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Excitonic and shallow-donor states in semiconducting quantum wells: a fractional-dimensional space approach

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Abstract. A systematic study of shallow-donor and excitonic states in semiconducting quantum wells within a fractional-dimensional space approach is presented. In this scheme, the Schrödinger equation is solved in a noninteger-dimensional space in which the interactions are assumed to occur in an isotropic effective environment, and the fundamental quantity is the parameter D, which defines the fractional dimension associated with the effective medium and the degree of anisotropy of the interactions. The fractional dimensionality of the isotropic effective space is derived via an unambiguous procedure in which one may obtain the exact solution for the energies of the actual physical system under consideration. Explicit calculations of the fractional-dimensional parameter are made in the case of shallow donors and excitons in finite-barrier GaAs–(Ga, Al)As quantum wells, with impurity and exciton binding energies found in good agreement with previous variational results and available experimental data.

1. Introduction

In the last few years, modern growth techniques such as molecular-beam epitaxy, chemical-beam epitaxy, and metal–organic chemical vapour deposition have made possible the realization of high-quality semiconducting heterostructures [1] consisting of layers of different semiconductors with sharp interfaces and controlled layer thicknesses. The unique physics character of the electronic states in semiconducting superlattices and heterostructures and the wide range of potential device applications associated with these systems resulted in a great deal of work devoted to the understanding of the nature of the electronic, excitonic, and impurity states in semiconducting heterostructures. In particular, work on impurity properties in quantum wells (QWs) was pioneered by Bastard [2], with several other more detailed investigations performed by Greene and Bajaj [3], Mailhiot *et al* [4], Tanaka *et al* [5], Fraizzoli *et al* [6], Masselink *et al* [7], Oliveira and Falicov [8], and others, in which the energy spectrum of the ground state and low-lying excited states of shallow impurities in GaAs–(Ga, Al)As QWs was studied taking into consideration the finite size of the barrier potential, the influence of the effective-mass and dielectric constant mismatches, nonparabolicity effects, etc. In general, these theoretical investigations are based on a variational approach. Experimentally, various measurements of the properties

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of impurity states in GaAs–(Ga, Al)As QWs, under different physical conditions, have been reported. Recent study [9] on the field contains a detailed list of theoretical and experimental work on general properties of shallow impurities in QWs and semiconducting heterostructures. Similar work, both theoretically [10–14] and experimental [15, 16], on excitonic states in GaAs–(Ga, Al)As QWs has been reported. Bastard *et al* [10] and Greene *et al* [11] performed variational calculations of the energy levels of Wannier–Mott excitons in GaAs–(Ga, Al)As and InAs–GaSb heterostructures, whereas Pereira *et al* [12] studied the exciton binding energies in semiconductor superlattices (SLs) using an anisotropic-effective-medium approach. An accurate theory of excitons in GaAs–(Ga, Al)As QWs including valence-band mixing, Coulomb coupling between excitons belonging to different subbands, nonparabolicity effects, and the difference in dielectric constants between well and barrier materials was performed by Andreani and Pasquarello [13]. Leavitt and Little [14] neglected valence-band mixings and presented a simple method for calculating exciton binding energies in quantum-confined structures. A recent account of experimental work on excitons may be found in the studies by Oelgart *et al* [15] and Voliotis *et al* [16].

Recently, the concept of fractional-dimensional space [17] has been successfully used in the study of the excitonic properties and the optical spectra of anisotropic semiconducting heterostructures [18]. A systematic work, within the fractional-dimensional space approach, on the excitonic states and absorption spectra in GaAs–(Ga, Al)As QWs, quantum-well wires (QWWs), SLs, and double QWs has been made by Mathieu *et al* [19–21], and by Zhao *et al* [22]. In this scheme, the Schrödinger equation is solved in a noninteger-dimensional space, where the interactions are assumed to occur in an isotropic effective environment, i.e., in the fractional-dimensional model, the fundamental quantity is the parameter D which defines the fractional dimension associated with the effective medium, and with the degree of anisotropy of the interactions. However, up to now, all theoretical proposals have been essentially based on an *ansatz* for the fractional dimension D. In this study, we propose a systematic and unambiguous procedure to determine the fractional dimensionality of the isotropic effective space used to model the actual system (a brief account of this work has been reported elsewhere [23]).

