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Infrared-absorption line shapes of shallow donors in cylindrical quantum-well-wire structures

A. Latgé
Instituto de Física, Universidade Federal Fluminense, 24020 Niterói, Rio de Janeiro, Brazil

Luiz E. Oliveira[a)]
Instituto de Física, Universidade Estadual de Campinas-Unicamp, CP 6165, Campinas, São Paulo 13083-970, Brazil

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A theoretical study of the intraimpurity infrared-absorption properties associated to donor-doped cylindrical GaAs–(Ga,Al)As quantum-well wires is presented. Donor binding energies and envelope wave functions are calculated within a variational scheme in the effective-mass approximation, and line strengths for intradonor transitions to excited states of $2s$-, $2p_z$-, and $3p_z$-like symmetries are obtained for different photon polarizations and for donor positions varying along the radial direction of the wire. The donor-related absorption coefficients are evaluated in the case of $1s \rightarrow 2p_z$ and $1s \rightarrow 3p_z$ transitions for z-polarized radiation, and for different donor profiles in the quantum wire. © *1995 American Institute of Physics.*

In recent years, there has been considerable experimental and theoretical interest in the understanding of the nature of isolated hydrogenic-impurity states in confined geometries.[1–5] In particular, intraimpurity transitions have been studied in some detail in GaAs–(Ga,Al)As quantum wells (QWs) via far-infrared magnetospectroscopy. Jarosik *et al.*[1] have observed broad absorption lines which they assigned to $1s-2p_{\pm}$ intradonor transitions in GaAs–(Ga,Al)As QW structures, whereas Fraizzoli, Bassani, and Buczko[3] computed the donor-related far-infrared-absorption coefficient taking into account the spatial impurity distribution and found good agreement with the experimental data. The line strengths for transitions from the $1s$-like ground state to some excited states were discussed by Fraizzoli, Bassani, and Buczko[3] and by Greene *et al.*,[4] who considered x and y polarization of the incident radiation for the case of GaAs–(Ga,Al)As QWs. Latgé *et al.*[5] have calculated the binding energies and envelope wave functions of the ground and some excited states of hydrogenic donors, and the line strengths of transitions from the $1s$- to the $2s$- and $2p_z$-like donor states in GaAs–(Ga,Al)As cylindrical quantum-well wires (QWWs). It was then suggested that although the $1s \rightarrow 2s$ donor transition is forbidden in bulk materials, this transition is allowed for incident radiation polarized along the y-radial direction of the wire with a quite considerable oscillator strength—comparable to the strength of the $1s \rightarrow 2p_z$ transition—for impurities away from the wire axis.

The experimental work by Jarosik *et al.*[1] and the theoretical study by Fraizzoli, Bassani, and Buczko[3] on GaAs–(Ga,Al)As QWs have motivated us to investigate the donor-related absorption coefficients of $1s \rightarrow 2p_z$ and $1s \rightarrow 3p_z$ transitions for z-polarized radiation, and for different donor profiles, in the case of GaAs–(Ga,Al)As cylindrical QWWs.

We consider a single, isolated donor impurity in a cylindrical GaAs–(Ga,Al)As QWW with radius R and adopted a variational procedure within the effective-mass approximation, with a finite-barrier potential. Effects of dielectric mismatch and difference of values of the effective mass across the interface are neglected. The origin of the coordinate system was chosen at the center of the wire well, and the impurity position to vary along the y axis. In what follows, the ground- and excited-donor states are labeled by their corresponding bulk hydrogenic limit with variational envelope wave functions[5] taken as products of hydrogenic functions with the ground-state wave function of the GaAs–(Ga,Al)As QWW.

The line strength for transitions from the donor ground state (i) to excited states (f) is proportional to the square of the momentum matrix elements between the initial and final states, which may alternatively be obtained by calculating the corresponding position matrix elements. Within the framework of the effective-mass approximation, the position matrix elements of $i \rightarrow f$ donor transitions may be expressed as[6]

$$|\langle i|\mathbf{r}|f\rangle|^2 = (\hbar^2/m^* E_{fi})^2 |\langle i|\nabla|f\rangle|^2, \qquad (1)$$

where $\mathbf{r}$ is the carrier position with respect to the impurity, and E_{fi} is the difference in energy between the initial and the final states involved in the intradonor transition.

