Fractional-dimensional approach for excitons in GaAs-$Ga_{1-x}Al_xAs$ quantum wells

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The fractional-dimensional approach, in which the real semiconductor heterostructure system is substituted by an effective isotropic environment with a fractional dimension, was used in the study of ground and excited excitonic states in GaAs-(Ga,Al)As quantum wells. The fractional-dimensional formalism was extended to include the possibility of dealing with excited states and varying effective masses across the heterostructure interfaces, with the fractional dimension chosen in a systematic way. Theoretical fractional-dimensional results for ground-state 1*s*-like exciton states in GaAs-(Ga,Al)As quantum wells were shown to be in good agreement with previous detailed calculations and recent experimental measurements. Moreover, theoretical results within the fractional-dimensional scheme were found in excellent agreement with the recent experimental high-resolution spectroscopic studies on excited-exciton states of shallow GaAs-$Ga_{1-x}Al_xAs$ quantum wells with Al concentration in the range of 1–4.5 %. [S0163-1829(98)07828-X]

I. INTRODUCTION

In the past two decades, a great deal of work has been devoted to the understanding of the unique physics nature of the electronic, excitonic, and impurity properties of semiconductor heterostructures, such as quantum wells (QW's), quantum-well wires (QWW's), quantum dots (QD's), periodic and quasiperiodic semiconductor superlattices (SL's), etc. Such interest has arisen due to the wide range of potential device applications associated with these systems. In particular, due to their large binding energies, oscillator strengths, and confinement effects, excitons may have a large influence on a variety of physical phenomena observed in such heterostructures, and have attracted considerable attention from the experimental, theoretical, and technological points of view.[1–13]

Following the experimental work on excitonic properties by Miller *et al.*[1] in GaAs-(Ga,Al)As QW's, some theoretical and pioneering work,[2] using variational schemes, was performed in the calculation of binding energies of excitons in these systems. Photoluminescence excitation measurements[4–6] have provided information about the *s*-like excited states of the lowest confined exciton in GaAs-(Ga,Al)As QW's. Exciton binding energies in semiconductor SL's were theoretically investigated by Pereira Jr. *et al.*,[7] in which an anisotropic medium characterized by effective masses parallel and perpendicular to the plane of the layers was used. A quite accurate study of excitons in GaAs-(Ga,Al)As QW's was performed by Andreani and Pasquarello,[8] who included valence-band mixing, Coulomb coupling between excitons belonging to different subbands, nonparabolicity of the bulk conduction band, and the mismatch in dielectric constants between well and barrier materials. These effects were shown to be of comparable size and result in very high exciton binding energies, particularly in narrow QW's. A simple method for evaluating exciton binding energies in quantum-confined structures, although neglecting valence-band mixings, was proposed by Leavitt and Little.[9] More recently, a number of experimental works has been performed in GaAs-(Ga,Al)As QW's: excitonic transition energies,[10] excitons in both shallow[11] and narrow[12] QW's, and magnetic-field dependence of internal transitions of confined excitons[13] in GaAs-(Ga,Al)As QW's.

In the past decade, systematic studies, within the fractional-dimensional formalism,[14,15] have been performed on the optical spectra and excitonic properties of anisotropic heterostructure systems.[16–18] In the fractional-dimensional space approach, the Schrödinger equation is solved in a noninteger-dimensional space, where the interactions are assumed to occur in an isotropic effective environment, and the fundamental quantity is the fractional dimension associated with the effective medium and to the degree of anisotropy of the actual system. In particular, a systematic study has been done in the area of excitonic states and absorption spectra[16–18] in semiconductor QW's, QWW's, SL's, and double QW's, in which one assumes an *ansatz* for the fractional dimension D. Recently, de Dios-Leyva *et al.*[19] have proposed a systematic procedure to determine the appropriate fractional dimensionality of the isotropic-effective space that would model the real system, and it was successfully used in the study of some excitonic and shallow-impurity properties. Also, the fractional-dimensional formalism has been recently applied in the understanding of exciton properties by Thilagam[20] and in the study of the complex dielectric constant by Tanguy *et al.*[21]

