Impurity Excited States and $1s \rightarrow 2s(2p_z)$ Line Strengths in Quantum-Well Wires

A. Latgé
Instituto de Física, Universidade Federal Fluminense
24020 Niterói, RJ, Brasil

M. de Dios-Leyva and Luiz E. Oliveira
Instituto de Física, Universidade Estadual de Campinas
Cx. Postal 6165, 13083-970 Campinas, SP, Brasil

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We present a variational calculation in the effective - mass approximation of the ground and lowest excited states of a. donor confinecl in a cylindrical GaAs-(Ga,Al)As quantum-well wire. The donor binding energies are calculated for different GaAs-(Ga,Al)As quantum-wire radii aiid donor positions within the wire. We have also calculated the line strengths of transitions from the donor ground state to excited states of $2s$-like and $2p_z$-like symmetries as the donor position varies along the radial direction in the wire, for polarizations of the incident radiation perpendicular and parallel to the wire axis, respectively. We found that tlie $1s \rightarrow 2s$ donor transition, which is forbidden in bulk materials, is allowed for incident radiation polarized along the y-radial direction of tlie wire with a quite considerable oscillator strength - comparable to the strength of the $1s \rightarrow 2p_z$ transition - for donors away from the wire axis.

Tlie understanding of the properties of impurity energy levels il1 low - dimensional semiconductor structures is a subject of interest due to possible technological aplications in electronic devices. The electronic configuration for the impurity differs from the correspon-clent bulk results and vary both with tlie well size and the impurity position along the low-dimensional heterostructures. GaAs-(Ga,Al)As quantum wells (QWs) are the most investigated systems and a number of studies[1-4] concerned with impurity-related properties are reported in tlie literature. Experimentally, Jarosik et al.[3] have observed broad absorption lines which appear to be related to $1s \rightarrow 2p_{\pm}$ transitions at on-center hydrogenic donors in GaAs-$Ga_{0.75}Al_{0.25}As$ QW structures. Far-infrared absorption spectrum of lightly doped GaAs-$Ga_{0.7}Al_{0.3}As$ superlattices were investigated by Helm et a~.[']

A considerable theoretical understanding of the properties of impurities in quantum-well wires (QWWs) has been achieved[6-8]. In particular, spectral features dominated by free carrier to acceptor - impurity recombinations have appeared in the photoluminescence measurements of GaAs quantum wire microcrystals by Hiruma et al.[9] and were attributed[10] to the presence of carbon acceptors in the wire microcrystal.

The experimental work of Helm et al.[5] on far - infrared spectroscopy of confined donors in GaAs - (Ga,Al)As superlattices has motivated us to investigate the properties of excited states associated to confined donors in cylindrical GaAs - (Ga,Al)As QWWs; the Hamiltonian for a donor-impurity in a cylindrical GaAs - (Ga,Al)As QWW with radius R may be written in the effective-mass approximation as

$$H = \frac{p^2}{2m^*} - \frac{e^2}{\epsilon_0[|\vec{\rho} - \vec{\rho}_i|^2 + z^2]^{1/2}} + V(\rho), \qquad (1)$$

where $V(\rho)$ is the confinement potential, ϵ_0 is the dielectric constant, and m* is the donor effective mass. We have considered the Al concentration x equal to 0.3 which corresponds to a potential barrier approximately equal to 224 meV.

We adopted a variational approach within the effective - mass approximation with the trial wave functions labeled by their correspondent bulk hydrogenic limit

and taken as products of hydrogeiiic functions with the ground-state wave function of the QWW, i.e.,

$$_{i} \qquad \vec{r}_i) = N_{nl}\phi_R(\rho)\Gamma_{nl}(\vec{r},\vec{r}_{i,i} \qquad \beta_{nl,i} \qquad (2)$$

