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Shallow donors in semiconductor heterostructures: Fractal dimension approach and the variational principle

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We propose a simple method for calculating the energies of the shallow donor *S* states in semiconductor heterostructures. The trial function is taken as a product of the wave equation for an unbound electron in the heterostructure corresponding to the lowest level with a variational function that depends only on electron-ion separation. Starting from variational principle, we find that the latter is a solution of the radial wave equation for a hydrogen-like atom in an effective space with a non-power-law dependence of the Jacobian volume element on the ion-electron separation. By using the relation between the Jacobian volume element and the dimension of the space similar to the one proposed by Mandelbrot for fractal geometric objects, we find that the fractional dimension is related with the density of charge distribution for the electron ground state within the heterostructure. An excellent agreement between our results for donor binding energies in GaAs-(Ga,Al)As quantum wells, quantum well wires (QWW's), and quantum dots with a square-well potential and those previously obtained by means of the variational, Monte Carlo, and series-expansion methods is found when we use the fractal dimension defined locally. Additionally, donor binding energies curves versus GaAs-(Ga,Al)As QWW radius, for models with soft-edge-barrier and double-step potentials are presented.

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I. INTRODUCTION

In the past two decades the theoretical analysis of the low-dimensional systems have attracted a great deal of attention[1–11] due to the technological progress in the generation of semiconductor structures, such as quantum wells (QW's), wires (QWW's), dots (QD's), and superlattices (SL's). The strong quantum-confinement effect produced on bound carriers (donor and acceptor impurities, excitons, etc.) in these structures widen the range of possibilities for electro-optical and electronic devices. The electronic spectra of shallow donor impurities in low-dimensional systems have been studied theoretically by using the variational,[1–6] series-expansion,[7] perturbative,[8] dimension scaling,[9] trigonometric sweep[10] and Monte Carlo[11] methods.

Several advances in the interpretation of experimental results and the theoretical calculations have been reached within the framework of the fractional-dimensional space approach in which the anisotropic interactions in a three-dimensional environment are treated as isotropic in an effective fractional-dimensional space and the value of the fractional dimension D (only parameter used in this theory) is associated with the degree of anisotropy of the actual three-dimensional system.[12–18] This approach was first applied to analyze solid-state problems by He[12] who, using the hydrogen-like Hamiltonian in effective fractional space proposed by Stillinger,[13] treated the interband optical transitions and bound excitons in strongly anisotropic semiconductors. Lefebvre and co-workers[14,15] applied this method to analyze the exciton energy states and the absorption spectra in GaAs/Ga$_{1-x}$Al$_x$As QW's and QWW's, considering D as a phenomenological parameter related to the heterostructure geometry. They proposed a formula that relates the fractional dimension to the average electron-hole distance within the heterostructure in the unbound state by a simple exponential law. A different method to determine the appropriate fractional dimension for D^0, in QW's, QWW's, QD's, and SL's by fitting the ground-state energy of the isotropic hydrogenic model in the fractional-dimensional space to an actual three-dimensional system has been proposed recently in a series of theoretical works of Oliveira and co-workers.[17,18]

In the last decade, the model of the fractional-dimensional space has been successfully used to describe shallow donor, exciton properties, absorption spectra, and the exciton-phonon interaction in semiconductor heterostructures.[12,14–18] However, as it was established previously,[18] this simple approach breaks down when the confinement or the magnetic field become too strong.[18] Moreover, the discrepancy between the calculation results for the D^0 binding energies in narrow QWW's and QD's and other theoretical calculations is more significant than the one in a QW.[18] A possible reason for these difficulties consists of the fact that the charge density in the heterostructures presents a complicated object whose exact value of the dimension may not be absolutely well defined.

The concept of the fractional dimension was first introduced by Mandelbrot,[19] who studied different geometric objects with self-similar structure and gave them name exact fractals. The formula proposed by Mandelbrot for the fractional dimension gives the same value for all parts of the self-similar objects. In contrast, the charge density within a heterostructure has not self-similar structure and therefore its exact dimension may be well defined only locally. From this point of view the fractional-dimension approach proposed by He[12] should be considered as an approximation in which the dimension of the effective space is defined only on the average.

In this paper, we propose a general variational procedure which we call fractal-dimension method. In this method, we consider the charge density within a semiconductor heterostructure as a fractal object and try to find the relation between the shape of this object and its local fractional dimension starting from the variational principle. By using the method of the functional derivation, we found that the problem of a donor in any semiconductor heterostructure can be reduced to a simple problem of a hydrogen-like atom in an isotropic space with a non-power-law dependence of the radial part of the Jacobian volume element on the ion-electron distance. In our formalism, the local noninteger dimension D^* appears in a natural form and can be found directly by using the fractal-dimension definition of Mandelbrot.[19] This paper is organized as follows. In Sec. II, we describe the fractal-dimension method. In Sec. III, we compare our results with the corresponding calculations by using the variational,[5,20,21] fractional-dimensional,[17,18] Monte Carlo,[11] and series-expansion[7,22] methods. A summary of the results and conclusions are presented in Sec. IV.