The recent experimental measurements on the 1*s*-like ex-

citon binding energies[10–12] and the high-resolution spectroscopic studies[11] with information on excited exciton states of shallow GaAs-$Ga_{1-x}Al_xAs$ QW's with Al concentration in the range of 1–4.5 % have motivated the present theoretical work. In what follows, we extend previous work[19] on the fractional-dimensional scheme in order to include varying effective masses across the heterostructure interfaces, and to take into account both ground and excited states. We emphasize that in this procedure the D fractional-dimensional parameter is chosen in a systematic way and would depend on the exciton state under consideration, as different exciton wave functions would experience different effective media. Within that fractional-dimensional scheme, one is then able to obtain, in a very simple way and with quite good accuracy, the $1s-$ and $2s$-like exciton energies in good overall agreement with available[10–12] experimental data. Also, this procedure avoids either an *ansatz* for the D fractional-dimensional parameter or *a priori* variational estimation of the exciton binding energy that involves tedious and extensive numerical work.

The work is organized as follows. In Sec. II we present the theoretical framework of the fractional-dimensional scheme used in the calculations, together with a systematic procedure to be used in the determination of the fractional dimension D for both ground and excited states. Theoretical results are compared with experiment in Sec. III, and conclusions are in Sec. IV.

II. THEORETICAL FRAMEWORK

We consider the problem of an exciton confined in a semiconductor GaAs-(Ga,Al)As QW (growth axis along the z direction), within the effective-mass and nondegenerate-parabolic band approximations. The Hamiltonian for the exciton may be given by

$$\mathbf{H}=-\frac{\hbar^2}{2}\nabla_e\cdot\left(\frac{1}{m_e(z_e)}\nabla_e\right)-\frac{\hbar^2}{2}\nabla_h\cdot\left(\frac{1}{m_h(z_h)}\nabla_h\right)+V_e(z_e)+V_h(z_h)-\frac{e^2}{\varepsilon|\mathbf{r}_e-\mathbf{r}_h|},\tag{2.1}$$

where m_e and m_h are the z-dependent (barrier or well) effective masses of the electron and hole, respectively, and V_e and V_h are the confining potentials. The eigenfunction of Eq. (2.1) may be taken as $e^{i\mathbf{K}\cdot\mathbf{R}}/\sqrt{S}\psi_E(\boldsymbol{\rho},z_e,z_h)$, where S is the transversal area of the QW, $\mathbf{K}$ is the exciton in-plane wave vector, $\boldsymbol{\rho}$ is the xy relative coordinate, and $\mathbf{R}$ is the in-plane coordinate of the exciton center 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 Eq. (2.1) and assuming the relative motion of the carriers and that of the center of mass are independent,

$$\left(-\frac{\hbar^2}{2\mu_w h(z)}\nabla\cdot[u(z)\nabla]-\frac{e^2}{\varepsilon r}\right)\phi_E=E\phi_E,\tag{2.2}$$

with

$$h(z)=\int_{-\infty}^{\infty}f_e^2(\xi)f_h^2(\xi-z)d\xi,\tag{2.3}$$

$$u(z)=\mu_w\int_{-\infty}^{\infty}\frac{f_e^2(\xi)f_h^2(\xi-z)}{\mu(\xi,z)}\,d\xi,\tag{2.4}$$

$$\mu^{-1}(\xi,z)=\frac{1}{\mu_w}+\left(\frac{1}{m_{eb}}-\frac{1}{m_{ew}}\right)\Theta[|\xi|-L_w/2]+\left(\frac{1}{m_{hb}}-\frac{1}{m_{hw}}\right)\Theta[|\xi-z|-L_w/2],\tag{2.5}$$

where μ_w is the reduced mass of the exciton in the well, b and w are labels for the barrier and well (of width L_w) regions, respectively, Θ is the Heaviside function, ε is the dielectric constant of the QW material (taken as the value for bulk GaAs and constant throughout the heterostructure), $z=z_e-z_h$, 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.[22] One may write Eq. (2.2), for $m=0$ and in spherical coordinates, as