2. Theoretical framework

We consider the problem of a shallow hydrogenic donor confined in a semiconducting GaAs–(Ga, Al)As QW (growth axis along the z-direction), within the effective-mass and non-degenerate-parabolic band approximations. The Hamiltonian for the donor is therefore given by [23–26]

$$\boldsymbol{H} = -\frac{\hbar^2}{2m^*}\nabla^2 + V(z) - \frac{e^2}{\varepsilon r} \tag{2.1}$$

where m^* is the conduction-band effective mass of the donor electron, ε is the dielectric constant of the QW material (m^* and ε are assumed constant throughout the heterostructure and equal to the GaAs bulk value), $V(z)$ is the corresponding confining potential, $r = \sqrt{x^2 + y^2 + (z - z_i)^2}$, and the donor is located at the position z_i. The eigenfunctions of (2.1) may be taken as $\psi_E(\boldsymbol{r}) = f(z)\phi_E(\boldsymbol{r})$, where $f(z)$ is the z-part of the $n = 0$ ($\boldsymbol{k} = 0$) electron-envelope wave function, for the QW in the absence of the Coulomb potential, and find, after using (2.1),

$$\left(-\frac{\hbar^2}{2m^*}\nabla^2 - \frac{e^2}{\varepsilon r}\right)\phi_E - \frac{\hbar^2}{2m^*}\frac{1}{h(z+z_i)}\frac{\mathrm{d}h(z+z_i)}{\mathrm{d}z}\frac{\partial\phi_E}{\partial z} = E\phi_E \tag{2.2}$$

where

$$h(z) = f^2(z) \tag{2.3}$$

z (and r) is now taken relative to the donor position, and E is the shallow-donor energy (with respect to the bottom of the $n = 0$ first conduction subband). (2.2) may be written, in spherical coordinates, and taking $m = 0$ (m is the magnetic quantum number), as

$$(H_D + W)\phi_E = E\phi_E \tag{2.4}$$

where

$$H_D = -\frac{\hbar^2}{2m^*}\left[\frac{1}{r^{D-1}}\frac{\partial}{\partial r}\left(r^{D-1}\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin^{D-2}(\theta)}\frac{\partial}{\partial\theta}\left(\sin^{D-2}(\theta)\frac{\partial}{\partial\theta}\right)\right] - \frac{e^2}{\varepsilon r} \tag{2.5}$$

and

$$W = -\frac{\hbar^2}{2m^*}\left[\left(\frac{\beta}{r} + \frac{1}{h}\frac{\partial h}{\partial r}\right)\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\frac{\beta\cos\theta}{\sin\theta} + \frac{1}{h}\frac{\partial h}{\partial\theta}\right)\frac{\partial}{\partial\theta}\right] \tag{2.6}$$

with $\beta = 3 - D$ and $h = h(r\cos\theta + z_i)$. One should note that (2.4) is *exact*, and depends on a D parameter which was introduced for convenience. Also, note that the Hamiltonian (2.5) corresponds to the $m = 0$ hydrogen Hamiltonian in a fractional-D-dimensional space, a problem which may be solved analytically [17, 18]. If one denotes by ϕ_j and E_j the eigenfunctions and eigenvalues of (2.5), i.e.,

$$H_D\phi_j = E_j\phi_j \tag{2.7}$$

the donor energy (with respect to the bottom of the $n = 0$ first conduction subband) may be written, after some straightforward algebraic manipulation of (2.4) and (2.7), as

$$E = E_j + \left(\int hr^2\sin\theta\phi_E^* W\phi_j\,\mathrm{d}r\,\mathrm{d}\theta\right)\left(\int hr^2\sin\theta\phi_E^*\phi_j\,\mathrm{d}r\,\mathrm{d}\theta\right)^{-1} \tag{2.8}$$

where ϕ_E is the corresponding donor eigenfunction. Note that (2.8) is still *exact*, and valid for *any value* of the D fractional-dimensional parameter, and *holds for arbitrary pairs* of (ϕ_E, E) and (ϕ_j, E_j).

If one now is interested in evaluating the donor binding energy, which is associated with the ground state E_{1s}, one may choose the D parameter such that the second term in the RHS of (2.8) is zero for ϕ_j chosen as the ground state associated with (2.7), so that both ground states coincide. The condition for D is therefore that

$$\int hr^2\sin\theta\phi_E^* W\phi_j\,\mathrm{d}r\,\mathrm{d}\theta = 0 \tag{2.9}$$

with ϕ_E being the *exact* ground-state solution of (2.4). One should stress that the above equation provides an *exact* expression for determining the dimension of the D-fractional-dimensional space which would model the actual system, and which would give the *exact* solution for the donor binding energy. Similar conditions could be obtained for the *exact* D parameters which could be used for obtaining any energies of the excited states of the actual physical system under consideration.