II. THE FRACTAL-DIMENSION METHOD FOR ONE-PARTICLE PROBLEMS

A. Donor impurities in semiconductor heterostructures

We consider the problem of a neutral donor impurity in the center of a semiconductor GaAs-(Ga,Al)As heterostructure (such as a QW, QWW, QD, or a SL) in the presence of an uniform magnetic field. Within the effective-mass and nondegenerate parabolic band approximations, the Hamiltonian for the donor can be written as

$$H=\frac{1}{2m^*}\left[\vec{p}+\frac{e}{c}\vec{A}\right]^2-\frac{e^2}{\varepsilon r}+V(\vec{r}), \tag{1}$$

where $V(\vec{r})$ is the confining potential. The material parameters m^*, the conduction-band effective mass and ε, the dielectric constant of the semiconductor heterostructure are assumed to be uniform throughout the heterostructure. The values of the physical parameters pertaining to GaAs ($m^*=0.067m_0$, and $\varepsilon=12.53$, where m_0 is the free-electron mass) are used in our calculations.[3] We choose the vector potential $\vec{A}=\frac{1}{2}(\vec{B}\times\vec{r})$, and the magnetic field $\vec{B}$ oriented along the z axis, so that the Hamiltonian (1) for the impurity S states may be written in cylindrical coordinates[2] as

$$\hat{H}=\hat{H}_0-\frac{2}{r}, \tag{2a}$$

$$\hat{H}_0=-\nabla^2+\tilde{V}(\vec{r}), \tag{2b}$$

$$\tilde{V}(\vec{r})=V(\vec{r})+\frac{1}{4}\gamma^2\rho^2. \tag{2c}$$

Here, we have introduced the effective Bohr radius $a_0^*=\varepsilon\hbar/m^*e^2$ as the unit of length, the effective Rydberg $R_y^*=e^2/2a_0^*\varepsilon$ as the energy unit, and $\gamma=e\hbar B/2m^*cR_y^*$ as the dimensionless unit of the magnetic-field strength. The ground-state wave function $f_0(x,y,z)$, for a free electron confined in the heterostructure corresponding to the lowest energy E_0 can be found as the solution of the eigenvalue problem

$$\hat{H}_0 f_0(x,y,z)=E_0 f_0(x,y,z). \tag{3}$$

If the heterostructure has a particular symmetry (for example, axial for a QW and QWW or spherical for a QD) then the Hamiltonian $\hat{H}_0$ becomes separable and the three-dimensional problem (3) can be solved exactly. On the contrary, the Schrödinger equation for the donor impurity (bound electron)

$$\hat{H}\Psi(\vec{r})=E\Psi(\vec{r}), \tag{4}$$

does not completely separate if the symmetry of the two terms on the right side of Eq. (2a) does not coincide. It is, therefore, of interest to eliminate the one-particle potential in the Schrödinger equation (4) by using the following substitution:

$$\Psi(\vec{r})=f_0(x,y,z)\Phi(\vec{r}), \tag{5}$$

where $\Phi(\vec{r})$ is a function that describes the properties of the intrinsic electron bound state. Substituting Eqs. (2) and (5) in Eq. (4) and taking into account the relation (3) one obtains an equation for $\Phi(\vec{r})$,

$$\hat{H}_{ren}\Phi(\vec{r})=(E-E_0)\Phi(\vec{r}), \tag{6a}$$

$$\hat{H}_{ren}=-\frac{1}{P_0(\vec{r})}\vec{\nabla}[P_0(\vec{r})\vec{\nabla}]-\frac{2}{r}, \tag{6b}$$

$$P_0(\vec{r})=f_0^2(\vec{r}), \tag{6c}$$

where the renormalized Hamiltonian $\hat{H}_{ren}$ does not include explicitly both the confinement potential and the external field. In general, Eq. (6a) corresponds to a central force problem for hydrogen-like atom in an anisotropic and nonhomogeneous space with $P_0(\vec{r})$ being the charge density in the heterostructure that defines the dimension of the effective space. It can clearly be seen that the renormalized Schrödinger equation (6) can be written as a variational problem of the following functional:

$$F[\Phi]=\int\left\{[\vec{\nabla}\Phi(\vec{r})]^2-\left(\frac{2}{r}-E_b\right)\Phi^2(\vec{r})\right\}f_0^2(\vec{r})d\vec{r}$$
$$\to\min,\qquad E_b=E_0-E. \tag{7}$$

Let us consider as an example a QW where the ground-state wave function $f_0(x,y,z)$ for a free electron depends only on coordinate z:

$$F[\Phi]=\int_{-\infty}^{\infty} f_0^2(z)dz\int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}\left[\left(\frac{\partial\Phi}{\partial x}\right)^2+\left(\frac{\partial\Phi}{\partial y}\right)^2+\left(\frac{\partial\Phi}{\partial z}\right)^2 -\left(\frac{2}{r}-E_b\right)\Phi^2\right]dy\to\min. \tag{7a}$$

It is seen that for small electron-donor separations, $(r\to 0)$ the Jacobian, $f_0^2(z)$ in this expresion can be considered as a constant, and the expression (7a) coincides with the functional for the three-dimensional hydrogen-like atom. On the other hand, as $r\to\infty$ the Jacobian can be approximated by a δ funcion, $f_0^2(z)\approx\delta(z)$, and the expression (7a) transforms into the functional for a two-dimensional hydrogen-like atom. Since the dimensionality of the charge density varies from 3 in the center of the QW to 2 in the barriers it can be defined only locally. To derive a formula for locally defined fractional dimension one should analyze in more detail the structure of the Jacobian factor in the functional (7) which controls the dimensionality of the effective space.