$$(H_D+W)\phi=E\phi,\tag{2.6}$$

where H_D and W are given by

$$H_D=-\frac{\hbar^2}{2\mu_w}\left[\frac{1}{r^{D-1}}\frac{\partial}{\partial r}\left(r^{D-1}\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin^{D-2}(\theta)}\frac{\partial}{\partial\theta}\left(\sin^{D-2}(\theta)\frac{\partial}{\partial\theta}\right)\right]-\frac{e^2}{\varepsilon r},\tag{2.7}$$

and

$$W=-\frac{\hbar^2}{2\mu_w h(z)}\left[\left(\frac{\beta u(z)}{r}+\frac{\partial u(z)}{\partial r}\right)\frac{\partial}{\partial r}+\frac{1}{r^2}\left(\beta u(z)\cot\theta+\frac{\partial u(z)}{\partial\theta}\right)\frac{\partial}{\partial\theta}\right]+\frac{\hbar^2}{2\mu_w}\left(1-\frac{u(z)}{h(z)}\right)\left[\frac{1}{r^{D-1}}\frac{\partial}{\partial r}\left(r^{D-1}\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin^{D-2}(\theta)}\frac{\partial}{\partial\theta}\left(\sin^{D-2}(\theta)\frac{\partial}{\partial\theta}\right)\right],\tag{2.8}$$

with $\beta=3-D$ and $z=r\cos\theta$.

One should note that Eq. (2.6) is exact, and depends on a D parameter that was introduced for convenience. Also, note that the Hamiltonian (2.7) corresponds to the $m=0$ hydrogen Hamiltonian in a fractional D-dimensional space, a problem which may be solved analytically.[14,15] If one denotes as ϕ_j and E_j the eigenfunctions and eigenvalues of Eq. (2.7), i.e.,

$$H_D\phi_j=E_j\phi_j,\tag{2.9}$$

the exciton binding energy may be written, after some straightforward algebraic manipulation of Eqs. (2.6) and (2.9), as

$$E = E_j + \frac{\int hr^2 \sin\theta \phi_E^* W \phi_j dr d\theta}{\int hr^2 \sin\theta \phi_E^* \phi_j dr d\theta}, \tag{2.10}$$

where ϕ_E is the corresponding exciton eigenfunction. One should notice that Eq. (2.10) is still exact, and valid for any value of the D fractional-dimensional parameter and for arbitrary pairs of (ϕ_E, E) and (ϕ_j, E_j).

If one now is interested in evaluating the exciton binding energy, which is associated with the $1s$-like ground state E_{1s}, one may choose the D parameter such that the second term in the right-hand side of Eq. (2.10) is zero for ϕ_j chosen as the ground state associated with Eq. (2.6), so that both ground states coincide. The condition for D is therefore that

$$\int hr^2 \sin\theta \phi_E^* W \phi_j dr d\theta = 0, \tag{2.11}$$

with ϕ_E being the ground-state solution of Eq. (2.6). One should stress that the above equation provides an exact expression for determining the dimension of the D fractional-dimensional space that would model the actual system in the case of obtaining the exciton ground-state solution. Similar conditions could be obtained for the D parameters that could be used for obtaining any energies of the excited states of the actual physical system under consideration. Of course, the solutions ϕ_E of Eq. (2.6) are not known, and approximate values for the fractional-dimensional parameter D may be obtained if one uses approximate solutions for ϕ_E. One 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 Eq. (2.7)], use Eq. (2.11) to find D, and obtain the ground-state exciton energy of the problem under consideration by solving the D-dimensional equivalent Hamiltonian. One would expect that this simple choice would give an appropriate physical solution for the ground-state exciton energy, provided that the actual system is not strongly anisotropic. In practice, therefore, the fractional-dimensional parameter D may be obtained, as a first approximation, if one takes ϕ_E as the $1s$ exciton ground-state solution of the D-dimensional Hamiltonian, and solves Eq. (2.11) for D. For excited states, one may choose for ϕ_E a linear combination of ϕ_j [properly orthonormalized with weight $h(z)$, which follows from Eq. (2.2)], and proceed in a similar way to obtain the appropriate D fractional-dimensional parameter.

