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Exciton states and diamagnetic shifts in symmetric coupled double GaAs–$Ga_{1-x}Al_xAs$ quantum wells within the fractional-dimensional approach

A Matos-Abiague†‡, L E Oliveira§ and M de Dios-Leyva‡

† Departamento de Física, Universidad de Oriente, P Lumumba s/n, 90500, Santiago de Cuba, Cuba

‡ Department of Theoretical Physics, University of Havana, San Lazaro y L, Vedado, 10400, Havana, Cuba

§ Instituto de Física, Unicamp, CP 6165, Campinas, São Paulo, 13083-970, Brazil

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Abstract. We have extended the fractional-dimensional space approach to study exciton states and diamagnetic shifts in symmetric coupled double GaAs–$Ga_{1-x}Al_xAs$ quantum wells. In this scheme, the fractional dimension is chosen using an analytical procedure, and the real anisotropic 'exciton + double quantum well' semiconductor system is mapped, for each exciton state, into an effective fractional-dimensional isotropic environment. We have performed calculations within the fractional-dimensional space scheme for the binding energies of 1s-like heavy-hole direct excitons and for the energy difference between 1s- and 2s-like direct heavy-hole exciton states in GaAs–$Ga_{1-x}Al_xAs$ symmetric coupled double quantum wells. Also, theoretical results were obtained for the magnetic-field dependence of the 1s-like heavy-hole exciton energy shift and for the exciton diamagnetic coefficient in quantum wells and symmetric coupled double quantum wells. Fractional-dimensional theoretical results are shown to be in good agreement with available experimental measurements and previous theoretical calculations.

1. Introduction

Artificial low-dimensional electron systems, such as semiconductor heterostructures, are of considerable interest due to their interesting basic physical properties and use in a wide range of semiconductor devices. Of course, the study of the optical properties of semiconductor heterostructures provides information on the nature of confined electrons and holes, and is of relevance for potential application in optoelectronic devices. Excitons essentially dominate the optical properties of semiconductor systems [1–6]. In particular, the physical behaviour of coupled double quantum wells (CDQWs) is strongly related to their excitonic properties, and semiconductor CDQWs have been the subject of intense experimental [7–13] and theoretical [11, 14–17] investigations in the last decade or so.

Fox *et al* [8] have used photocurrent spectroscopy to measure the intrawell and interwell exciton splittings in GaAs–$Ga_{1-x}Al_xAs$ coupled QW structures. The mixing of symmetric and antisymmetric exciton states in GaAs–$Ga_{0.7}Al_{0.3}As$ symmetric coupled double quantum wells (SCDQWs) was investigated by Westgaard *et al* [9] by photoluminescence (PL) and photoluminescence excitation (PLE) spectroscopy. Zhao *et al* [10] used unpolarized and polarized PLE measurements to determine the 1s–2s splitting of symmetric heavy-hole excitons in GaAs–$Ga_{1-x}Al_xAs$ SCDQWs. The diamagnetic shift [5, 11, 18] for free excitons was obtained experimentally by Zhao *et al* [11] through PL studies for single quantum wells (SQWs) and CDQWs. Butov *et al* [12] studied direct and indirect magnetoexcitons in symmetric $In_xGa_{1-x}As$–GaAs coupled QWs by PL and PLE spectroscopy. Similar experimental studies in GaAs–$Ga_{1-x}Al_xAs$ superlattices were performed by Tartakovskii *et al* [13]. From the theoretical point of view, most work on exciton states in semiconductor CDQWs have used the effective-mass envelope function approach and variational procedures [8, 14–16]. Of particular interest for the present work is the theoretical study of Zhao *et al* [11], who have extended to semiconductor SCDQWs the fractional-dimensional space approach developed by Stillinger [19], He [20], Mathieu *et al* [21], and Lefebvre *et al* [22]. In this approach, the Schrödinger equation for a given anisotropic system is solved in a noninteger-dimensional space where the interactions are assumed to occur in an isotropic effective environment. This approach has been recently used with success in the understanding of a number of physical situations [23–25]. The essential quantity in this scheme is the fractional dimension associated with the effective medium and the degree of anisotropy of the real system under consideration. Recently, de Dios-Leyva *et al* [26–28] have proposed a systematic procedure to determine the appropriate fractional dimension of the isotropic space which would model the actual system, in the case of shallow impurities and exciton states in QWs and superlattices. As Zhao *et al* [11] have assumed a quite cumbersome *ansatz* for the fractional dimension in SCDQWs, we were motivated to extend our previous work [26–28] in QWs and superlattices within the fractional-dimensional space approach to the case of semiconductor SCDQWs.