Figure 1 shows the line strengths $|\langle i|\mathbf{r}|f\rangle|^2$ for infrared transitions from the $1s$-like donor ground state to $2s$, $2p_z$, and $3p_z$ excited states in the case of a GaAs–$Ga_{0.7}Al_{0.3}As$ QWW of radius $R=100$ Å. The incident radiation was considered to be y polarized for the $1s \rightarrow 2s$ transition, and z polarized in the case of $1s \rightarrow 2p_z$ and $1s \rightarrow 3p_z$ transitions. Results for $|\langle i|\mathbf{r}|f\rangle|^2$ are calculated either directly [Fig. 1(a); position form] or via the RHS of Eq. (1) [Fig. 1(b); momentum form]. Of course, Eq. (1) is only exact for true solutions of the donor problem and is **not** valid[7] for a variational solution as in the present case. Nevertheless, it is apparent from the results in Fig. 1 that the overall behavior of the different line strengths are quite the same. Also, the donor-related ab-

[a)]E-mail: oliveira@ifi.unicamp.br

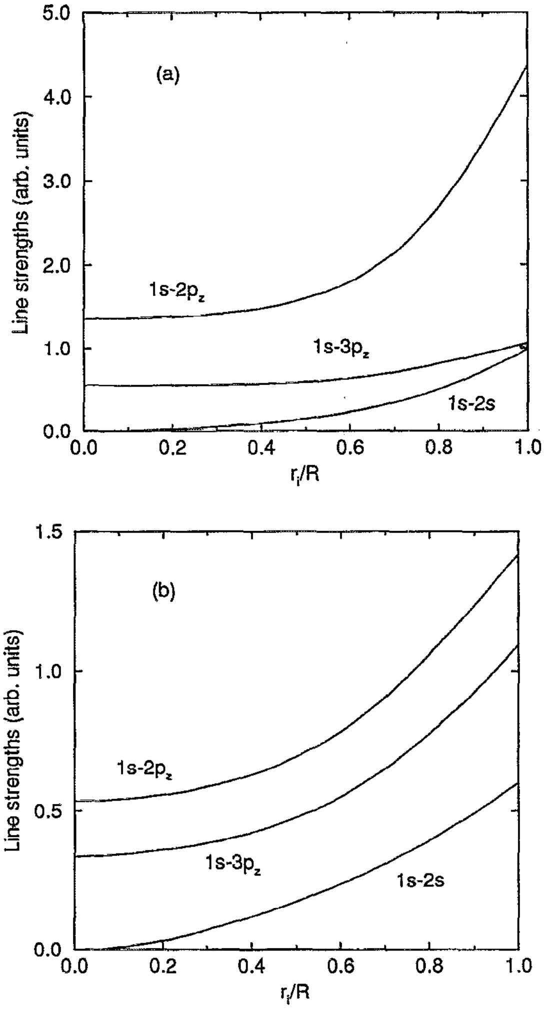

FIG. 1. Line strengths $|\langle 1s|z|2p_z\rangle|^2$ and $|\langle 1s|z|3p_z\rangle|^2$ for the $1s\rightarrow 2p_z$ and $1s\rightarrow 3p_z$ transitions, respectively (with z-polarized radiation), and $|\langle 1s|y|2s\rangle|^2$ for the $1s\rightarrow 2s$ transition (with y-polarized radiation) as functions of the donor position along the radial direction, for a GaAs–$Ga_{0.7}Al_{0.3}As$ QWW of radius $R=100$ Å. Results shown in (a) and (b) are calculated using the position and momentum forms, respectively.

sorption coefficient (see below) calculated by using the momentum or the position forms of the line strengths $|\langle i|\mathbf{r}|f\rangle|^2$ gives essentially the same result. Notice that the strength of the transition (y-polarized radiation) between $1s$ and $2s$ states is zero (as in the bulk case) for on-center donors. Away from the center, the $|\langle 2s|y|1s\rangle|^2$ matrix elements increase[3,4] but remain smaller than that of the $1s\rightarrow 2p_z$ transition.