III. RESULTS AND DISCUSSION

The solutions of Eq. (2.11) for the D fractional-dimensional parameter may then be obtained, as explained above, and the binding energies of excitons in GaAs-(Ga,Al)As QW's may be obtained through[16,17]

$$E_B = \frac{R_y^*}{\left[n + \dfrac{D-3}{2}\right]^2}, \tag{3.1}$$

where R_y^* is the effective Rydberg (with the exciton reduced-effective mass of the well material).

Theoretical results for the fractional-dimensional parameter D, in the case of $1s$- and $2s$-like heavy-hole excitons are displayed in Fig. 1, as functions of the GaAs-(Ga,Al)As QW width, and compared with the ansatz used by Mathieu, Lefebvre, and Christol.[16] Notice that, in contrast to the previous fractional-dimensional studies,[16–18] the D fractional-dimensional parameter we use (within the exact procedure described above), for a given heterostructure, would depend on the exciton state under consideration, as one should expect, as different wave functions ''see'' different effective media. Of course, it is clear from Fig. 1, that one recovers the obvious three-dimensional limit in both cases of extremely narrow and large QW widths. Notice that the D parameter of the $2s$-like exciton state is larger than that of the $1s$-like state for wide wells, whereas $D(2s)$ is almost equal to 2 [and much smaller than $D(1s)$] for narrow QW's. We believe the result for narrow QW's is due to the fact that the $2s$-like state (with naturally larger extension) is more ''compressed'' by the QW barrier.

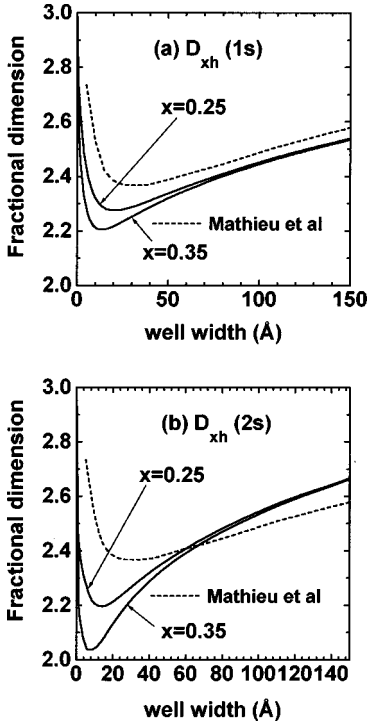

FIG. 1. Well-width dependence of the fractional-dimensional parameter corresponding to a confined HHl-CBl exciton in GaAs-$Ga_{1-x}Al_xAs$ QW's for the $1s$-like ground state (a) and $2s$-like state (b). Dashed curves are from Mathieu, Lefebvre, and Christol (Ref. 16) for $x = 0.25$.

The fractional-dimension heavy-hole $1s$-like exciton results of this work, for the binding energies in GaAs-(Ga,Al)As QW's, are shown in Fig. 2(a), and compared with the detailed calculation of Andreani and Pasquarello.[8] Figure 2(b) shows our results, compared with the theoretical values of Mathieu, Lefebvre, and Christol[16] (results for $x = 0.3$ by Mathieu, Lefebvre, and Christol[16] were obtained via a linear interpolation for the value of x from results in their Fig. 6) and with experimental measurements by Oelgart *et al.*,[10] Sanders and Chang,[3] and Voliotis *et al.*[12] One notices in Fig. 2(a) that the fractional-dimensional exciton binding energies with the effects of the effective-mass mismatches[20] are, for narrow QW's, in better agreement with the predictions by Andreani and Pasquarello[8] than the calculation with constant effective masses throughout the QW, and are both in quite