B. Radial part of the Jacobian volume element

It should be noted that $\hat{H}_{ren}$ is separable only if the symmetry of the two terms on the right-hand side of Eq. (6b) coincides, i.e., for heterostructures with a spherical symmetry (e.g., a spherical QD in the zero-magnetic-field case). In the other cases (such as QW's, QWW's, and SL's), the Hamiltonian $\hat{H}_{ren}$ is nonseparable and the exact equation (6a) does not provide any advantage in comparison with the initial eigenvalue problem (4). Hence, to simplify the problem, we have to approximate the first term in the Hamiltonian (6b) by one with spherical symmetry. In this way, we propose to replace the exact wave function (5) by the following approximation:

$$\Psi(\vec{r})=f_0(\vec{r})\overline{\Phi}(r), \tag{8}$$

where the unknown isotropic function $\overline{\Phi}(r)$ should be interpreted as the mean value of the exact function $\overline{\Phi}(\vec{r})$ averaged over all the directions. The representation of the trial function in the form (8) is valid only for donor S states and in what follows we will be considering only the donor states which correspond to this symmetry.

This approximation permits us to simplify the expression (7) which after integrating over all angles can be rewritten as

$$F[\overline{\Phi}]=\int_0^{\infty}J(r)\left\{\left[\frac{d\overline{\Phi}(r)}{dr}\right]^2-\frac{2}{r}\overline{\Phi}^2(r)+E_b\overline{\Phi}^2(r)\right\}dr \to\min,\qquad \frac{\delta F[\overline{\Phi}]}{\delta\overline{\Phi}}=0, \tag{9}$$

where $\delta/\delta\overline{\Phi}$ denotes the functional derivative and $J(r)$ is the radial part of the Jacobian volume element related to the radial charge probability distribution $P(r)$ by means of the formula

$$J(r)=r^2P(r), \tag{9a}$$

$$P(r)=\int_0^{2\pi}d\varphi\int_0^{\pi}\sin\theta d\theta f_0^2 \times(r\sin\theta\cos\varphi, r\sin\theta\sin\varphi, r\cos\theta). \tag{9b}$$

Here, the value $r^2P(r)dr$ is the probability of finding an unbound electron within a spherical shell of radii r and $r+dr$.

Calculating the functional derivative, one can obtain the Euler-Lagrange equation for the envelope function $\overline{\Phi}(r)$ that minimizes the functional (9):

$$\hat{\overline{H}}_{red}\overline{\Phi}(r)=-E_b\overline{\Phi}(r), \tag{10a}$$

$$\hat{\overline{H}}_{red}=-\frac{1}{J(r)}\frac{d}{dr}\left[J(r)\frac{d}{dr}\right]-\frac{2}{r}, \tag{10b}$$

$$E_b=E_0-E. \tag{10c}$$

Of course, the solution of Eq. (10) defines an approximated value of the donor binding energy E_b and a wave function that is not exact, but *it is the best among all the functions presented in the form* (8). The reduced wave equation (10) describes a hydrogen-like atom in an effective space with a variable dimension. Such an interpretation arises from the property of orthogonality of the eigenfunctions $\overline{\Phi}_n(r)$ of the self-conjugate equation (10) for different S states:

$$\int_0^{\infty}\overline{\Phi}_n(r)\overline{\Phi}_m(r)J(r)dr=\int\overline{\Phi}_n(r)\overline{\Phi}_m(r)dV=\delta_{n,m}. \tag{11}$$

It should be noted that the relation (11) together with the definition of the radial part of the Jacobian volume element (9a) provides automatically the orthogonality of all trial functions $\Psi_n(\vec{r})=f_0(\vec{r})\overline{\Phi}_n(r)$ corresponding to different donor S states. In Eq. (11), $dV=J(r)dr$ represents the volume element in the functional effective space and $J(r)$ can be considered as the frontier-surface area of an infinitesimal spherical shell of radii r and $r+dr$ in this space. For example, for one-, two-, and three-dimensional homogeneous spaces, the function $J(r)$ will be equal to 1, $2\pi r$, and $4\pi r^2$, respectively. If the dependence of $J(r)$ on r were a power law, e.g., $J(r)=Cr^{D-1}$, then the Eq. (10) would coincide with the Schrödinger equation for S states of a hydrogen-like atom in an effective isotropic and homogeneous D-dimensional space, D being an integer or fractional number.[13] In general, the function $J(r)$ has no power-law dependence on the ion-electron separation r due to the factor $P(r)$ and Eq. (10) could be considered as a wave equation for hydrogen-like atom in an isotropic and nonhomogeneous space with a variable dimension that depends on the ion-electron distance r. We will call this dimension fractal and it can be calculated once the radial part of the Jacobian volume element $J(r)$ is found.