In this work we are concerned with direct exciton states and diamagnetic shifts [5, 11, 18] in GaAs–$Ga_{1-x}Al_xAs$ SCDQWs within the fractional-dimensional space approach [19–28]. In section 2 the theoretical basis of the fractional-dimensional scheme, developed by de Dios-Leyva *et al* [26–28] for excitons and shallow impurities in QWs and superlattices, is extended to the case of GaAs–$Ga_{1-x}Al_xAs$ SCDQWs. Results and discussion are in section 3, and conclusions in section 4.

2. The fractional-dimensional space approach

We consider the problem of a direct exciton in a semiconductor GaAs–$Ga_{1-x}Al_xAs$ SCDQW (growth axis along the z-direction), within the effective-mass and non-degenerate-parabolic band approximations. The dielectric constant ε of the SCDQW is assumed constant throughout the heterostructure and equal to the 12.5 GaAs bulk value, and we use a 65% (35%) rule for the conduction- (valence-) barrier potential with respect to the total band-gap difference. Also, the effective masses were taken, in units of the free-electron mass, as $m_{ew} = 0.0665$, $m_{eb} = 0.0665 + 0.0835x$, $m_{hw} = 0.34$, and $m_{hb} = 0.34 + 0.42x$, in which w and b are labels for well and barrier, respectively, and e and h denote electron and heavy hole, respectively.

Within the fractional-dimensional scheme, the system 'exciton + semiconductor GaAs–$Ga_{1-x}Al_xAs$ SCDQW' may be realistically modelled by an equivalent isotropic hydrogenic system in a fractional D-dimensional space, a problem which may be solved analytically. The theoretical extension for GaAs–$Ga_{1-x}Al_xAs$ SCDQWs of the framework developed by Matos-Abiague *et al* [27] in the case of QWs is straightforward. For a given state of the anisotropic system, one may choose the D parameter in order to map the actual system into an equivalent isotropic D-dimensional space via the condition

$$\int hr^2 \sin\theta \phi_E^* W \phi_j \, \mathrm{d}r \, \mathrm{d}\theta = 0 \tag{2.1}$$

where we have used the same notation as Matos-Abiague *et al* [27], and now the confining potential is a SCDQW potential. The operator W is defined as the difference of the real

Hamiltonian and the fractional-dimensional approximate Hamiltonian, and is given (see [27]) in terms of the fractional dimension D and functions h and u which depend upon f_e and f_h (the z part of the electron and hole ground-state envelope wavefunctions for the SCDQW—see Thoai [29]):

$$h(z) = \int_{-\infty}^{\infty} f_e^2(\xi) f_h^2(\xi - z)\, \mathrm{d}\xi \tag{2.2a}$$

$$u(z) = \mu_w \int_{-\infty}^{\infty} \frac{f_e^2(\xi) f_h^2(\xi - z)}{\mu(\xi, z)}\, \mathrm{d}\xi \tag{2.2b}$$

with $\mu(\xi, z)$, for the case of a SCDQW, given by

$$\mu^{-1}(\xi, z) = \frac{1}{\mu_w} + \left(\frac{1}{m_{eb}} - \frac{1}{m_{ew}}\right)(\Theta[L_b/2 - |\xi|] + \Theta[|\xi| - (L_w + L_b/2)]) \\ + \left(\frac{1}{m_{hb}} - \frac{1}{m_{hw}}\right)(\Theta[L_b/2 - |\xi - z|] + \Theta[|\xi - z| - (L_w + L_b/2)]) \tag{2.2c}$$