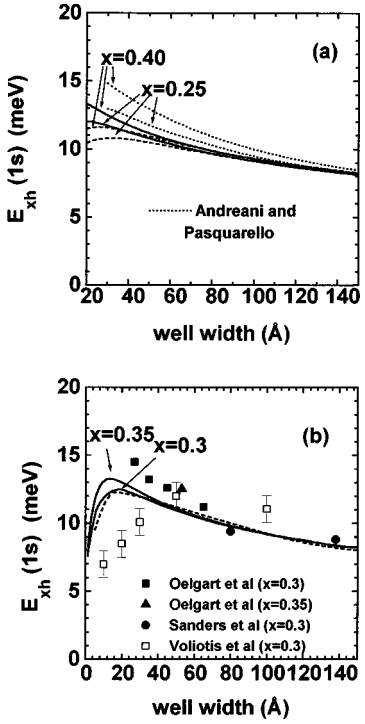

FIG. 2. (a) Heavy-hole exciton binding energies as a function of the width of GaAs-$Ga_{1-x}Al_xAs$ QW's, for different Al concentrations. Fractional-dimensional results of this work: dashed curves obtained using constant GaAs effective masses throughout the heterostructure, whereas solid curves take into account the effective-mass mismatches. Dotted lines correspond to theoretical results by Andreani and Pasquarello (Ref. 8); (b) Well-width dependence of the fractional-dimensional heavy-holes exciton binding energies (full curves; this work) together with the experimental data from Oelgart *et al.* (Ref. 10), Sanders and Chang (Ref. 3), and Voliotis *et al.* (Ref. 12). Dashed line is the theoretical result for $x=0.3$ by Mathieu, Lefebvre, and Christol (Ref. 16) (linear interpolation for the value of x from results in their Fig. 6).

good agreement with the values of Andreani and Pasquarello[8] for large values of the QW width. Also, the overall agreement between our calculated fractional-dimensional exciton results and experimental measurements[10–12] is quite apparent in Fig. 2(b), if one considers the large spread in the experimental data. We have also evaluated, within the fractional-dimensional scheme, the $2s$-like excited heavy-hole exciton energy in GaAs-$Ga_{0.65}Al_{0.35}As$ QW's as a function of the well width, and our results for the energy difference $E_{xh}(1s)-E_{xh}(2s)$ between the $1s$ and $2s$ heavy-hole exciton states are in quite good agreement with both the available experimental measurements[1,4–6] and the accurate calculations of Andreani and Pasquarello,[8] as displayed in Fig. 3, which also shows the theoretical results (dotted line) obtained by Mathieu, Lefebvre, and Christol.[16] Notice that the results in Figs. 2(b) and 3 by Mathieu, Lefebvre, and Christol[16] agree not less satisfactorily with experimental data than those of this work, although their calculations are based on an *ansatz* for the D fractional-dimensional parameter.

In order to quantitatively understand the recent experimental high-resolution spectroscopic studies by Simmonds *et al.*[11] with information on excited exciton states of shallow multiple large-barrier 200-Å GaAs-$Ga_{1-x}Al_xAs$ QW's with

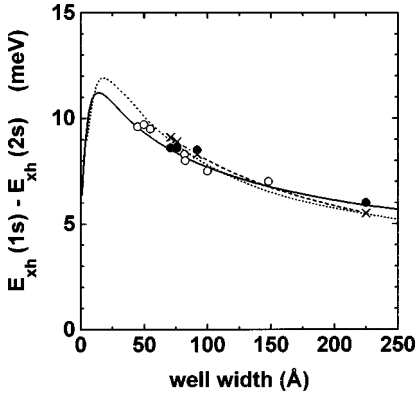

FIG. 3. Energy difference between $1s$ and $2s$ states of the heavy-hole exciton in GaAs-$Ga_{0.65}Al_{0.35}As$ QW's as a function of the well width. The solid curve corresponds to our fractional-dimensional results, the dotted line is the theoretical result by Mathieu, Lefebvre, and Christol, and crosses (dashed line is a guide for the eye) are the theoretical results by Andreani and Pasquarello (Ref. 8). Open dots are the experimental results by Miller *et al.* (Ref. 1), and full dots are the experimental data by Dawson *et al.* (Ref. 4), Reynolds *et al.* (Ref. 5), and Molenkamp *et al.* (Ref. 6).