The general expression (9) for $J(r)$ can be simplified for heterostructures with any type of symmetry. For heterostructures with a spherical symmetry, e.g., a QD with confining potential $\tilde{V}(\vec{r})\equiv V(r)$ in the absence of magnetic field,

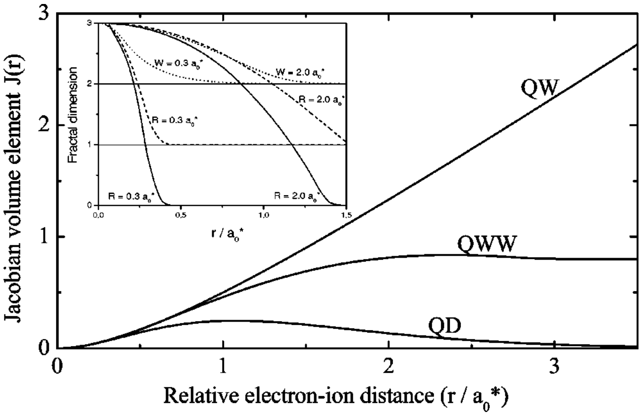

FIG. 1. The radial part of the Jacobian volume element in different GaAs/Ga$_{0.7}$Al$_{0.3}$As heterostructures, as a function of the electron-ion separation. In the inset the fractal dimension D^* as a function of the ion-electron separation for on-center donors in QW's, QWW's, and QD's is plotted for different sizes of the heterostructures.

$$J(r)=4\pi r^2 f_0^2(r), \tag{12a}$$

where the wave function $f_0(r)$ is the solution of the one-dimensional Schrödinger equation

$$\left[-\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}+V(r)\right]f_0(r)=E_0 f_0(r) \tag{12b}$$

corresponding to the lowest-energy level E_0. For heterostructures with a cylindrical symmetry such as a QW, double QW, multiple QW, SL, cylindrical QWW, coaxial QWW, quantum disk, or a quantum ring,

$$J(r)=2\pi r\int_{-r}^{r} f_0^2(\sqrt{r^2-z^2},z)\,dz, \tag{13a}$$

where $f_0(\rho,z)$ is the solution of the two-dimensional Schrödinger equation

$$\left[-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}-\frac{\partial^2}{\partial z^2}+V(\rho,z)+\frac{\gamma^2\rho^2}{4}\right]f_0(\rho,z)=E_0 f_0(\rho,z), \tag{13b}$$

for the lowest-energy level E_0. Since $V(\rho,z)\equiv V(z)$ in heterostructures with the growth axis along the z direction (such as a QW, SL, and so on) and $V(\rho,z)\equiv V(\rho)$ in cylindrical QWW's, Eq. (13b) becomes separable and splits into a pair of the independent one-dimensional equations, whose solutions can be found numerically.

For a model with square-well potential, one can calculate $J(r)$ directly by using the relations (12a) and (13a) and the well-known analytical expressions for the wave functions of an unbound electron in a QW,[2] cylindrical QWW,[3] and a spherical QD.[20] Figure 1 shows the typical behavior of the radial part of the Jacobian volume element $J(r)$ obtained for these three models of confinement. For small values of the electron-ion separation r, the three curves behave as parabolic ($J\sim r^2$). As electron-ion distance increases, the curves transform into a linear function ($J\sim r$) for a QW, into a constant ($J\sim r^0$) for QWW, and in a decreasing exponential function ($J\sim 0$) for a QD. Such behavior of $J(r)$ is typical of an effective space with a variable dimension which falls as r increases.

C. Fractal dimension

According to the theory of Mandelbrot[19] for exact fractals that have the property of self-similarity, the dimension D is determined uniquely by a power-law dependence of its mass M upon its size L as $M=CL^D$. On the contrary, for non-self-similar fractals there are an infinite number of ways to measure the "size" and therefore there are different definitions and each may give a somewhat different answer. The fractal dimension is often defined by using a set of measuring boxes in the form of geometric figures whose shapes reproduce the contour of the object and whose sizes gradually approach zero. It is reasonable to have the shape of the boxes to correspond to the basic physics of the problem and be congruent with the symmetry of the analyzed system. If we consider the charge density within a heterostructure as a fractal object, then due to the symmetry of the donor S states, the boxes natural set will be spheres with the center in the donor location. Therefore, we can postulate that the dimension D of this object is determined by the dependence of the charge Q enclosed within the sphere upon its radius R of this box as $Q=CR^D$. In this relation, the parameters C and D are constants only for exact fractals otherwise they vary slowly with R.

Let us consider a charge dQ within a thin spherical shell with the inner and outer radii r and $r+dr$. For a free electron in the heterostructure, this charge is related to the density of probability $P(r)$, and the radial part of the Jacobian volume element $J(r)$, defined by the formulas; $dQ=r^2P(r)dr=J(r)dr$. If we assume that the charge density can be considered as a spherical fractal with a finite dimension $D^*(r)$, then the charge dQ enclosed within a spherical shell and its radius r should be related by means of the quasi-power-law dependence $dQ=C(r)r^{D^*(r)-1}dr$ with the functions $C(r)$ and $D^*(r)$ varying more slowly than any power function. If one define the fractal dimension as

$$D^*(r)=1+r\frac{d\ln J(r)}{dr}=3+r\frac{d\ln P(r)}{dr}, \tag{14a}$$

with the additional condition

$$\frac{d\ln C(r)}{dr}+\ln r\frac{dD^*(r)}{dr}=0, \tag{14b}$$

then both expressions for dQ coincide

$$J(r)=C(r)r^{D^*(r)-1}. \tag{14c}$$

Note that this definition also includes the case of exact fractals for which the functions $C(r)$ and $D^*(r)$ are constant. In this way, the Jacobian factor in the Laplacian of the renormalized wave Eq. (10) is related to the fractal dimension of the free-electron charge density in the heterostructure by means of the relations (14c) and (14a), therefore, Eq. (10)

can be interpreted as the wave equation for the *S* states of a hydrogen-like atom in an effective space with fractal dimension (14a). This is the reason why the procedure of finding a donor binding energy by solving Eqs. (9) and (10) is referred as the *fractal-dimension method.*