where $\phi_R(\rho)$ is tlie ground-state QWW solution[6] without tlie impurity potential, N_{nl} are the normalization constants and the Γ_{nl} are hydrogenic functions. The corresponding excited states were referred to as $2s$, $2p_{x,y,z}$, $3s$, $3p_{x,y,z}$ ($n = 1,2$, and 3 with $1 = 1,2$), although tliey should not be identified with actual hydrogeiiic states since in general the above wave functions (Eq. 2) are distorted by the barrier potential. $\{\lambda_{nl}, \beta_{nl}, \alpha_{nl}\}$ is tlie set of variational parameters of the hydrogenic wave functioiis. The origin of tlie coordinate systeni was chosen at the center of tlie wire-well, the axis of the QWW was chosen as tlie z-axis, and tlie impurity pos tion is taken to vary within the y-axis. In this coordinate system tlie distance from tlie impurity-electron to t ıe donor is $r = (|\vec{\rho} - \vec{\rho}_i|^2 + z^2)^{1/2}$. The hydrogenic wave functions uscd in Eq. 2 are

$$\Gamma_{1s} = \exp(-\lambda_{1s}r), \qquad (3.a)$$

$$\Gamma_{2s} = (1 - \beta_{2s}r)\exp(-\lambda_{2s}r), \qquad (3.b)$$

$$\Gamma_{2p_x} = \rho\sin\varphi\exp(-\lambda_{2p_x}r), \qquad (3.c)$$

$$\Gamma_{2p_y} = (\rho\cos\varphi - \rho_i)\exp(-\lambda_{2p_y}r), \qquad (3.d)$$

$$\Gamma_{2p_z} = z\exp(-\lambda_{2p_z}r), \qquad (3.e)$$

$$\Gamma_{3s} = (3 - 6\beta_{3s}r + 2\alpha_{3s}^2r^2)\exp(-\lambda_{3s}r), \qquad (3.f)$$

$$\Gamma_{3p_x} = (2 - \beta_{3p_x}r)\rho\sin\varphi\exp(-\lambda_{3p_x}r), \qquad (3.g)$$

$$\Gamma_{3p_y} = (2 - \beta_{3p_y}r)(\rho\cos\varphi - \rho_i)\exp(-\lambda_{3p_y}r), \qquad (3.h)$$

$$\Gamma_{3p_z} = (2 - \beta_{3p_z}r)z\exp(-\lambda_{3p_z}r), \qquad (3.i)$$

where φ is tlie angle between $\vec{\rho}$ and $\vec{\rho}_i$. We have determined tlie impurity ground and excited states via a variational procedure which involves minimizing $< \Psi_{nl}|H|\Psi_{ni} >$ witli respect to tlie variational parameters $\{\lambda_{n'}, \beta_{nl}, \alpha_{nl}\}$ with the requirement[11] that the liydrogeiiic functioiis Γ_{nl}, form a set of orthogonal functioiis. This procedure leads to the exact bulk hydrogeiiic results in the limit of large-radius QWW. Of course, one should be aware that an appropriate calculation[12] within the effective-mass approximation would involve tlie diagonalization of tlie hamiltonian matrix written in a basis of functions which also include excited states of the QWW without the impurity. As usual, tlie binding energies for all hydrogenic-like states are obtained by subtracting the correspondiiig minimized $\epsilon_{nl} =< \Psi_{nl}|H|\Psi_{nl} >$ from the first coiiduction - subband energy ohtained from the solution of tlie QWW without the impurity. In what follows we present our results in reduced effective units of length and energy, which correspond to an effective Bohr radius $a_B = \hbar^2\epsilon_0/m^*e^2$ and an effective Rydberg $R_B = m^*e^4/2\hbar^2\epsilon_0^2$, respectively (for donors in GaAs-(Ga,Al)As QWWs, these units are $a_B \simeq 100$ Å and $R_B \simeq 5.7$ meV).