Al concentration in the range of 1–4.5 %, we have calculated, within the fractional-dimensional scheme, both the $1s$- and $2s$-like heavy-hole exciton energies for 200-Å GaAs-(Ga,Al)As QW's in the range of Al concentrations appropriate for comparison with the experimental data. Results are displayed in Fig. 4, and compared with the experimental and

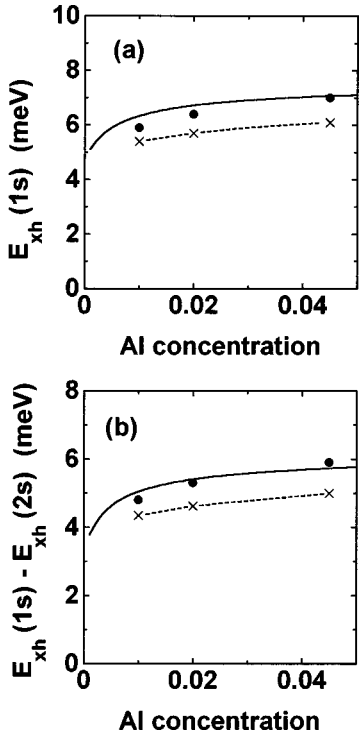

FIG. 4. Al-concentration dependence of the $1s$-like heavy-hole exciton (a) and energy difference between $1s$-like and $2s$-like heavy-hole excitons (b) in 200-Å GaAs-$Ga_{1-x}Al_xAs$ QW's. Full curves correspond to fractional-dimensional results, whereas crosses (dashed line is a guide for the eye) and full dots are the theoretical and experimental values, respectively, by Simmonds *et al.* (Ref. 11).

theoretical values of Simmonds *et al.*[11] One should notice the signature of quasi-two-dimensionality in the strong enhancements in the 1*s*-like exciton heavy-hole binding energies even for very low $Ga_{1-x}Al_xAs$ barrier heights. Also, Fig. 4 makes clear the excellent agreement between our fractional-dimensional theoretical results and the experimental values of Simmonds *et al.*[11]

IV. CONCLUSIONS

In summary, we have used the fractional-dimensional approach, in which the real semiconductor heterostructure system is substituted by an effective isotropic environment with a fractional dimension, in the study of ground and excited excitonic states in GaAs-(Ga,Al)As QW's. The fractional dimensional formalism, in which the fractional dimension is chosen[19] in a systematic way, was extended to include the possibility of dealing with excited states and varying effective masses across the heterostructure interfaces. It is shown that different exciton states would experience different effective media through different fractional dimensionalities. Fractional-dimensional results for 1*s*-like exciton states in GaAs-(Ga,Al)As QW's were shown to be in quite good agreement with previous *ansatz*-based fractional-dimensional calculations,[16] detailed[8] theoretical results,[8] and available experimental measurements.[3–6,10–12] Moreover, the present theoretical results within the fractional-dimensional scheme were found in excellent agreement with the recent experimental high-resolution spectroscopic studies by Simmonds *et al.*[11] on excited-exciton states of shallow GaAs-$Ga_{1-x}Al_xAs$ QW's with Al concentration in the range of 1–4.5 %.

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[22] We follow Andreani and Pasquarello (Ref. 8), and take a GaAs dielectric constant $\varepsilon = 12.53$, and a 65% (35%) rule for the conduction (valence)-barrier potential with respect to the total band-gap difference, which was taken as $\Delta E_g\ (\mathrm{eV}) = 1.247x$, where x is the Al concentration. 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. Unless otherwise stated, all theoretical results in this work take into account the effect of effective-mass mismatches.