where μ_w is the reduced mass of the exciton in the GaAs QW (L_b and L_w are the widths of the barrier and well regions of the SCDQW, respectively), and Θ is the Heaviside function. Notice that $\mu(\xi, z)$ is a kind of two variable-reduced effective mass calculated with the local electron and hole masses, which accounts for changes in the effective masses between barrier and well materials. Moreover, $u(z)/\mu_w$ may be interpreted as an average inverse reduced mass for a given electron–hole z separation with the confinement wavefunctions $f_{e,h}^2$ as weights, and this is a way to account for the broken translational invariance in the z direction. In (2.1), E is the direct exciton energy with respect to the bottom of the first SCDQW conduction subband, ϕ_E is associated with the exciton envelope wavefunction, and ϕ_j and E_j are the eigenfunctions and eigenvalues of the D-dimensional Hamiltonian [19, 20]. One should notice that equation (2.1) provides an analytical and systematic procedure for obtaining the D fractional-dimensional parameter associated with the ground and excited states of the actual anisotropic system. For evaluating the 1s-like direct exciton binding energy, which is associated with the ground state E_{1s}, as the ϕ_E exact solution is not known one chooses $\phi_E = \phi_{j=0}$ in equation (2.1), where $\phi_{j=0}$ is the 1s exact solution of the D-dimensional Hamiltonian, i.e. $\phi_{j=0} = \phi_{1s}(\boldsymbol{r}) = \mathrm{e}^{-\lambda r}$, with $\lambda = 2/[a_0^*(D-1)]$, where a_0^* is the effective heavy-hole exciton Bohr radius. One then obtains (from equation (2.1) and after some algebra) the following transcendental equation to be solved for the fractional-dimensional parameter D,

$$(2\beta - 3)L(\alpha) + G(\alpha) - \alpha \frac{\mathrm{d}[L(\alpha) + G(\alpha)]}{\mathrm{d}\alpha} = 0 \tag{2.3}$$

with

$$L(\alpha) = \int_0^{\infty} \mathrm{e}^{-\alpha z} h(z)\, \mathrm{d}z \tag{2.4}$$

$$G(\alpha) = \int_0^{\infty} \mathrm{e}^{-\alpha z} u(z)\, \mathrm{d}z \tag{2.5}$$

$\beta = 3 - D$, and $\alpha = 4/[a_0^*(D-1)]$. Once the D fractional dimension is obtained, the 1s-like heavy-hole exciton binding energies may then be obtained in a straightforward way through [19, 20] $E_B = 4/(D-1)^2\,\mathrm{Ryd}^*$, where Ryd^* is the exciton effective Rydberg. Finally, we would like to stress that, in the above scheme, the fractional dimension is chosen via an analytical procedure (cf equation (2.1)), and involves no *ansatz* [11, 21, 22], and no fitting with experiment [20, 23] or previous variational calculations [22]. Notice that, for excited states, one may choose for ϕ_E a linear combination of ϕ_j (properly orthonormalized with weight $h(z)$), and proceed in a similar way to obtain the appropriate D fractional-dimensional parameter.

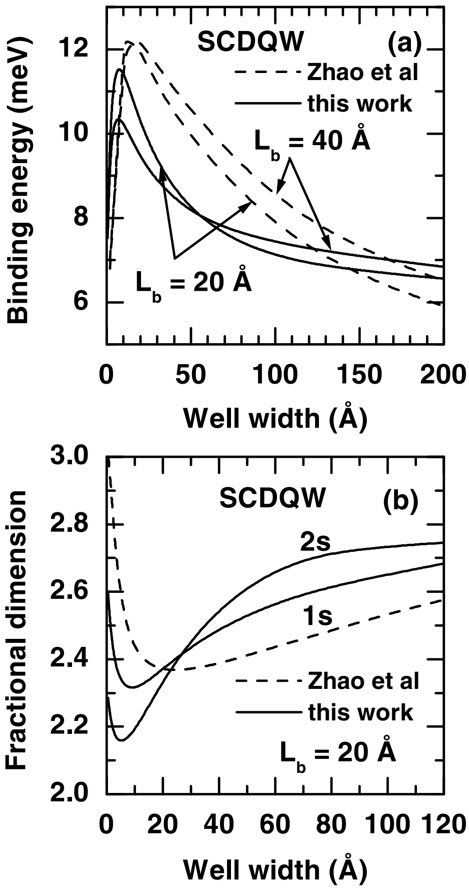

Figure 1. Well-width dependence of 1s-like binding energies (a) and fractional-dimensional parameters (b) for heavy-hole direct excitons in GaAs–$Ga_{0.7}Al_{0.3}As$ SCDQW heterostructures for fixed L_b barrier thicknesses. Fractional-dimensional parameters obtained in this work are shown for both the 1s-like and 2s-like exciton states. Full curves correspond to the present fractional-dimensional results, whereas dashed lines are the theoretical calculations by Zhao *et al* [11].