Of course, the exact solutions ϕ_E of (2.4) are not known, and approximate values for the fractional-dimensional parameter D may be obtained if one uses approximate solutions for ϕ_E. The obvious simple choice is to take $\phi_E = \phi_{j=0}$ (where $\phi_{j=0}$ is the 1s ground-state solution [17, 18] of the D-dimensional Hamiltonian in (2.5)), use (2.9) to find D, and obtain the energy states of the full problem under consideration by solving the D-dimensional equivalent Hamiltonian. One would expect, of course, that this simple choice would give an appropriate physical solution for the energy states, provided that the actual system is not

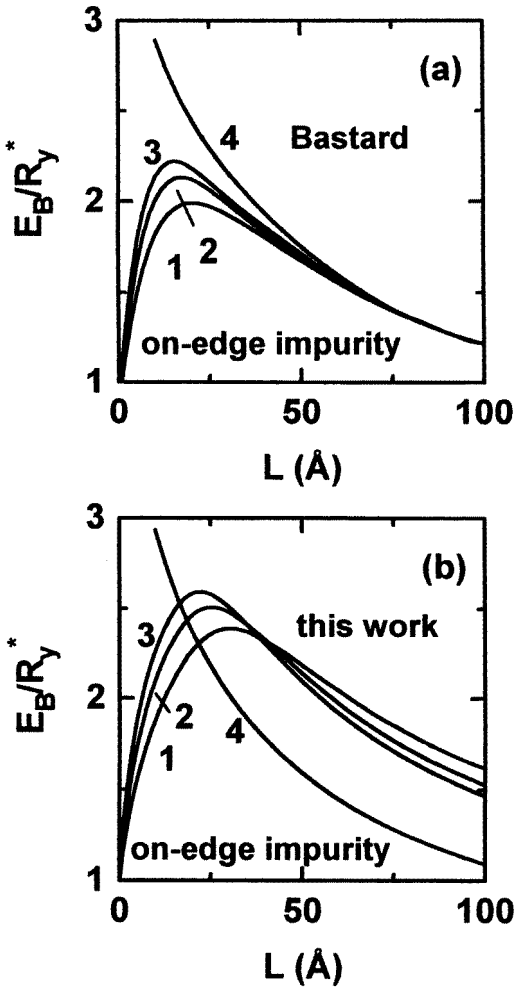

Figure 1. Thickness dependence of the on-edge donor binding energies in GaAs–(Ga, Al)As QWs. The curves in (a) are from Bastard [24], whereas the curves in (b) were calculated within the fractional-dimensional approach. The curves labelled 1, 2, 3, and 4 correspond to conduction barriers of 212 meV, 318 meV, 424 meV, and infinite barriers, respectively.

strongly anisotropic. If one considers the problem of a Wannier–Mott exciton confined in a semiconducting QW, a similar condition for D may be found, and the excitonic energies may be readily obtained (see the appendix).

3. Results and discussion

The solutions of (2.9) for the D fractional-dimensional parameter may be obtained, as explained before, for the case of donors at the general position z_i in QWs, and also for excitons in QWs. The binding energies may then be obtained through [17, 18]

$$E_B = \frac{4}{(D-1)^2} R_y^* \tag{3.1}$$

where R_y^* is the effective Rydberg, either for donors or for excitons.

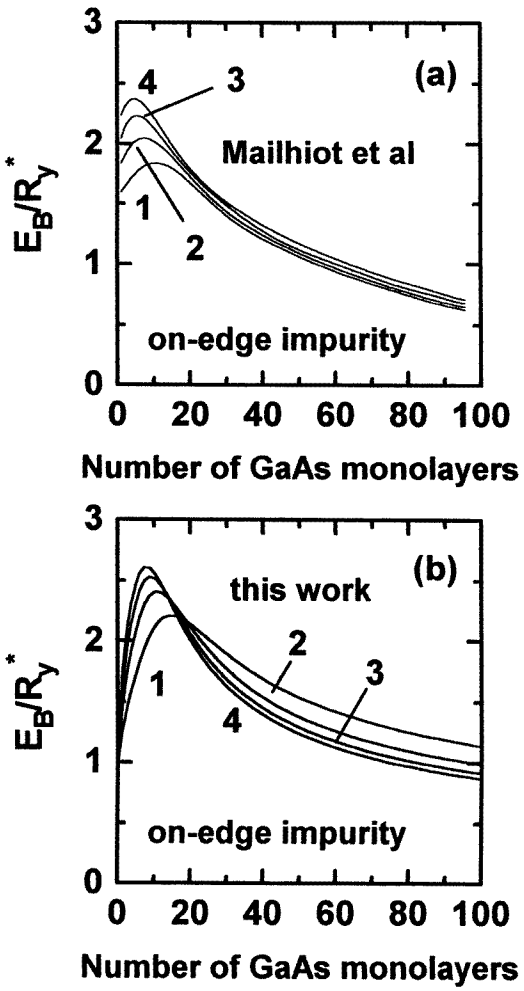

Figure 2. Thickness dependence of the on-edge donor binding energies in GaAs–$Ga_{1-x}Al_xAs$ QWs for different x alloy compositions. The curves in (a) are from Mailhiot *et al* [4], whereas the curves in (b) were calculated within the fractional-dimensional approach. The curves labelled 1, 2, 3, and 4 correspond to conduction barriers of 106 meV, 212 meV, 318 meV, and 424 meV, respectively.

