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E. Reyes-Gómez, L. E. Oliveira, and M. de Dios-Leyva

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Shallow impurities in semiconductor superlattices: A fractional-dimensional space approach

E. Reyes-Gómez
Departamento de Física, ISPJAE, Calle 127 s/n, Marianao, 19390, Havana, Cuba

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

M. de Dios-Leyva
Department of Theoretical Physics, University of Havana, San Lazaro y L, Vedado, 10400, Havana, Cuba

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A thorough detailed study of donor and acceptor properties in doped GaAs–(Ga,Al)As semiconductor superlattices is performed within the fractional-dimensional approach, in which the real anisotropic ''impurity+semiconductor superlattice'' system is modeled through an effective isotropic environment with a fractional dimension. In this scheme, the fractional-dimensional parameter is chosen via an analytical procedure and involves no *ansatz*, and no fittings either with experiment or with previous variational calculations. The present fractional-dimensional calculated results for the donor and acceptor energies in GaAs–(Ga,Al)As semiconductor superlattices are found in quite good agreement with previous variational calculations and available experimental measurements. © *1999 American Institute of Physics.* [S0021-8979(99)04408-4]

I. INTRODUCTION

Semiconductor heterostructures, such as quantum wells, quantum-well wires, quantum dots, and superlattices (SLs), are unique man-made systems with physical phenomena not typically accessible in naturally occurring solids. In particular, the understanding of the role played by impurities in semiconductor heterostructures is an area of considerable scientific and technological relevance. For example, the prospects for building physical devices based on selectively doped semiconductor heterostructures opens up a number of possibilities in the development of semiconductor systems with prescribed properties appropriate for technological applications. Shallow-impurity properties in GaAs–(Ga,Al)As quantum wells have been extensively studied in the last few years,[1–8] whereas theoretical and experimental work in GaAs–(Ga,Al)As doped-semiconductor SLs have received considerably less attention.[9–12]

Lane and Greene[9] have studied the effects of finite-width barriers upon the binding energies of shallow donor states in GaAs–(Ga,Al)As SLs, by using an expansion in Gaussian functions for the variational donor envelope wave functions. Results of their calculations have shown that, for the ground state, the strongest effects occur for donor impurities near the semiconductor interfaces or within the barrier regions, whereas the lowest excited states can show relatively large effects due to neighboring wells for all donor locations. The vertical transport in semiconductor GaAs–(Ga,Al)As SLs probed by miniband-to-acceptor magnetoluminescence was studied by Skromme *et al.*[10] in magnetic fields up to 13 T, applied either parallel or perpendicular to the layers, with experimental results obtained for SLs with different ratios of well to barrier widths. Also, Helm *et al.*[11] have performed a far-infrared spectroscopy study of minibands and confined donors in lightly doped GaAs–(Ga,Al)As SLs, together with a variational calculation via hydrogenic-like functions for the impurity trial wave functions, and found good agreement between experiment and theory. Moreover, Ivchenko and Kavokin[12] have used the miniband effective-mass approximation and allowed for nonparabolicity effects in the calculation of the donor binding energy in short-period SLs, and obtained qualitative agreement with results reported by Lane and Greene.[9]

In the last few years, a simple method, based on the concept of fractional-dimensional space,[13] has emerged and been successfully used in the study of the excitonic and impurity properties, and the optical spectra of anisotropic semiconducting heterostructures.[14–22] 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. In this scheme, the fundamental quantity is the parameter D that defines the fractional dimension associated to the effective medium and to the degree of anisotropy of the interactions. In particular, a systematic work has been made in the study of excitonic states and absorption spectra[14–17] in semiconductor quantum wells, quantum-well wires, SLs, and double quantum wells, in which one assumes an *ansatz* for the choice of the fractional dimension. Moreover, the fractional-dimensional formalism has been recently[18] applied in the understanding of some exciton-complex properties and in the study of the complex dielectric constant of low-dimensional structures. Recently, de Dios-Leyva *et al.*[19–21] have proposed a systematic and unambiguous procedure to

[a]Electronic mail: oliveira@ifi.unicamp.br

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determine the appropriate fractional dimensionality of the isotropic-effective space which would model the real semiconductor-heterostructure system, and it has been successfully used in the study of some excitonic and shallow-impurity properties in semiconductor quantum wells.