The inset in Fig. 1 shows the fractal dimension $D^*(r)$ calculated as a function of the ion-electron separation for on-center donors in GaAs/Ga$_{0.7}$Al$_{0.3}$As QW's, QWW's, and QD's (barrier height $40R_y^*$) with square-well potential. In this model of confinement, the explicit expressions for $f_0(\vec{r})$ in QW, QWW, and QD are well known and therefore, one can calculate $D^*(r)$ directly by using the relations (9) and (14). It can be seen from Fig. 1 that the fractal dimension $D^*(r)$ falls from 3 for small electron-ion distances to 2 for a QW (dotted line), to 1 for a QWW (dashed line), and to 0 for a QD (solid line) as the distance ion-electron become larger and the electron is placed in the barrier of the heterostructure. Such dependence of the dimension on the electron-ion separation is typical for quasi-zero, one-, and two -dimensional heterostructures, respectively.

Within our formalism, it is also possible to introduce the average value of the fractional dimension $\overline{D}$ of the effective space. There are different ways to define $\overline{D}$ and one of them is proposed in the papers.[17,18] We propose to define the $\overline{D}$ of the donor *S* states as the mean value of the fractal dimension given by Eq. (14a) which is calculated by using the radial probability distribution corresponding to the states for a hydrogen-like atom in a *D*-dimensional space.

$$\overline{D}=\frac{\int_0^\infty D^*(r)R_n^2[r,D^*(r)]J(r)dr}{\int_0^\infty R_n^2[r,D^*(r)]J(r)dr}. \tag{15}$$

Here, $R_n(r,D)$ is the radial part of the hydrogen-like atom wave function in *D*-dimensional space for the ns state ($n=1,2,\dots$) which is given by the expression[13]

$$R_n(r,D)=\exp(-\kappa r)M(1-n,D-1,2\kappa r),$$

$$\kappa=\frac{1}{n+\dfrac{(D-3)}{2}}, \tag{16}$$

with $M(a,b,z)$ being the confluent hypergeometric function. Once the value $\overline{D}$ is found the ns-state donor binding energy E_b and the corresponding wave function $\Psi_n(\vec{r})$ can be obtained in a straightforward way through[13]

$$E_b=\frac{4}{\left[n+\dfrac{\overline{D}-3}{2}\right]^2},\qquad \Psi_n(\vec{r})=f_0(\vec{r})R_n(r,\overline{D}). \tag{17}$$

We have performed the calculations of $\overline{D}$ for a QW, a cylindrical QWW, and a spherical QD with square-well confining potentials as a function of the heterostructures size by using relations (9), (14), and (15). In all the cases, we have results similar to those obtained previously in Refs. 17,18 in spite of the fact that our calculation method is absolutely different. Therefore, it is clear that different definitions of the average fractional dimension provide similar results and any improvement of this approximation can be achieved only by taking into account the fact that the dimension is not the same in all parts of the heterostructure.

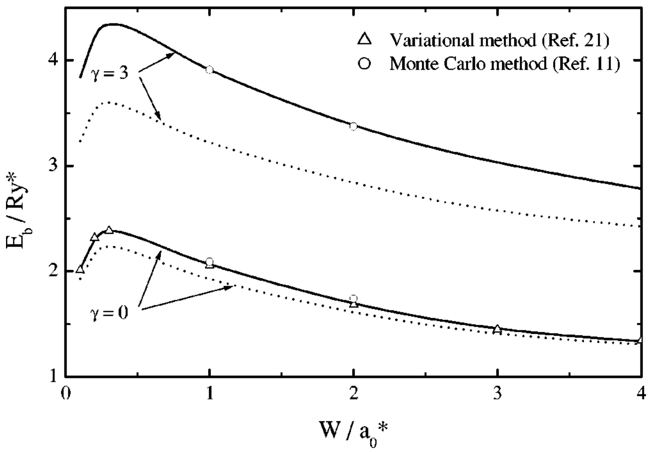

FIG. 2. D^0 Binding energy in a GaAs/Ga$_{0.7}$Al$_{0.3}$As QW with square-well potential, as a function of the well width for two strengths of the magnetic field ($\gamma=0$ and $\gamma=3$) obtained by using the fractal-dimension (solid lines) and fractional-dimension (dotted lines) methods.