Calculated results, within the fractional-dimensional approach, for the on-edge donor binding energies are displayed in figures 1–3 as functions of the GaAs–(Ga, Al)As QW width, and for different conduction-barrier potentials (or concentrations of Al) [27], and compared with theoretical variational calculations by Bastard [24], Mailhiot *et al* [4], and Oliveira [25] for on-edge donors. As already discussed by Oliveira [25], in the large-L limit and infinite barrier potentials, the *exact* binding energy of on-edge impurities is $R_y^*/4$, whereas for infinitely large L and vanishingly small Al concentrations (or barrier potentials), one should obtain the limiting value of $1R_y^*$ for the on-edge binding energy, implying that, for large values of the QW width, the on-edge binding energies *increase* as the barrier potential *decreases*, a prediction which contrasts with the theoretical behaviour obtained by Bastard [24] and Mailhiot *et al* [4], and which is in agreement with the variational

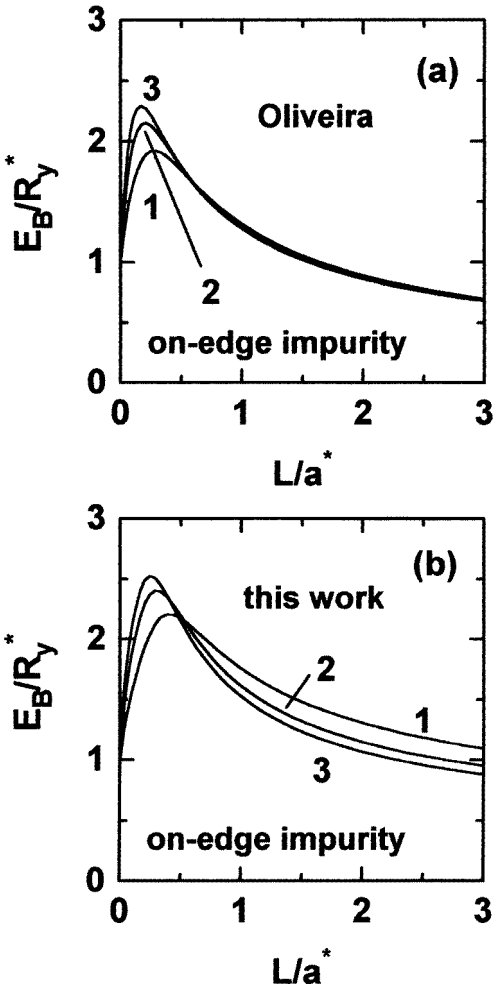

Figure 3. Thickness dependence of the on-edge donor binding energies in GaAs–$Ga_{1-x}Al_xAs$ QWs for different x alloy compositions. The curves in (a) were obtained as in the work of Oliveira [25] (using a constant screening), whereas the curves in (b) were calculated within the fractional-dimensional approach. The curves labelled 1, 2, and 3 correspond to an Al concentration $x = 0.15$, 0.30, and 0.45, respectively.

calculation by Oliveira [25] and with the results of the present calculation in the fractional-dimensional scheme. Moreover, in figure 3, it is apparent the overall quantitative agreement between the on-edge binding energies calculated within a variational calculation [25] and via the fractional-dimensional scheme, with the fractional dimension D calculated as described in the previous section.

In figure 4, we compare the theoretical results for the on-centre donor binding energies, both in the case of the variational calculation [25] and the fractional-dimensional scheme. For finite conduction-potential barriers, both theoretical calculations give the *exact* results of $1R_y^*$ for the on-centre donor binding energies, in the limiting cases of QW widths $L = 0$, and infinite, respectively, whereas for infinite barriers, one also recovers the exact limiting value of $4R_y^*$ for the $L = 0$ case. The overall agreement between both calculations is apparent for