As mentioned by Greene and Bajaj,[4] the far-infrared intradonor absorption line shape for z-polarized incident radiation is given by

$$I(\omega)\simeq\omega\sum_f \int_0^R 2\pi r_i P(r_i)|\langle f|z|i\rangle|^2\delta(\omega-\omega_{fi})dr_i, \quad (2)$$

where $\hbar\omega$ is the photon energy, $P(r_i)$ defines the impurity distribution in the QWW, r_i gives the donor distance to the wire axis, and $\omega_{fi}=(E_f-E_i)/\hbar$ is the energy difference between the final and initial donor states. We calculated the contribution to the absorption line shape from $1s\rightarrow 2p_z$ and $1s\rightarrow 3p_z$ donor transitions for a GaAs–$Ga_{0.7}Al_{0.3}As$ QWW of radius $R=100$ Å. We consider both an homogeneous donor distribution inside the QWW as well as an on-center Gaussian donor distribution of half width$=R/3$. Also, following Fraizzoli, Bassani, and Buczko,[3] we have introduced a phenomenological width $\Gamma=0.7$ meV by replacing the δ function $\delta(\omega-\omega_{fi})$ in Eq. (2) by a Lorentzian function in the calculation of the absorption line shape. Our results for the intradonor absorption line shapes are displayed in Fig. 2. The absorption line shape associated to the homogeneous donor distribution [cf. Fig. 2(a)] in the QWW shows essentially two structures loosely corresponding to on-center and on-edge intradonor transitions, respectively. For the on-center Gaussian donor distribution [cf. Fig. 2(b)], the absorption coefficient shows a peaked structure at a photon energy slightly below the on-center intradonor $1s\rightarrow 2p_z$ transition energy,

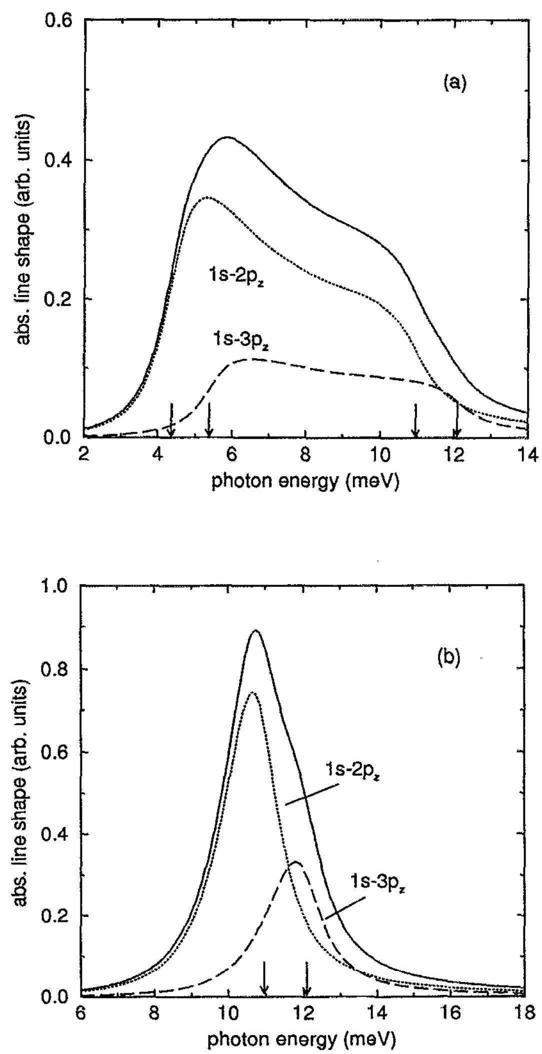

FIG. 2. Donor-related absorption coefficients for $1s\rightarrow 2p_z$ and $1s\rightarrow 3p_z$ transitions (z-polarized radiation). Results are shown for (a) an homogeneous donor distribution in the $R=100$ Å GaAs–$Ga_{0.7}Al_{0.3}As$ quantum wire, and (b) an on-center Gaussian donor distribution of half width$=R/3$. Full curves correspond to the total contribution for both transitions. Arrows in the figures indicate on-center and on-edge donor transition energies corresponding to $E(2p_z)-E(1s)$ and $E(3p_z)-E(1s)$.

whereas the $1s \rightarrow 3p_z$ transitions essentially contribute to the asymmetry of the peak. Our result in Fig. 2(b) should be compared to the calculation by Fraizzoli, Bassani, and Buczko[3] (cf. their Fig. 6) in GaAs–(Ga,Al)As quantum wells.

In conclusion, we have presented a theoretical study of the intradonor far-infrared-absorption coefficients of cylindrical GaAs–(Ga,Al)As QWWs in the case of $1s \rightarrow 2p_z$ and $1s \rightarrow 3p_z$ transitions for z-polarized radiation, and for different donor profiles in the wire. Our results are qualitatively comparable with theoretical[3] and experimental[1] work in GaAs–(Ga,Al)As QWs. As no experimental data in QWWs is available, we do hope that the present calculation might motivate future far-infrared spectroscopic experiments in selectively impurity-doped GaAs–(Ga,Al)As QWWs.

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