The beliavior of the theoretical binding energies as functions of the GaAs-$Ga_{0.7}Al_{0.3}As$ QWW radius for tlie states $2s$, $3s$, $2p_z$, and $3p_z$ are very similar with tlie result obtained[6,8] for the $1s$ state. For on-center donors and very large QWW radii (R >> a_B), the bound electrons no longer interact with the wire boundary and beliave as tliree-dimensional electrons in GaAs. Also, as tlie QWW radius diminishes, the binding energies, for any donor positioii in the wire, 'increase up to a maximum value as tlie donor wavefunction (for states with tlie above symmetries) beconies more compressed in tlie QWW which leads to more binding. One should notice that tlie states labeled by $2p_z$ and $3p_z$ behave in tlie same qualitative way as 1s, 2s, and $3s$, as the electron wave function of a p_z-like state is essentially concentrated aloiig tlie wire axis and are affected in a similar inaniier by the coiifinement effects. For very small wire radii, tlie donor-electrons leak out of the wire and behave as three-dimensional electrons in $Ga_{0.7}Al_{0.3}As$ aiid tlie exact bulk liydrogenic values are again recovered as expected. The behavior of tlie donor binding energies as the impurity position changes along tlie wire radial directioii is shown in Fig. 1 for these same states and for R = 10 nm. As the donor approaches the wire boundary, the binding energy decreases due to the repulsion of tlie doiior-electroii wavefunction by the barrier potential. This effect is clearly more pronounced for states labeled as s-like than for p_z-like states, as one would expect. Our results in Fig . 1 are very similar to the corresponding theoretical results for donors in GaAs-(Ga,Al)As quantum wells although the spread of the binding eiiergies as tlie donor position varies is larger in QWWs than in QWs because of the larger

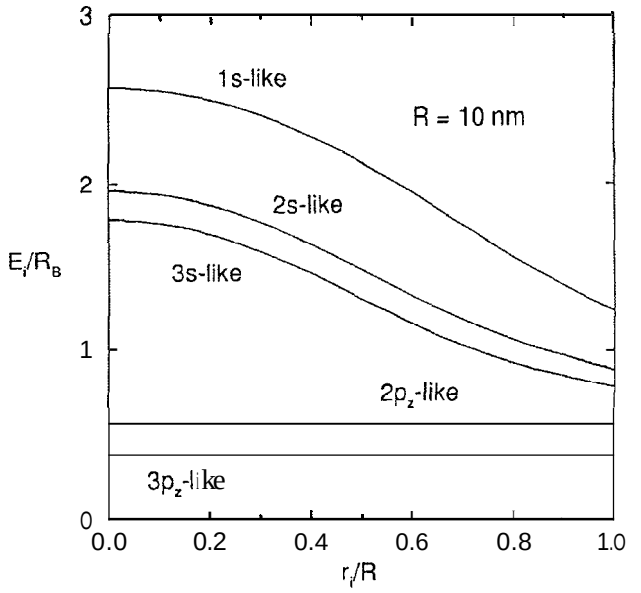

Figure 1: Doiior binding energies as functions of the impurity position for a GaAs-$Ga_{0.7}Al_{0.3}As$ QWW with radius of 10nm for different impurity states, labeled by their bulk hydrogenic limits.

confinement.

Fig. 2 shows our theoretical results for the donor binding energies for the states labeled as $2p_x$, $2p_y$, $3p_x$, and $3p_y$ in the case of varying GaAs-$Ga_{0.7}Al_{0.3}As$ QWW radii and for on-center and on-edge donors. Tlie np_x - and np_y-like states have electron densities essentially distributed around the xy-plane and are clearly degenerated (by symmetry) iii the case of donors located at the wire axis, as a comparison between Figs. 2(a) and 2(c)(for $n = 2$) and Figs. 2(b) and (d) (for $n = 3$) shows. As tlie impurity position changes from $r_i = 0$ (on-center donor) to $r_i = R$ (on-edge tlonor), the presence of the wire-barrier potential breaks tlic symmetry between x ancl y and lifts these degeneracies. Independently of the doiior position within tlic QWW, the behavior of these $2p_{x,y}$ and $3p_{x,y}$ states are very similar in the sense that for the QWW radius smaller than some particular value (which depends on the impurity position), they become unbound due to the rather large increase in the donor-electron kinetic energy as the electron wavefunction is compressed by the wire potential barrier (this occurs even for the $2p_y$-like on-edge case shown in Fig. 2(c), although this is not explicitly shown in the figure). This unbound-donor behavior was also theoretically found for donors in quantum wells by Greene and Bajaj[2,13] and Fraizzoli et al.[4] Perhaps it is worthwhile to mention that the rather peculiar behavior, for a given QWW radius, of the tlonor binding energies with impurity position of the $2p_y$ - and $3p_y$ -like states is probably related to an interplay between donor position, QWW radius, and spatial extension and nodes of the $2p_y$ - and $3p_y$ -like electron radial wavefunction.