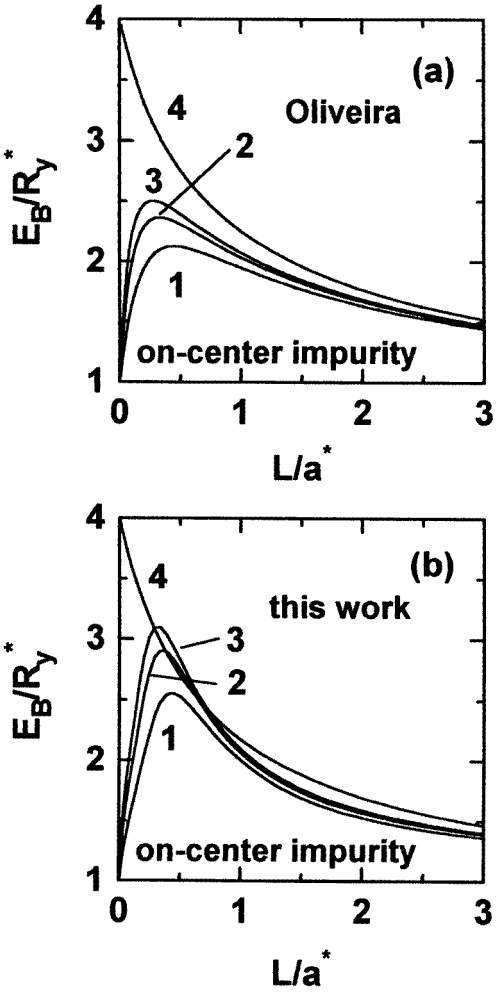

Figure 4. Thickness dependence of the on-centre donor binding energies in GaAs–$Ga_{1-x}Al_xAs$ QWs for different x alloy compositions. The curves in (a) were obtained as in the work of Oliveira [25] (using a constant screening), whereas the curves in (b) were calculated within the fractional-dimensional approach. The curves labelled 1, 2, 3, and 4 correspond to $x = 0.15$, 0.30, 0.45, and infinite barriers, respectively.

QW widths larger than the donor effective Bohr radius ($\cong$100 Å), and results quantitatively differ for small QW widths as the QW heterostructure is then strongly anisotropic, and most certainly both methods (as well the effective-mass approximation itself) are not quantitatively reliable. The donor binding energies in the fractional-dimensional scheme are shown in figure 5, in the case of the impurity position varying within the GaAs–(Ga, Al)As QW, for different QW widths, as compared with the results of variational calculations by Oliveira [25] and Greene and Bajaj [26]. Again, the overall quantitative agreement is good, except in the case of the $L = 50$ Å QW, in which the anisotropy is stronger.

The fractional-dimensional parameters D (cf (2.9)) used to obtain the theoretical binding energies of figures 4(b) and 5(b) are displayed in figure 6, where one may note that the appropriate physical dimension $D = 3$ is recovered (see figure 6(a)) in the limiting cases

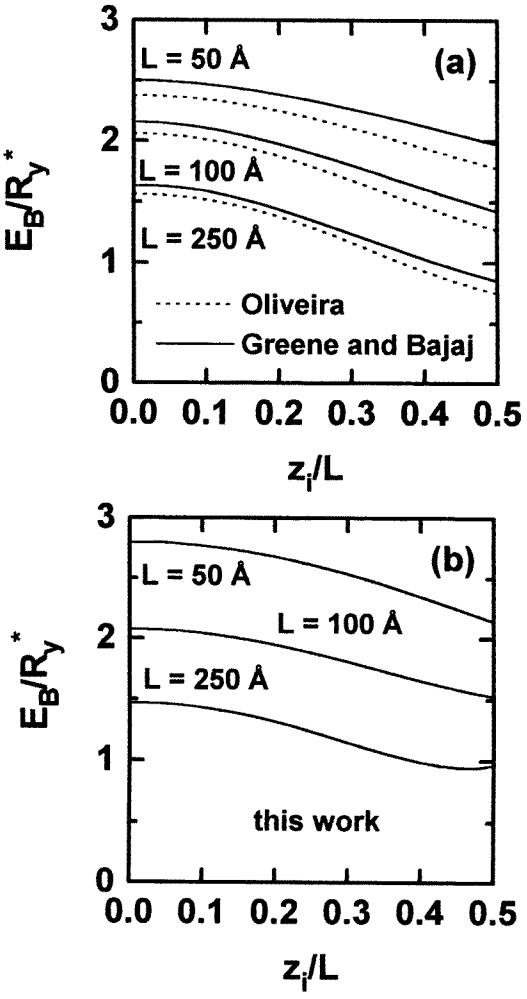

Figure 5. Impurity-position dependence of the donor binding energies in GaAs–$Ga_{1-x}Al_xAs$ QWs for three different GaAs well thicknesses and for a conduction-barrier potential of 323 meV. The dashed and solid curves in (a) are from Oliveira [25] (using a constant screening) and Greene and Bajaj [26], respectively, whereas the curves in (b) are calculated within the fractional-dimensional approach.

of QW widths $L = 0$ and infinite, although for small values of L the D parameter almost goes to two (the two-dimensional behaviour appropriate for small values of the width L), and it recovers as $L \to 0$ to the value $D = 3$ as the donor wave function penetrates the barrier and the system reduces to the appropriate three-dimensional barrier-bulk limit.