III. RESULTS AND DISCUSSION

A. Comparison of calculation methods

As it was pointed out above, we have two different algorithms for calculating the binding energy of the donor *S* states in semiconductor heterostructures. The first of them consists of solving the one-dimensional wave equation (10) that takes into account the spatial dependence of the fractal dimension. In our calculations, the eigenvalue problem (10) is solved by using the numerical procedure of trigonometric sweep.[10] We refer this algorithm as the fractal-dimension method. The second algorithm referred as the fractional-dimension approach, is based on the approximated formulas (15)–(17) in which the fractal dimension is defined only on average. In order to compare the accuracy of these two methods, we have calculated the ground-state binding energies of a donor in a QW, QWW, and a QD with the square-well potential. Figure 2 displays the binding energy of a donor in a GaAs-(Ga,Al)As QW as a function of the well width and for different magnetic-field strengths. Our results are compared with the corresponding calculations by Pang *et al.*[11] (Monte Carlo method), and Fraizzoli *et al.*[21] (variational method) and some of them are also listed in Table I.

It is seen from Fig. 2 and Table I that the agreement between our results obtained by using the fractal-dimension approach (from Eq. (10), [solid line and column (b)]) and those of the Monte Carlo method [open circles and column (c)] is excellent if we take into account the relative simplicity of our procedure and the fact that the error bar for the Monte Carlo method is $0.02R_y^*$. Moreover, this agreement notably

TABLE I. Binding energy of a shallow on-center donor in a GaAs/$Ga_{0.75}Al_{0.25}As$ QW, present results obtained by using (a) fractional-dimension, (b) fractal-dimension, and (c) Monte Carlo methods (Ref. 11).

W/a_0^*	$E_b/Ry^*(\gamma=0)$			$E_b/Ry^*(\gamma=3)$			$E_b/Ry^*(\gamma=3)$		
	(a)	(b)	(c)	(a)	(b)	(c)	(a)	(b)	(c)
1.0	1.87	2.04	2.09	2.35	2.88	2.92	3.04	3.88	3.89
2.0	1.53	1.67	1.74	1.99	2.47	2.52	2.63	3.35	3.36

improves in the strong magnetic fields. Similarly, an excellent agreement between our results (solid line) and those of the previous variational calculations[21] (open triangles) is observed in Fig. 2 for the case of zero-magnetic field. In contrast, the agreement between our results obtained by using the fractional-dimension approach [dotted lines and column (a)] and Monte Carlo calculations is poor and even still worse in the strong magnetic fields [cf. columns (a) and (c) in Table I]. This result underlines again the fact that the fractional-dimension method breaks down for strong magnetic fields (fact emphasized also in Refs. 17 and 18).

The ground-state binding energies E_b, of a donor located at the axis of a cylindrical GaAs/$Ga_{0.6}Al_{0.4}As$ QWW in the presence of a uniform magnetic field are shown in Fig. 3. Our results obtained by using fractal-dimension approach (solid lines) are in an excellent agreement with the previous variational calculations[3] (open diamond). The dotted lines in Fig. 3 show the donor binding energies calculated by using the fractional-dimension approach, which are considerably lower than the corresponding results obtained by the variational method (Ref. 3). It should be noted that in a QWW the confining potential $[V(\vec{r})=V(\rho)]$ and the term $\gamma^2\rho^2/4$ that describes the external magnetic field in Hamiltonian (2c) have the same type of symmetry and therefore they produce a similar effect. As it is seen from Fig. 3, for small values of the QWW radius $(R/a_0^*<1)$, the binding energy is relatively insensitive to the magnetic fields used here since the diamagnetic energy of the electron strongly confined in the radial direction tends to zero. In this range of radii, the effect of the geometrical or spatial localization overcomes the effect of the magnetic field. As the QWW radius increases and surpasses the cyclotron radius value, the effect of the magnetic field becomes considerable. The increase of the binding energy in a strong magnetic field observed for large values of the QWW radius can be ascribed to the electron localization related to the cyclotron radius reducing. For all the cases in Fig. 3, E_b increases as the wire radius decreases up to a critical radius $R_c \approx 0.24a_0^*$ when the ground-state level is pushed up and the electronic wave-function leakage into the barrier region becomes significant. The obtained results indicate that the fractal-dimension method provides a wave function flexible enough to transform its symmetry from spherical to cylindrical as the wire radius decreases and to change its asymptotic behavior from exponential to Gaussian in the presence of magnetic field.

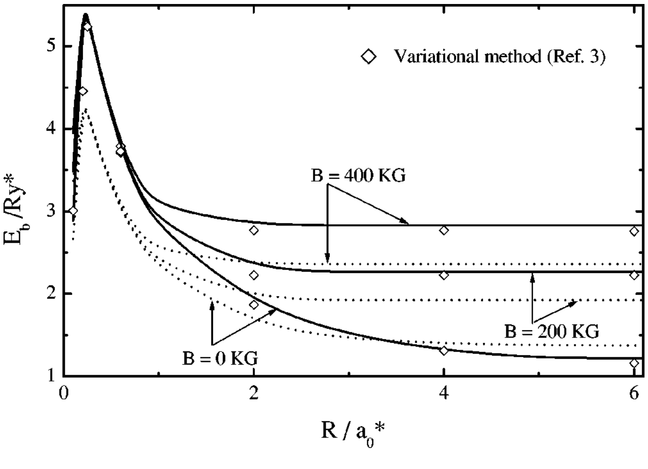

FIG. 3. Binding energy of a donor in a GaAs/$Ga_{0.6}Al_{0.4}As$ QWW with square-well potential, as a function of the wire radius, for different magnetic-field strengths obtained by using the fractal-dimension (solid lines) and fractional-dimension (dotted lines) methods.