This work is concerned with an extension of the fractional-dimensional scheme in order to include periodicity and barrier-penetration tunneling effects in the study of shallow-impurity properties in semiconductor SLs. Within the fractional-dimensional scheme, one is able to obtain, in a very simple way and with quite good accuracy, the ground-state impurity binding energies in good overall agreement with available[9–11] theoretical and experimental data. Also, this procedure avoids either an *ansatz* for the D fractional-dimensional parameter or a prior variational calculation of the impurity binding energy that would involve previous and extensive numerical work.

The work is organized as follows. In Sec. II we present the theoretical framework of the fractional-dimensional scheme appropriate for the study of impurity properties of semiconductor SLs. Theoretical results are compared with previous theoretical work and experimental data in Sec. III, and conclusions are in Sec. IV.

II. THEORETICAL FRAMEWORK

In this work, we are concerned with the properties of a shallow impurity in a semiconductor GaAs–(Ga,Al)As SL, grown along the z direction. We adopt a parabolic-band scheme, and consider the impurity located at the position z_i in the SL. Both the dielectric constant ϵ of the SL material and the conduction- (or valence-) band effective mass m^* of the impurity carrier are assumed constant throughout the heterostructure and equal to the GaAs bulk value.

Within the fractional-dimensional scheme, the system ''shallow impurity+semiconductor SL'' may be realistically modeled by an equivalent isotropic hydrogenic system in a fractional D-dimensional space, a problem which may be solved analytically. The theoretical extension for SLs of the framework developed by de Dios-Leyva *et al.*[20] in the case of quantum wells 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

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

where we have used the same notation as de Dios-Leyva *et al.*,[20] except that now the confining potential is a SL potential, and $f(z)$ is the periodic electron (hole)-envelope wave function[11] corresponding to the bottom (top) of the first conduction (valence) miniband for the SL in the absence of the Coulomb potential (the functions W and h are defined[20] in terms of f and the parameter D). In the above, E is the shallow-impurity energy [with respect to the bottom (top) of the first conduction (valence) miniband], ϕ_E is the corresponding impurity eigenfunction, and ϕ_j and E_j are the eigenfunctions and eigenvalues of the D-dimensional Hamiltonian H_D.

As an application, if one is interested in evaluating the impurity binding energy, which is associated with the $1s$-like ground-state energy E_{1s}, one chooses $\phi_E = \phi_{j=0}$ in Eq. (2.1), where $\phi_{j=0}$ is the $1s$ ground-state exact solution of the D-dimensional Hamiltonian, i.e., $\phi_{j=0} = \phi_{1s}(\mathbf{r}) = e^{-\lambda \mathbf{r}}$, with $\lambda = 2/[a_0^*(D-1)]$, where a_0^* is the effective impurity Bohr radius. One then obtains [from Eq. (2.1)] the following transcendental equation to be solved for the fractional-dimensional parameter D,

$$(\beta-1)L(\alpha,z_i) - \alpha \frac{dL(\alpha,z_i)}{d\alpha} = 0, \tag{2.2}$$

where $\alpha = 2\lambda$, $\beta = 3-D$, and

$$L(\alpha,z_i) = \int_0^\infty [h(z_i+r) + h(z_i-r)] e^{-\alpha r} \, dr, \tag{2.3}$$

or, equivalently,

$$L(\alpha,z_i) = \frac{1}{(1-e^{-\alpha d})} \int_0^d [h(z_i+r) + h(z_i-r)] e^{-\alpha r} \, dr, \tag{2.4}$$

where d is the SL period. Once the fractional-dimensional parameter is obtained, the impurity binding energies may then be obtained in a straightforward way through[13,14] $E_B = 4/(D-1)^2 \, \mathrm{Ry}^*$, where Ry^* is the impurity effective Rydberg, either for donors or for acceptors. Finally, we would like to stress that, in the above scheme, the fractional-dimensional parameter D is chosen via an analytical procedure [cf. Eq. (2.1)], and involves no *ansatz*-based[15,16] fractional dimension, or fitting with experiment[22] or previous variational calculations.[16] Of course, the procedure proposed here is not aimed to compete with some very accurate variational schemes; rather, it is intended to provide a simple and physical procedure which gives quite satisfactory agreement with both experimental and variational results, and avoids tedious computer calculations.