In the case of excitons, we used effective masses of 0.067 m_0 and 0.34 m_0, for the electron and hole, which give a value of 4.85 meV for the exciton effective Rydberg (we take the dielectric constant $\varepsilon_0 = 12.53$). For ideal infinite-barrier [23] QWs, we obtain values for the fractional-dimensional parameter D of 2.18 and 2.55 for reduced L/a^* well widths of 0.4 and 1.6, respectively, in very good agreement with the 2.20 and 2.49 results obtained by Lefebvre *et al* [21] via a comparison with a full calculation. For finite-barrier GaAs–(Ga, Al)As QWs, our results for the 1s exciton binding energy, within the

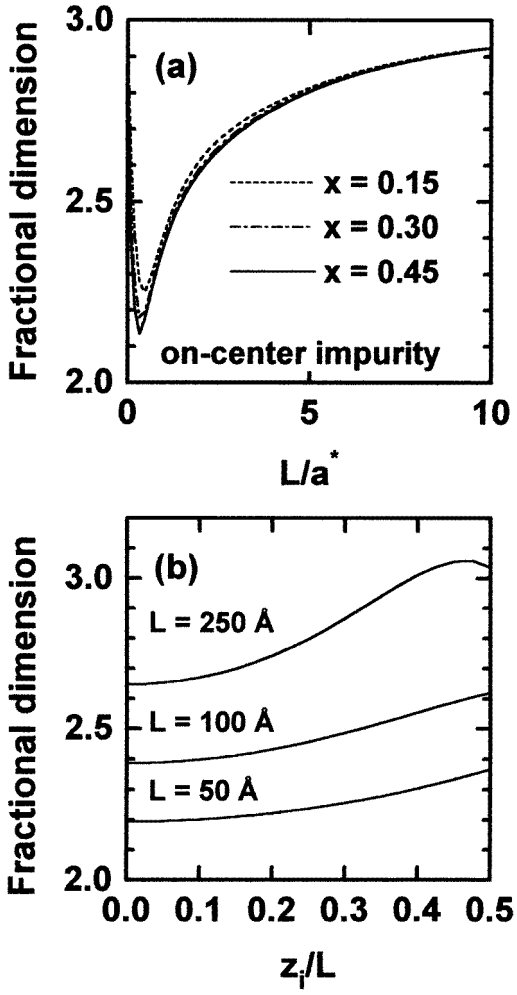

Figure 6. (a) Thickness dependence of the fractional-dimensional parameter corresponding to on-centre donors in GaAs–$Ga_{1-x}Al_xAs$ QWs for different x alloy compositions (as in figure 4(b)); (b) donor-position dependence of the fractional-dimensional parameter for three different GaAs well thicknesses and for a conduction-barrier potential of 323 meV (as in figure 5(b)).

fractional-dimensional scheme and for two values of the Al concentration, are presented in figure 7, and are in very good agreement with a full calculation by Andreani and Pasquarello [13]. Figure 8 presents a comparison between the exciton fractional-dimensional theoretical binding energies and data from two recent experiments, where the good agreement with the most recent experiment by Voliotis *et al* [16] is apparent.

4. Conclusions

Summing up, we have developed a *systematic and unambiguous procedure* for determining the fractional dimensionality of the isotropic effective space which would model and give the *exact* solution (8) for the energies of the actual physical system under consideration. Of

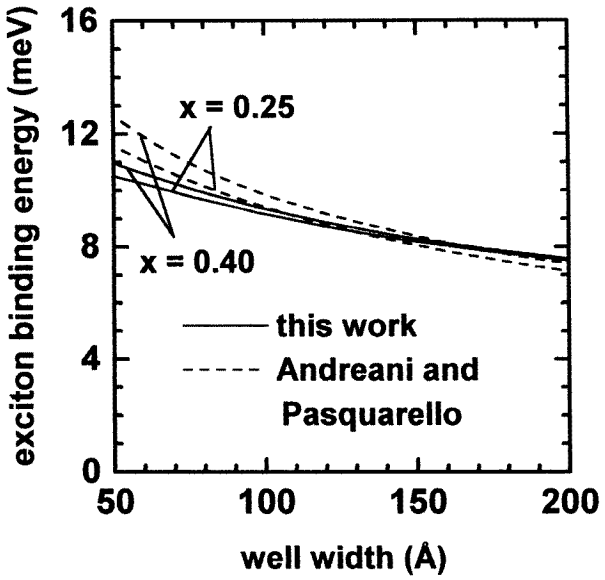

Figure 7. Exciton binding energies for GaAs–$Ga_{1-x}Al_xAs$ QWs as a function of the well width and for $x = 0.25$ and 0.40. The dashed curves are the theoretical results of a full calculation by Andreani and Pasquarello [13]. The solid curves were calculated within the fractional-dimensional approach.