3. Results and discussion

Results in this section were then obtained following the procedure just discussed above. The direct 1s-like heavy-hole exciton binding energy was then obtained within the fractional-dimensional space approach (by using equation (2.3)), and our exciton theoretical results for GaAs–$Ga_{0.7}Al_{0.3}As$ SCDQW heterostructures are compared in figure 1(a) with the corresponding calculations by Zhao *et al* [11]. One should notice that our calculated exciton binding energies are significantly different from the results obtained by Zhao *et al* [11], who used an *ansatz* for the fractional dimension. We have also obtained the fractional dimension for 2s-like heavy-hole exciton states (using equation (2.1)), and our results for both the 1s- and 2s-like exciton states are compared with the fractional dimension *ansatz* by Zhao *et al* [11] in figure 1(b). Note that, in contrast with Zhao *et al* [11], we obtain different fractional-dimension parameters for different exciton states, as one would physically expect, since a given exciton wavefunction would 'see' different effective isotropic media, depending on its anisotropy and

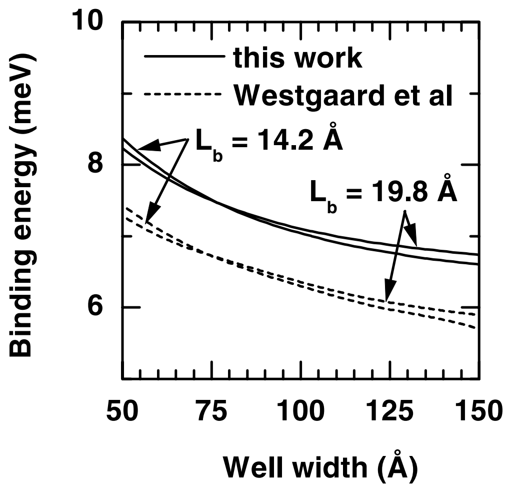

Figure 2. Binding energies for 1s-like heavy-hole excitons in GaAs–$Ga_{0.7}Al_{0.3}As$ SCDQWs with 14.2 Å or 19.8 Å barrier thicknesses (L_b) as functions of the GaAs well width. Full curves correspond to the present fractional-dimensional results whereas dashed lines are the variational calculations by Westgaard *et al* [9].

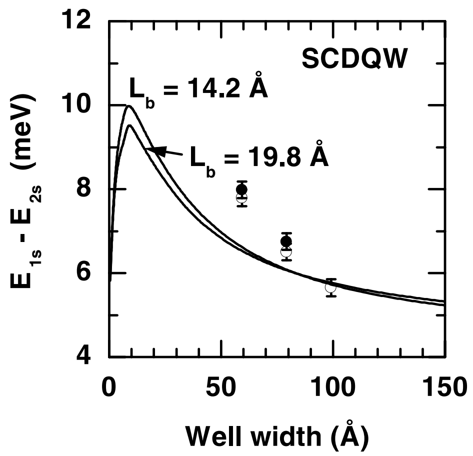

Figure 3. Energy difference between 1s- and 2s-like direct heavy-hole exciton states in GaAs–$Ga_{0.7}Al_{0.3}As$ SCDQWs as a function of the well width, for two different L_b barrier thicknesses. Full curves correspond to the present fractional-dimensional results, whereas open and full dots are experimental values for barrier thicknesses of 14.2 Å and 19.8 Å, respectively, by Zhao *et al* [11].

spatial extension. Also, one should notice that the crossing of the two calculated $L_b = 20$ Å and $L_b = 40$ Å GaAs–$Ga_{0.7}Al_{0.3}As$ SCDQW exciton binding energies occurs for a larger value of the SCDQW well width in our results than in the calculation by Zhao *et al* [11]. In order to further investigate this, we compare in figure 2, for two different SCDQW barrier widths, the fractional-dimensional 1s direct exciton present results for the binding energies with the calculated variational exciton binding energies by Westgaard *et al* [9] (without mixing of excitonic states), and apart from a small shift ($\leqslant 1$ meV), both calculations are in quite good agreement. Also note that, for an $L_b = 20$ Å SCDQW, results for the exciton binding