III. RESULTS AND DISCUSSION

As a first application of the fractional-dimensional scheme to impurities in a semiconductor SL, we consider the ground state of a donor impurity in a periodic GaAs–(Ga,Al)As SL. The periodic dependence of the ground-state binding energy with the impurity position in the semiconductor SL is clearly seen in Fig. 1. Also, a strong dispersion follows due to the large SL period ($d = 4a_0^*$) as compared with the effective-donor size $a_0^* \approx 100$ Å. On the other hand, when calculations are performed for well and barrier widths small compared with the effective Bohr radius, the donor-position dependence of the binding energy is flat, reflecting the three-dimensional character of the ''donor+SL'' system. Of course, the impurity binding energy is larger for donors at the well center (cf. Fig. 1), as expected due to the larger confinement of the donor-electron wave function. A larger confinement (due to the anisotropy caused by the SL potential) than in the isotropic hydrogen three-dimensional (3D) case corresponds to a fractional-dimensional parameter $D < 3$, as is the typical case of donors confined within the GaAs well, i.e., anisotropic situations with a ''larger-than-

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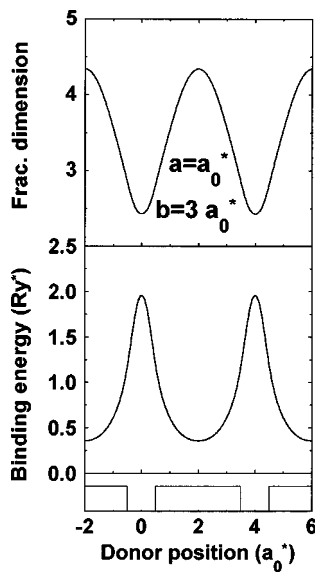

FIG. 1. Fractional-dimensional parameter and $1s$-like ground-state donor binding energy for a periodic GaAs–$Ga_{0.7}Al_{0.3}As$ superlattice with well width $a=a_0^*$ and barrier $b=3\ a_0^*$, where a_0^* is the donor-effective Bohr radius. The superlattice potential profile is shown schematically at the bottom.

isotropic'' 3D confinement lead to an ''effective'' isotropic medium with dimension $D<3$. On the other hand, for donors at the barrier region, the donor-electron wave function becomes partially trapped in the well region (far from the impurity nucleus) leading to a smaller confinement (and binding energy) than in the 3D situation, and to a fractional-dimensional parameter $D>3$, i.e., anisotropic situations with a ''smaller-than-isotropic'' 3D confinement lead to an effective isotropic medium dimension $D>3$.

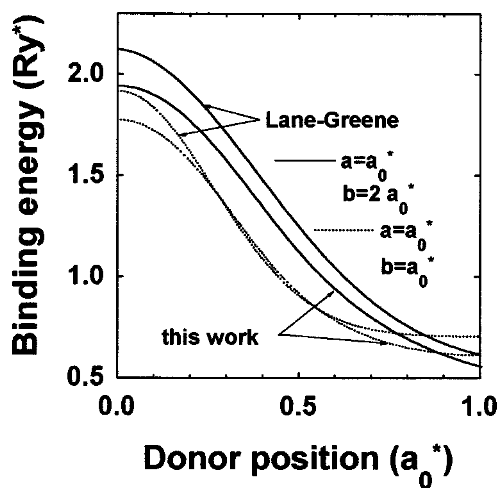

FIG. 2. Ground-state donor binding energies calculated within the fractional-dimensional formalism vs impurity position for a periodic GaAs–$Ga_{0.7}Al_{0.3}As$ superlattice with well width a and barrier b; full curves are for $a=a_0^*$ and $b=2\ a_0^*$, whereas dotted lines are for $a=b=a_0^*$, where a_0^* is the donor-effective Bohr radius. Also shown are the theoretical results by Lane and Greene (see Ref. 9). The position is measured from the GaAs well center (at $z=0$), and $z_i=0.5\,a_0^*$ corresponds to the well-barrier interface.