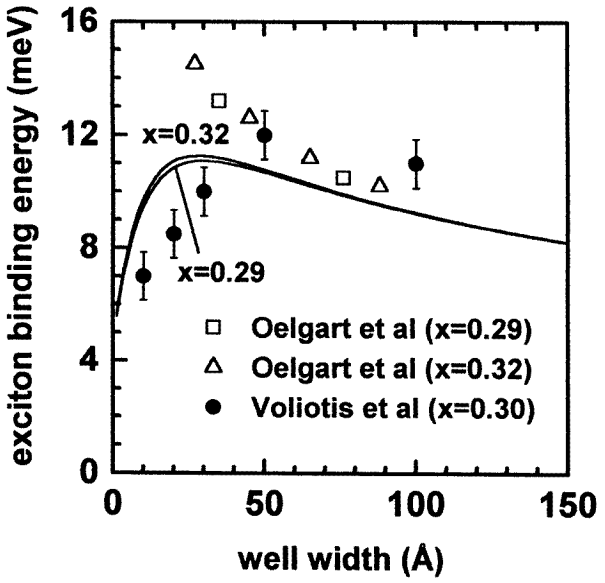

Figure 8. Exciton binding energies for GaAs–$Ga_{1-x}Al_xAs$ QWs as a function of the well width and for $x = 0.29$ and 0.32. The solid curves were calculated within the fractional-dimensional approach. Some experimental results of Oelgart *et al* [15] and Voliotis *et al* [16] are also shown.

course, although explicit calculations of the fractional-dimensional D parameter are made only in the case of excitons and impurities in finite-barrier QWs (with good agreement for

the exciton and impurity binding energies with previous variational results), our results may be readily generalized for other physical systems. One must stress that the study of excitons and impurities in QWs, QWWs, SLs, and semiconducting heterostructures in general, as well as absorption, optical, and photoluminescence properties such as lineshapes, etc, are readily obtained as straightforward applications of the above fractional-dimensional space approach on the physical properties of heterostructures.

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Appendix

The problem of an exciton confined in a semiconducting QW, within the effective-mass and parabolic band approximations, may be given by the Hamiltonian

$$\boldsymbol{H} = -\frac{\hbar^2}{2m_e}\nabla_e^2 - \frac{\hbar^2}{2m_h}\nabla_h^2 + V_e(z_e) + V_h(z_h) - \frac{e^2}{\varepsilon|\boldsymbol{r}_e - \boldsymbol{r}_h|} \tag{A.1}$$

where m_e and m_h are the effective masses of the electron and hole, respectively, and V_e and V_h are the confining potentials. The eigenfunction of (A.1) may be taken as $(\mathrm{e}^{\mathrm{i}\boldsymbol{K}\cdot\boldsymbol{R}}/\sqrt{S})\psi_E(\boldsymbol{\rho}, z_e, z_h)$, where S is the transversal area of the QW, $\boldsymbol{K}$ is the exciton in-plane wavevector, $\boldsymbol{\rho}$ is the xy relative coordinate, and $\boldsymbol{R}$ is the in-plane coordinate of the exciton centre of mass. One may write $\psi_E(\boldsymbol{\rho}, z_e, z_h) = f_e(z_e)f_h(z_h)\phi_E(\boldsymbol{\rho}, z_e, z_h)$, where f_e and f_h are the z-part of the electron and hole envelope wave functions, respectively, in the absence of the Coulomb potential, and find, after using (A.1) and assuming the relative motion of the carriers and that of the centre of mass are independent,

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 - \frac{e^2}{\varepsilon r}\right)\phi_E - \frac{\hbar^2}{2\mu}\frac{h'(z)}{h(z)}\frac{\partial\phi_E}{\partial z} = E\phi_E \qquad h(z) = \int_{-\infty}^{\infty} f_e^2(\xi)f_h^2(\xi - z)\,\mathrm{d}\xi \tag{A.2}$$

where μ is the reduced mass of the exciton, ε is the dielectric constant of the QW material, $z = z_e - z_h$, and E is the exciton energy with respect to $E_0 = E_g + E_{v,n=1} + E_{c,n=1}$, with E_g being the GaAs bulk gap, and $E_{v,n=1}$ ($E_{c,n=1}$) the confining (positive) energy of the top (bottom) of the first valence (conduction) subband. One may write (A.2), for $m = 0$ and in spherical coordinates, as $(H_D + W)\phi = E\phi$, where H_D and W are given by (2.5) and (2.6) with m^* substituted by μ. If one denotes by ϕ_j and E_j the eigenfunctions and eigenvalues of H_D, the exciton energy may be written in the form of (2.8), and one readily recovers (2.9). For evaluating the exciton ground-state binding energy, the fractional-dimensional parameter D may then be obtained if one takes ϕ_E as the 1s exciton ground-state solution of the D-dimensional Hamiltonian, and solves (2.9) for D.

