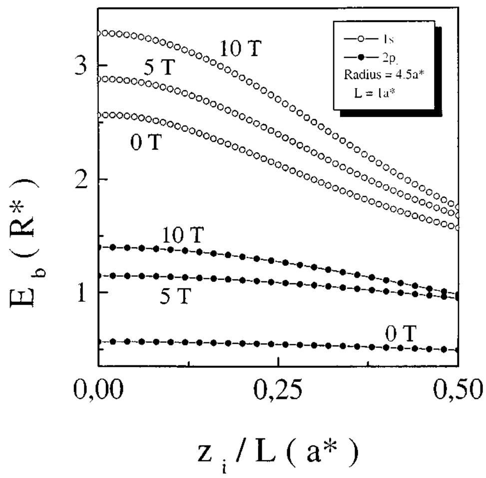

Figure 3. Binding energies for the ground and 2p$_-$-like states of a donor impurity as a function of the impurity position, z_i/L, in a disc-shaped GaAs QD with radius of 4.5 a^* and length of 1 a^*.

state shows a minimum in the range of the magnetic field in which the binding energy of the 3p$_-$-like state presents a maximum. The experimental data correspond to on-centre doped GaAs–$Ga_{0.7}Al_{0.3}As$ quantum wells with $L = 1.25\,a^*$. For all values of the magnetic field, the 1s $\to$ 2p$_-$ experimental values of the transition energy are between the theoretical results for the QDs with $L = 10\,a^*$ and $L = 1\,a^*$, as expected, bearing in mind that we are working with a dot with $R = 4\,a^*$, which does not exactly correspond to the experimental setup. As the magnetic field increases the wave function is more localized and for a QD with an additional radial confinement ($R = 4\,a^*$) the transition energy augments, due to the large extent of the 2p$_-$-like state. The same happens for 1s $\to$ 2p$_+$ transition energies in comparison with the experimental reports. Our theoretical results for the 1s $\rightarrow$ 3p$_+$ transition energy in the case of the QD with $L = 1\ a^*$, and for magnetic fields higher than 5 T, coincide quite well with the experimental data (QW with $L = 1.25\ a^*$). This is due to the fact that the strong magnetic field, independent of the radial confinement in the QD, confines the electronic wave function in a similar way in both structures.

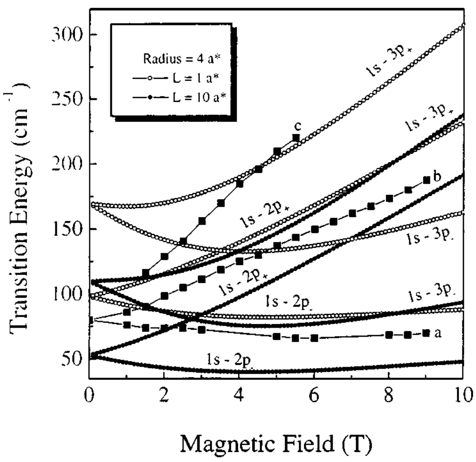

Figure 4. Infrared transition energies between the 1s-like and some excited states of a donor impurity located at the centre of a disc-shaped GaAs QD as a function of the magnetic field, and for disc lengths of $L = 1\ a^*$ (open circles) and $L = 10\ a^*$ (full circles). Experimental curves have been taken from [20] and are indicated by full squares: a, b, and c correspond to 1s $\rightarrow$ 2p$_-$, 1s $\rightarrow$ 2p$_+$, 1s $\rightarrow$ 3p$_+$, respectively.

4. Conclusions

In this work, we have considered the effects of an axial-applied magnetic field on the binding energy of some excited states and on the allowed transition energies between the 1s-like, and the 2p$_-$-like, 2p$_+$-like, 3p$_-$-like, 3p$_+$-like states of an on-centre shallow-donor impurity in a disc-shaped GaAs QD. In the calculations we have used the effective-mass approximation within a variational scheme and an infinite confinement potential model for all the boundaries of the QD. We have found that some excited states are not bounded for some values of the radius of the QD and of the applied magnetic field. Unfortunately, it is not possible to compare our results with experimental data, as measurements of the infrared transitions under applied magnetic fields have not been carried out so far in QDs. Despite of this fact, we have made a comparison with experimental reports in quantum wells [22], in order to stress the effects of the geometrical and magnetic confinement in the allowed transitions. Also, we have found that our results for the binding and transition energies are higher than those obtained in previous works in GaAs QWWs [15, 16]. Considering the potential device applications of the role of impurities in semiconducting heterostructures, we believe the present calculation will be of importance in the quantitative understanding of future experimental work in this subject. Although this work has been done for GaAs using the infinite potential model, its results could be used to discuss experimental results not only in vacuum–GaAs–vacuum, but in GaAs–Ga$_{1-x}$Al$_x$As QDs under the action of applied magnetic fields, whenever $0.30 < x < 0.45$ in order to have high enough potential barriers.

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References

[1] Cibert J, Petroff P M, Dolan G J, Pearton S J, Gossard A C and English J H 1986 *Appl. Phys. Lett.* **49** 1275
[2] Petroff P M, Cibert J, Gossard A C, Dolan G J and Tsu C W 1987 *J. Vac. Sci. Technol.* B **5** 1204
[3] Greene R L and Bajaj K K 1985 *Phys. Rev.* B **31** 913
[4] Bryant G W 1987 *Phys. Rev. Lett.* **59** 1140
[5] Brum J A 1991 *Phys. Rev.* B **43** 12 082
[6] Takagahara T 1987 *Phys. Rev.* B **36** 9293
[7] Lo L F and Sollie R 1991 *Solid State Commun.* **79** 775
[8] Johnson N F and Payne M C 1991 *Phys. Rev. Lett.* **67** 1157
[9] Chuu D S, Hsiao C M and Mei W N 1991 *Phys. Rev.* B **46** 3898
[10] Porras-Montenegro N, and Pérez-Merchancano S T 1992 *Phys. Rev.* B **46** 9780
[11] Porras-Montenegro N, Pérez-Merchancano S T, and Latgé A 1993 *J. Appl. Phys.* **74** 7624
[12] Ribeiro F J and Latgé A 1994 *Phys. Rev.* B **50** 4913
[13] Paredes-Gutirrez H, Cuero J C and Porras-Montenegro N 1994 *J. Appl. Phys.* **75** 5150
[14] Li G, Branis S V and Bajaj K K 1993 *Phys. Rev.* B **47** 15 735
[15] Villamil P and Porras-Montenegro N 1998 *J. Phys.: Condens. Matter* **10** 10 599
[16] Villamil P, Porras-Montenegro N and Granada J C 1999 *Phys. Rev.* B **59** 1605
[17] Brown J and Spector H 1986 *J. Appl. Phys.* **59** 1179
[18] Latgé A, Porras-Montenegro N and Oliveira L 1992 *Phys. Rev.* B **45** 9420
[19] Chaudhury S and Bajaj K 1984 *Phys. Rev.* B **29** 1803
[20] Greene R and Bajaj K 1988 *Phys. Rev.* B **37** 4604
[21] Bransden B H and Joachain C J 1991 *Physics of Atoms and Molecules* (New York: Longman)
[22] McCombe B D, Ranganathan R, Yoo B S and Cheng J-P 1990 *Proc. 20th Int. Conf. on Physics of Semiconductors* ed E M Anastassakis and J D Joannopoulos (Singapore: World Scientific) p 1337