We have also calculated the line strengths for infrared transitions from the 1s-like donor giound state to some excited states. The line strengths for these transitions were discussed by Greene et al.[14,15] who considered r- and y-polarization of the incident. radiation for the case of QWs, aiid by Fraizzoli et al.[4]. The line strengths of these infrared transitions are therefore proportional to the square of the dipole matrix elements between the initial and final states. In Fig. 3, we present the square of the dipole matrix element between the $1s$ and $2s$ states for radiation polarized in the y direction, $|<2s|y|1s>|^2$, aiid hetween the $1s$ and $2p_z$ states in the case of z-polarization, $|<2p_z|z|1s>|^2$, for all impurity positions within a GaAs-$Ga_{0.7}Al_{0.3}As$ QWW of radius R = 10 nm. Because of the symmetry of the Hamiltonian, tlie strength of the y-polarized radiation between $1s$ and 2s states is zero for on-center donors. Away from the center, the $<2s|y|1s>|^2$ matrix elements increase but remain smaller than that of the $1s - 2p_z$ transition. Our results for $<2s|y|1s>|^2$ and $<2p_z|z|1s>|^2$ are quite similar to those obtained by Greene and Lane[14] and Fraizzoli et al.[4] in GaAs-(Ga,Al)As quantum wells although no maximum is observed in the $<2s|y|1s>|^2$ QWW line strength in contrast with the result by Fraizzoli et al.[4] for L = 400 A QWs.

Summing up, me have presented a variational calculation within the effective - mass approximation of the states of a. donor impurity in a cylindrical GaAs-(Ga,Al)As QWW. The binding energies of the ground and lowest excited states - labeled for convenience by their bulk hydrogenic limits - wcre calculated for variou-values of the GaAs-(Ga.Al)As QWW radius and impurity positions within the quantum wire. Our results are very similar to those obtained in previous theoretical calculations[2,4] for impurity states in GaAs-(Ga,Al)As QWs, although one should take into account that confinement effects are larger in quantum wires than in QWs and therefore the spread of the

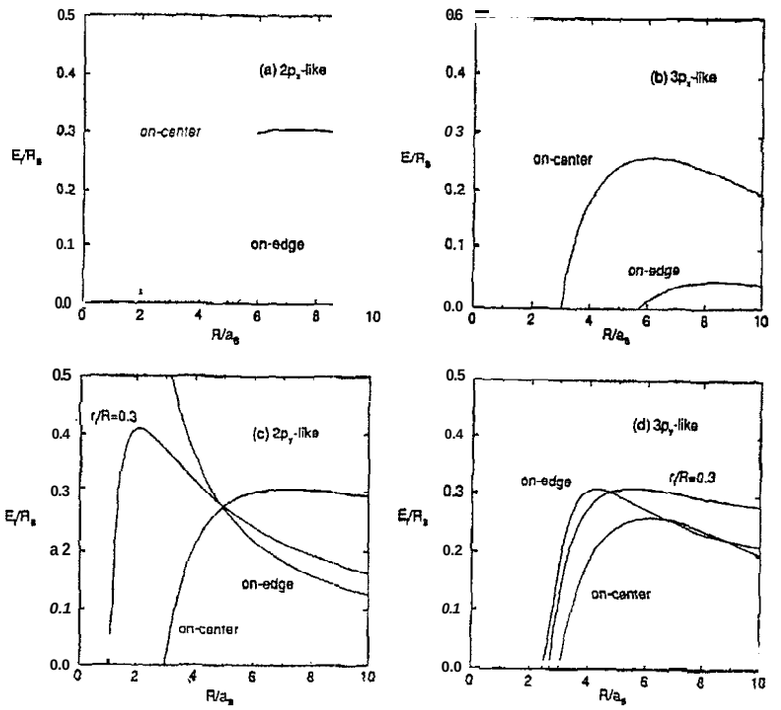

Figure 2: Bir ding energies of an electron bound to on-center and on-edge shallow-donor impuritiers in a GaAs-$Ga_{0.7}Al_{0.3}As$ QWW as a f inction of tlie QWW radii (given in units of the effective Bohr radius a_B i 100 Å): (a) $2p_x$-like, (b) $3p_x$-like, (c) $2p_y$-like, and (d) $3p_y$-like states.