References

[1] Esaki L and Tsu R 1969 *IBM Report* RC-2418
Esaki L and Tsu R 1970 *IBM J. Res. Dev.* **14** 61
[2] Bastard G 1981 *Phys. Rev.* B **24** 4714
[3] Greene R L and Bajaj K K 1985 *Solid State Commun.* **45** 825
[4] Mailhiot C, Chang Y-C and McGill T C 1982 *Phys. Rev.* B **26** 4449
[5] Tanaka K, Nagaoka M and Yamabe T 1983 *Phys. Rev.* B **28** 7068
[6] Fraizzoli S, Bassani F and Buczko R 1990 *Phys. Rev.* B **41** 5096

[7] Masselink W T, Chang Y-C and Morkoç H 1983 *Phys. Rev.* B **28** 7373
[8] Oliveira L E and Falicov L M 1986 *Phys. Rev.* B **34** 8676
[9] Latgé A, Porras-Montenegro N, de Dios-Leyva M and Oliveira L E 1996 *Phys. Rev.* B **53** 10 160 and references therein
[10] Bastard G, Mendez E E, Chang L L and Esaki L 1982 *Phys. Rev.* B **26** 1974
[11] Greene R L, Bajaj K K and Phelps D E 1984 *Phys. Rev.* B **29** 1807
[12] Pereira M F Jr, Galbraith I, Koch S W and Duggan G 1990 *Phys. Rev.* B **42** 7084
[13] Andreani L C and Pasquarello A 1990 *Phys. Rev.* B **42** 8928
[14] Leavitt R P and Little J W 1990 *Phys. Rev.* B **42** 11 774
[15] Oelgart G, Proctor M, Martin D, Morier-Genaud F, Reinhart F-K, Orschel B, Andreani L C and Rhan H 1994 *Phys. Rev.* B **49** 10 456
[16] Voliotis V, Grousson R, Lavallard P, Gourdon C and Planel R 1995 *22nd Int. Conf. on the Physics of Semiconductors (Vancouver, 1994)* vol 2, ed D J Lockwood (Singapore: World Scientific) p 1412
[17] Herrick D R and Stillinger F H 1975 *Phys. Rev.* A **11** 42
Stillinger F H 1977 *J. Math. Phys.* **18** 1224 and references therein
[18] He X-F 1987 *Solid State Commun.* **61** 53
He X-F 1990 *Phys. Rev.* B **42** 11 751
He X-F 1991 *Phys. Rev.* B **43** 2063
[19] Mathieu H, Lefebvre P and Christol P 1992 *J. Appl. Phys.* **72** 300
Mathieu H, Lefebvre P and Christol P 1992 *Phys. Rev.* B **46** 4092
[20] Lefebvre P, Christol P and Mathieu H 1992 *Phys. Rev.* B **46** 13 603
Lefebvre P, Christol P and Mathieu H 1993 *Phys. Rev.* B **48** 17 308
[21] Christol P, Lefebvre P and Mathieu H 1993 *J. Appl. Phys.* **74** 5626
Christol P, Lefebvre P and Mathieu H 1994 *IEEE J. Quantum. Electron.* **QE-30** 2287
Lefebvre P, Christol P, Mathieu H and Glutsch S 1995 *Phys. Rev.* B **52** 5756
[22] Zhao Q X, Monemar B, Holtz P O, Willander M, Fimland B O and Johannessen K 1994 *Phys. Rev.* B **50** 4476
[23] de Dios-Leyva M, Bruno-Alfonso A, Matos-Abiague A and Oliveira L E 1997 *J. Appl. Phys.* **82** at press
[24] Bastard G 1985 *J. Lumin.* **30** 488
[25] Oliveira L E 1988 *Phys. Rev.* B **38** 10 641
[26] Greene R L and Bajaj K K 1985 *Solid State Commun.* **53** 1103
[27] For donors, we assumed a 60% rule (used by Oliveira [25]) for the conduction-barrier potential with respect to the total band-gap difference, which was taken as ΔE_g (eV) $= 1.247x$, where x is the Al concentration; in the case of excitons, we followed Andreani and Pasquarello [13], and used a 65% rule.