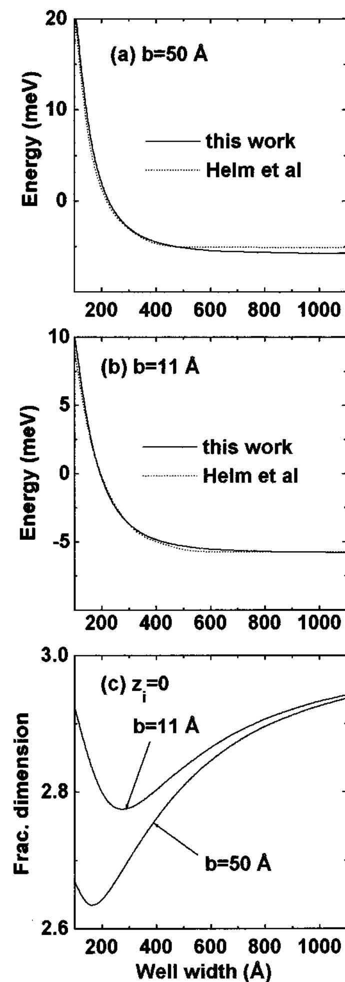

FIG. 3. Well-width dependence of the fractional-dimensional theoretical results (full curves) for the ground-state donor energy levels of an impurity in the center of a GaAs quantum well in a periodic GaAs–$Ga_{0.7}Al_{0.3}As$ superlattice with barrier widths $b=50$ Å [(a)] and $b=11$ Å [(b)]. Results by Helm *et al.* (see Ref. 11) are shown as dotted lines; (c) displays the fractional-dimensional parameter. The origin of energies is taken at the bottom of the conduction band of bulk GaAs.

The overall agreement between theoretical results for the position-dependent donor binding energies within the fractional-dimensional approach and those obtained by Lane and Greene[9] via a variational procedure (by using an expansion in Gaussian functions for the donor envelope wave function) is clear from Fig. 2 for two different GaAs–(Ga,Al)As SLs. Fractional-dimensional theoretical results for both the well- and barrier-width dependences of the well-centered ($z_i=0$) donor energies in GaAs–(Ga,Al)As SLs are also found in quite good agreement with the work by Helm *et al.*,[11] who used hydrogenic-like functions for the variational donor envelope wave functions, as indicated in Figs. 3 and 4. Notice [cf. Fig. 3(c)] that for large well widths, the system ''donor+SL'' exhibits essentially a three-dimensional behavior, whereas for decreasing well widths, as the donor wave function is increasingly confined, the system dimension diminishes up to a limiting well width for which the wave function begins to rapidly increase its penetration into the barrier, and the system dimension increases with the eventual recovery of the three-dimensional behavior. Of

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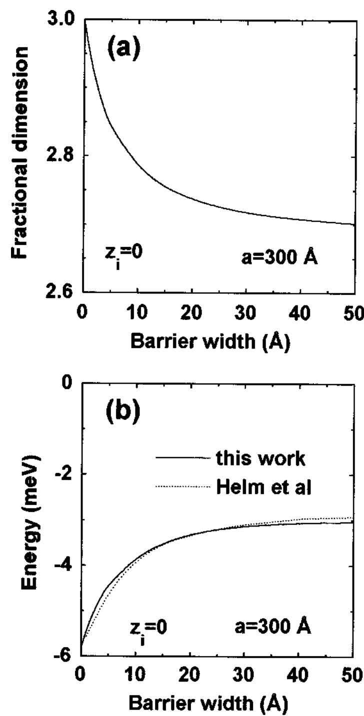

FIG. 4. Barrier-width dependence of the fractional-dimensional theoretical results (full curves) for the fractional-dimensional parameter [(a)] and ground-state donor energy levels [(b)] of an impurity in the center of a GaAs quantum well in a periodic GaAs–$Ga_{0.7}Al_{0.3}As$ superlattice with well width $a=300$ Å. Results by Helm *et al.* (see Ref. 11) are shown as dotted lines in (b). Origin of energies is taken at the bottom of the conduction band of bulk GaAs.