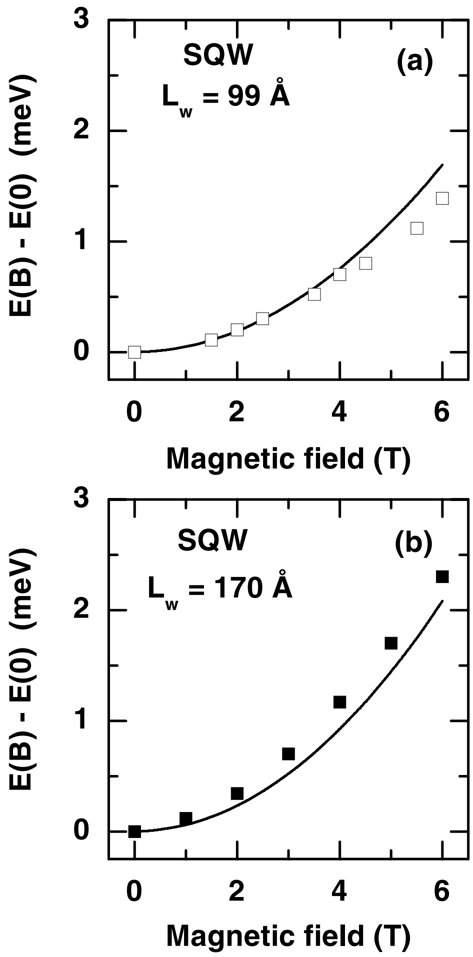

Figure 4. Fractional-dimensional theoretical results (solid curves) for the magnetic-field dependence of the 1s-like heavy-hole exciton energy shift for both a 99 Å wide GaAs–$Ga_{0.7}Al_{0.3}As$ SQW (a) and a 170 Å wide GaAs–$Ga_{0.77}Al_{0.23}As$ SQW (b). The corresponding experimental data are from Zhao *et al* [11] (open squares) and Aksenov *et al* [4] (full squares).

energies by Westgaard *et al* [9] are much smaller than the calculations by Zhao *et al* [11], in the available range of SCDQW well widths, in agreement with our fractional-dimensional results. Of course, as the present fractional-dimensional approach is not derived from an energy-minimum principle, one should bear in mind that having around 1 meV of 'additional binding energy' does *not* imply that we have a 'better' wavefunction than in the calculation by Westgaard *et al* [9].

The present fractional-dimensional results for the difference in energy between the 1s- and 2s-like direct heavy-hole exciton binding energies are shown in figure 3 in comparison with the experimental PLE measurements by Zhao *et al* [10, 11]. Although we obtain the same trend as in the experimental data, the agreement between theoretical calculations and experiment is only fair.

The fractional-dimensional approach may also be used to analyse the effect of applied magnetic fields on the exciton peak position in a PL or PLE experiment. The behaviour of

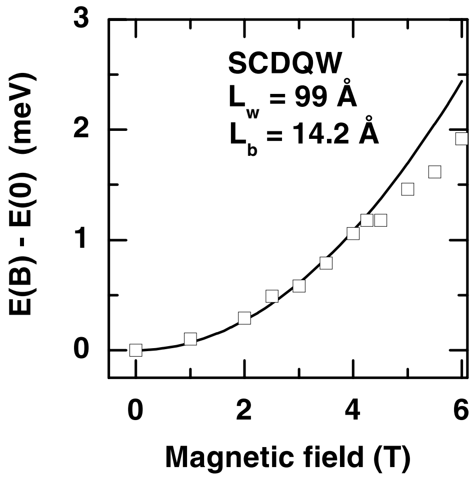

Figure 5. Magnetic-field dependence of the 1s-like heavy-hole exciton energy shift in a GaAs–$Ga_{0.7}Al_{0.3}As$ SCDQW with a 14.2 Å barrier and 99 Å wells. The solid line was calculated within the present fractional-dimensional approach whereas the open squares correspond to the experimental values by Zhao *et al* [11].