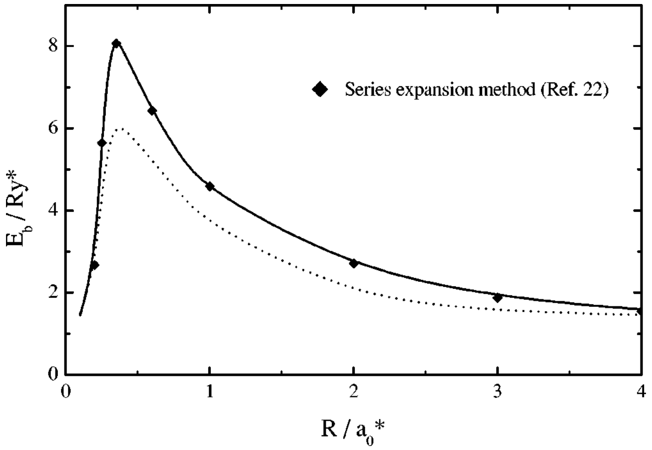

FIG. 4. Binding energy of a donor in a GaAs/$Ga_{0.7}Al_{0.3}As$ spherical QD with square-well potentials, as a function of the dot radius obtained by using fractal-dimension (solid lines) and fractional-dimension (dotted lines) methods.

In Fig. 4 we plot the donor binding energy as a function of the radius of a GaAs/$Ga_{0.7}Al_{0.3}As$ spherical QD. A total coincidence can be observed between the present calculations (solid line) and the results obtained previously by Zhu[22] (solid diamond), who found the exact solutions of donor states in a spherical QD by using a series-expansion method. The dotted line in Fig. 4 presents the calculation results by using the fractional-dimension approach. Although the solid and dotted lines have a similar behavior the energies obtained by means of this simple method are 25% lower than the corresponding exact values. This emphasizes once again the fact that the fractional-dimension approach in a strong confining limit breaks down.

It can be seen from Fig. 4 that, as the QD radius decrease to critical value $R_c \approx 0.33a_0^*$, the electron wave function becomes compressed in the narrowing well and the donor binding energy climbs up due to the decreasing of the average distance between the electron and the ion. The binding energy E_b reaches a maximum of $8.13R_y^*$ as it was already established in Ref. 22. As the QD radius further decreases the

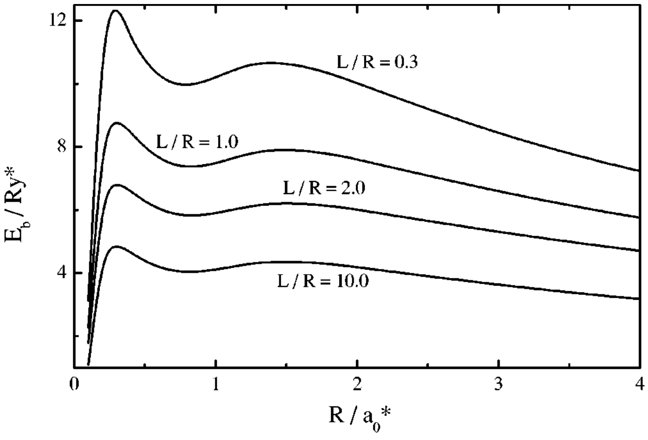

FIG. 5. Binding energy of a donor in a GaAs/$Ga_{0.8}Al_{0.2}$As/$Ga_{0.55}Al_{0.45}$ As coaxial QWW (double step potential), as a function of the outer radius *R*, and for different wire lengths.

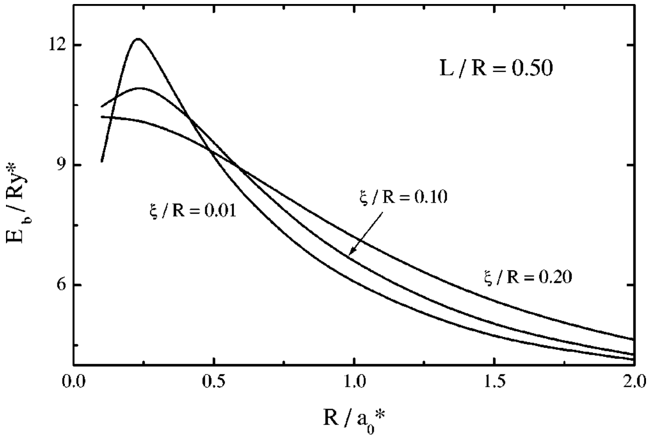

FIG. 6. Binding energy of a donor in a GaAs/$Ga_{0.6}Al_{0.4}$ cylindrical QWW with soft-barrier potentials, as a function of the wire radius, and for different thickness of the transition region in the junction.

wave function's three-dimensional character is restored and E_b begins to fall off sharply to $1R_y^*$.[10]