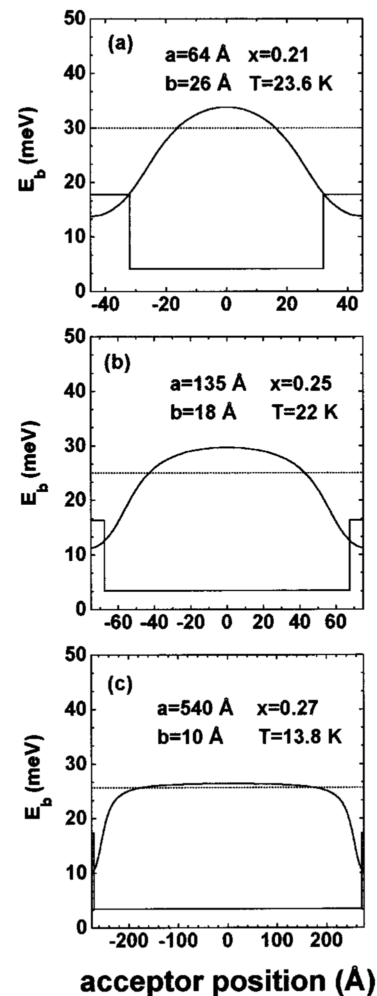

FIG. 5. Ground-state acceptor binding energies (full curves) within the fractional-dimensional formalism as a function of impurity position for various GaAs–(Ga,Al)As superlattices. Dotted lines correspond to the acceptor binding energies associated to the peak position in the photoluminescence measurements by Skromme *et al.* (see Ref. 10). The superlattice potential profile is also shown (not in scale).

course, in the small-barrier case ($b=11$ Å), the tunneling is more effective and the system dimension start to increase for a larger value of the well width than in the case of a wider barrier ($b=50$ Å). A similar analysis may be done in Fig. 4(a), where one sees that, for a fixed well width, the system dimension increases up to the three-dimensional limit for diminishing widths of the barrier, as the donor wave function tunneling becomes more effective.

We have also performed calculations for three different acceptor-doped GaAs–(Ga,Al)As SLs studied by Skromme *et al.*[10] via miniband-to-acceptor magnetoluminescence. We used the fractional-dimensional approach to calculate the impurity-position dependence of the acceptor binding energies in GaAs–(Ga,Al)As SLs, and compare our theoretical results with the experimental measurements by Skromme *et al.*,[10] in the case of vanishing applied magnetic field (see Fig. 5). One should notice that the experimental[10] (dotted lines) acceptor binding energies, obtained after taking into account the temperature-dependent[23] GaAs band gap and both the conduction and valence minibands confinement energies, fall within the calculated acceptor band, as one would expect. Of course, a detailed quantitative account of the experimental data should involve a full calculation of the acceptor-related (conduction miniband to acceptor transitions) photoluminescence line shape, together with the actual acceptor distribution along the SL and temperature effects on the population of acceptor states. Nevertheless, the present fractional-dimensional calculated profile of acceptor binding energies provides a clear physical picture of the zero-magnetic field experimental measurements. For the wider 540 Å well [Fig. 5(c)], the barrier is small enough that most of the acceptors essentially behave as ''bulk'' well-centered acceptors, and the experimental binding energy agrees very well with the well-centered calculated acceptor binding energy. On the other hand, when tunneling effects become important [Figs. 5(a) and 5(b)], the profile of the acceptor distribution becomes important and transitions to off-well-centered acceptors obviously begin to contribute to the photoluminescence line shape.

IV. CONCLUSIONS

In conclusion, we have performed a quite detailed study of some donor and acceptor properties in doped GaAs–(Ga,Al)As semiconductor SLs, within the fractional-dimensional approach. In this scheme, the actual anisotropic ''impurity+semiconductor SL'' system is modeled by an effective isotropic environment with a fractional dimension. In contrast to previous studies using the same scheme, the

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fractional-dimensional parameter D is chosen via an analytical procedure, and involves no *ansatz*-based[15,16] fractional dimension, or fitting with previous variational[16] calculations, or experimental fitting.[22] In that sense, the present work extends and complements our previous calculations[19–21] involving excitons and impurities in semiconductor quantum wells. Finally, the present fractional-dimensional results for the donor and acceptor energies are in quite good agreement with previous variational calculations and experimental measurements, when available.

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