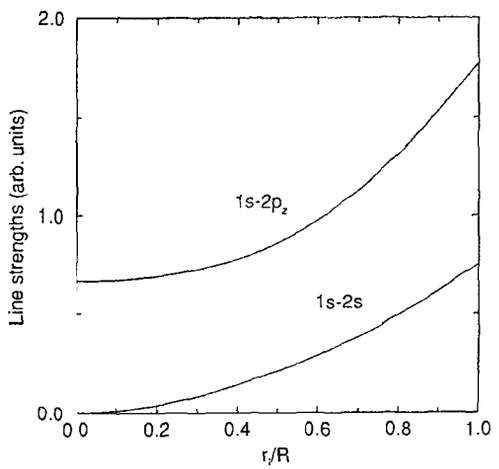

Figure 3: Lir e strengths $|< 1s|y|2s >|^2$ for the $1s - 2s$ transition (with y-polarized radiation), aiid $|<1s|z|2p_z>|^2$ for the $1s - 2p_z$ transition (with z-polarized radiation) as functions of the donor position along the radial direction, for a GaAs-$Ga_{0.7}Al_{0.3}$As QWW radius $R = 10$ nm.

donor binding energies as the donor position varies is larger in QWWs than in QWs of comparative dimensions. The line strengths of transitions from tlie donor ground state to excited states of $2s$-like and $2p_z$-like symmetries were calculated for a $R = 100$ Å GaAs-(Ga,Al)As QWW as the donor position varies along the radial direction in tlie wire. for polarizations of the incident radiation perpendicular and parallel to the QWW axis, respectively. Although tlie $1s \rightarrow 2s$ donor transition is forbidden in bulk material~this transition i~ allowed with a quite considerable oscillator strength (comparable to the strength of the $1s - 2p_z$ transition) for impurities amay from the wire axis in a GaAs-(Ga,Al)As QWW. Experiments in selectively donor-doped GaAs-(Ga,Al)As QWWs using far-infrared spectroscopy[5] should be performed in ordei. to investigate the detailed properties associated to impurity transitions.

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References

1. G. Bastard, Phys. Rev. B**24**, 4714 (1981).
2. R. L. Greene and K. K. Bajaj, Solid State Commun. 45, 825 (1983); Phys. Rev. B**31**, 913 (1985).
3. N. C. Jarosik, B. D. McCombe, R. V. Shanabrook, J. Comas, J. Ralston and G. Wicks, Phys. Rev. Lett. 54, 1283 (1985).
4. S. Fraizzoli, F. Bassani and R. Buczko, Phys. Rev. B**41**, 5096 (1990).
5. M. Helm, F. N. Peeters, F. DeRosa, E. Colas, J. P. Harbison and L. T. Florez, Phys. Rev. B 43, 13983 (1991).
6. J. W. Brown and H. N. Spector, J. Appl. Phys. 59, 1179 (1986).
7. G. W. Bryant, Phys. Rev. B29, 6632 (1984); *ibid.* **31**, 7812 (1985).
8. N. Porras-Montenegro, J. Lopez-Gondar and L. E. Oliveira, Phys. Rev. B 43, 1824 (1991); A. Latgé, N. Porras-Montenegro and L. E. Oliveira, ***ibid.*** B45, 9420 (1992).
9. K. Hiruina, T. Katsuyama, K. Ogawa., M. Koguchi, H. Kakibayashi and G. P. Morgan, Appl. Phys. Lett. 59, 431 (1991).
10. L. E. Oliveira, N. Porras-Montenegro and A. Latgé, Phys. Rev. B47, 13864 (1993).
11. S. Chaudhuri and K. K. Bajaj, Phys. Rev. B29, 1803 (1984).
12. R. A. Faulkner, Phys. Rev. 184, 713 (1969).
13. R. L. Greene and K. K. Bajaj, Phys. Rev. B**31**, 4006 (1985).
14. R. L. Greene and P. Lane, Phys. Rev. B**34**, 8639 (1086).
15. R. L. Greene and K. K. Bajaj, Phys. Rev. B 34, 951 (1986).
16. W. Kohn, in Solid *State* Physics, edited by F. Seitz and D. Turnbull (Academic, New York, 1957), Vol. 5.