excitons in a magnetic field [1] depends very much on the strength of the applied field. In the low-field case, i.e. when the cyclotron energy of the electrons and holes is smaller than the exciton binding energy, the exciton shows a quadratic, diamagnetic energy shift [5, 6] with increasing magnetic field essentially given by [5], in the case of quantum wells under magnetic fields applied perpendicularly to the growth direction,

$$\Delta E(B) = \gamma B^2 \tag{3.1}$$

with

$$\gamma = \frac{e^2}{8\mu_w c^2}\langle\rho^2\rangle \tag{3.2}$$

where the expectation value of the square of the in-plane electron-hole separation is with respect to the *zero-magnetic-field* state and γ is the diamagnetic coefficient. On the other hand, in the high-field case the cyclotron energy of the electron–hole pair is larger than the exciton binding energy, and the cyclotron motion becomes dominant, leading to Landau levels for electrons and holes [2, 6]. Therefore, the field-produced energy shift of the exciton peak position becomes essentially linear in the field strength.

We have used the fractional-dimensional approach and equations (3.1) and (3.2) to evaluate the magnetic-field dependence of the 1s-like exciton diamagnetic shift for the case of two isolated GaAs–$Ga_{1-x}Al_xAs$ SQWs (cf figure 4), and a GaAs–$Ga_{0.7}Al_{0.3}As$ SCDQW with a 14.2 Å barrier and 99 Å wells (see figure 5). For the 170 Å wide GaAs–$Ga_{0.77}Al_{0.23}As$ SQW (figure 4(b)) we found good overall agreement with experimental data by Aksenov *et al* [4] in the range of magnetic-field strengths considered. In the case of the 99 Å wide GaAs–$Ga_{0.7}Al_{0.3}As$ SQW (figure 4(a)) and the GaAs–$Ga_{0.7}Al_{0.3}As$ SCDQW (figure 5), the agreement with measurements by Zhao *et al* [11] is quite good in the low-field regime, and, for a magnetic-field strength of $B \geqslant 4$ T, one finds a clear deviation from the quadratic diamagnetic shift. A similar behaviour was also very recently found by Jaschinski *et al* [6] in the case of $In_{0.53}Ga_{0.47}As$–InP QWs.

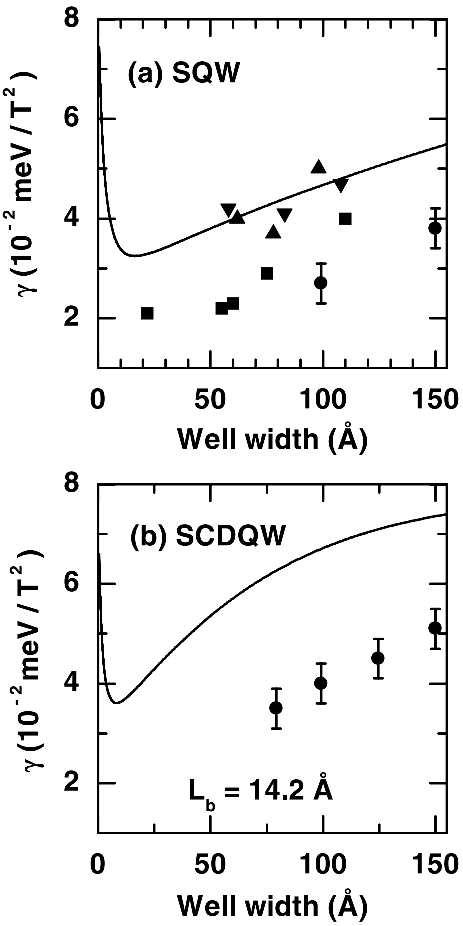

Figure 6. Well-width dependence of the 1s-like heavy-hole exciton diamagnetic coefficient for a GaAs–$Ga_{0.7}Al_{0.3}As$ SQW (a) and a 14.2 Å wide-barrier GaAs–$Ga_{0.7}Al_{0.3}As$ SCDQW (b). Fractional-dimensional results of the present work are presented as solid curves whereas experimental data are from Rogers *et al* [2] (full squares), Zhao *et al* [11] (full dots), Ossau *et al* [7] (up triangles) and Miura *et al* [7] (down triangles).

The well-width dependence of the 1s-like heavy-hole exciton diamagnetic coefficient γ (cf equations (3.1) and (3.2)) was evaluated for both GaAs–$Ga_{1-x}Al_xAs$ SQWs and SCDQWs, and theoretical fractional-dimensional results are shown in figure 6, in comparison with available experimental data [2, 7, 11]. The diamagnetic coefficient obtained by Zhao *et al* [11] was inferred from experimental measurements of the exciton peak energies and a fitting procedure with quadratic and linear terms in B. From the data by Zhao *et al* [11], it is straightforward to verify that a quadratic-only fitting would give larger values for the γ coefficient both in SQWs and SCDQWs than the ones displayed in figure 6. Moreover, the spread of 'experimental' diamagnetic coefficients from different studies is quite apparent, as already pointed out by Duggan [3]. Therefore, if one considers the uncertainty in the experimental determination of the diamagnetic coefficient, the agreement between calculated fractional-dimensional results and 'experimental' diamagnetic coefficients may be considered as fair. We have also evaluated the heavy-hole 1s-like exciton diamagnetic coefficient as a function of well width of GaAs–

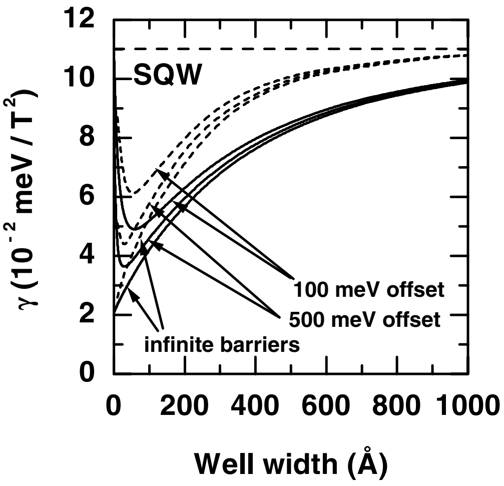

Figure 7. Heavy-hole 1s-like exciton diamagnetic coefficient as a function of well width of GaAs–$Ga_{1-x}Al_xAs$ SQWs for different values of the total (electron + hole) potential offset. The solid lines correspond to the present calculation whereas the dashed curves reproduce the theoretical results of Walck and Reinecke [5]. The bulk limit of 110.2 μeV T^{-2} is also shown as a horizontal dashed line.

$Ga_{1-x}Al_xAs$ SQWs for different values of the total electron + hole potential offset, and compared (see figure 7) the present theoretical fractional-dimensional calculations with the variational results by Walck and Reinecke [5]. Apart from a shift, the general trend is the same. Note that results from Walck and Reinecke [5] are larger than the ones obtained in the present work and much larger than the experimental results in figure 6(a). At the moment we do not know of a simple physical explanation of why the present fractional-dimensional results might be better than the variational calculations by Walck and Reinecke [5]. We believe, however, that the fractional-dimensional space approach may be extended to explicitly include magnetic-field effects in the Hamiltonian in both the cases of shallow-impurity and exciton states in GaAs–$Ga_{1-x}Al_xAs$ QWs and superlattices, and then one would obtain results beyond the quadratic magnetic-field dependence. The extension, however, is a non-trivial one, and work is in progress in that respect [30].

4. Conclusions

In conclusion, we have performed a quite detailed study of some properties of direct heavy-hole exciton states and diamagnetic shifts in semiconductor GaAs–$Ga_{1-x}Al_xAs$ QWs and SCDQWs. The fractional-dimensional space formalism was extended to the case of GaAs–$Ga_{1-x}Al_xAs$ SCDQWs. In this approach, the real anisotropic 'exciton + double QW' semiconductor system is modelled, for each exciton state, into an effective fractional-dimensional isotropic environment. In contrast to previous studies using the same fractional-dimensional scheme, in the present work the fractional dimension is chosen using an analytical procedure, and no *ansatz* or fitting with experiment is involved. Fractional-dimensional theoretical results were obtained for the binding energies of 1s-like direct heavy-hole excitons and the energy difference between 1s- and 2s-like direct heavy-hole exciton states in GaAs–$Ga_{1-x}Al_xAs$ SCDQWs. Theoretical results were also obtained for the magnetic-field dependence of the 1s-like heavy-hole exciton energy shift and the exciton diamagnetic coefficient in QWs and SCDQWs. Finally, fractional-dimensional theoretical results are shown to be in fair agreement with available experimental measurements.

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