B. Quantum wire with different potential shapes

The fractal-dimension approach is a simple and effective tool for calculating the ground-state binding energy of donors confined in semiconductor heterostructures with different potential shapes. Below we use our procedure to analyze the potential-shape effects on the binding energy of a shallow donor in a cylindrical QWW considering the models of one-step and double-step soft-edge-barrier potentials. To describe the conduction-band discontinuity in the GaAs/$Ga_{1-x}Al_x$As junction, we assume that in all the cases the displacement of the band bottom is related to the distribution of the Al concentration in the radial direction, $c(\rho)$ by means of the interpolation formula[3]

$$V_\rho(\rho)=0.6[1.36c(\rho)+0.22c^2(\rho)] \ \ \text{eV}, \qquad (18)$$

whereas $c(\rho)$ in the junction of the cylindrical QWW of radius *R* varies smoothly according to the relation

$$c(\rho)=x\,\frac{1-\exp(-\rho/\xi)}{1+\exp[-(\rho-R)/\xi]}\equiv F(\rho,R,x,\xi). \qquad (19)$$

The parameter ξ determines the thickness of the transition region in the heterostructure junction where the Al concentration increases smoothly from 0, at the axis of the wire ($\rho\rightarrow 0$) up to *x*, in the barrier as $(\rho-R)/\xi \gg 1$, while the confinement potential increases from 0 up to V_0, respectively $[V_\rho(\rho)=V_0$ as $c(\rho)=x]$. Different potential-barrier shapes[10] from almost rectangular ($\xi/R\rightarrow 0$) up to very smooth one ($\xi/R\rightarrow 1$) can be obtained by varying the dimensionless ratio ξ/R. The results obtained for a double-step potential corresponding to a coaxial structure of cylindrical GaAs/$Ga_{0.8}Al_{0.2}$As/$Ga_{0.55}Al_{0.45}$As QWW's are presented in Fig. 5, where we plot the donor binding energy E_b, as a function of the outer radius *R* for several values of the wire length *L*. We have simulated the distribution of the Al concentration in the radial direction for this heterostructure by using the following function:

$$c(\rho)=F(\rho,R_1,0.2,0.01)+F(\rho,R,0.25,0.01). \qquad (20)$$

We assume that the QWW radii, inner R_1 and outer *R* are related as $R_1=0.2R$. According to the relations (19) and (20), the Al concentration $c(\rho)$ has two almost rectangular jumps from 0 up to 0.2 in the first junction ($\rho=R_1$) and from 0.2 up to 0.45 in the second junction ($\rho=R$). The confinement potential $V_\rho(\rho)$ in these junctions jumps from 0 up to V_1 and from V_1 up to V_2, respectively (V_1 and V_2 are the values of V_ρ in Eq. (18) corresponding to the Al concentrations 0.2 and 0.45, respectively). From Fig. 5 the existence of two peaks in the E_b curves is evident. The main in each curve is associated with the wave-function leakage into the exterior barrier region, whereas the secondary peak can be ascribed to electronic wave-function leakage into the interior barrier region. A considerable increase of the binding energy is found as the wire length decreases due to transformation of the quasi-one-dimensional system (QWW) into quasi-zero-dimensional one (cylindrical QD).

The calculation results of the ground-state binding energy of a donor in a cylindrical GaAs/$Ga_{0.6}Al_{0.4}$As QWW are shown in Fig. 6 for three different thickness of the transition region in the heterostructure junction: $\xi/R=0.01,0.1,0.2$ corresponding to almost rectangular, smooth, and very smooth edge-barrier potentials, respectively. The curves crossover in the region $0.4<R/a_0^*<0.6$ is evident. It is apparent that for intermediate and large values of the QWW radius ($R/a_0^*>0.6$) the electronic orbital confinement is small and the energy level is situated close to the bottom of the conduction band. The electronic orbital confinement in this region for the smooth potential is stronger than for the rectangular one and the potential shape corresponding to $\xi/R=0.2$ gives the largest binding energy followed by $\xi/R=0.1$, whereas the corresponding to $\xi/R=0.01$ present the smallest confinement and binding energy. As the QWW radius decreases the energy level rises to the upper part of the conduction band where the electronic orbital confinement for the rectangular potential is the strongest. Therefore, as R is small ($R/a_0^* < 0.4$) the potential corresponding to $\xi/R=0.01$ presents the largest donor binding energy followed by $\xi/R=0.1$, while the corresponding to $\xi/R=0.2$ present the smallest binding energy.

IV. SUMMARY AND CONCLUSIONS

To sum up, we have developed a simple method to study the electronic *S* states of shallow donors confined in semiconductor heterostructures where the problem is reduced to the wave equation for a hydrogen-like atom in an effective space with a non-power-law dependence of the radial part of the Jacobian volume element on the ion-electron separation. By using the relation between the radial part of the Jacobian volume element and the dimension of the space similar to one proposed by Mandelbrot for fractal geometric objects, we find that the donor *S* states fractional dimension is related to the charge-density distribution for the free-electron ground state within the heterostructure and decreases from 3 for small electron-ion distances to 2 in QW's, to 1 in QWW's, and to 0 in QD's barriers.

All information about any anisotropic perturbation of the system (confinement due to the heterostructure or the magnetic field) is contained in the radial dependence of the Jacobian volume element for which we have found an analytical expression. One of the attractive features of the proposed method is its universality which is related to the simplicity of its application for different models of confinement in the framework of the same numerical procedure[10] (trigonometric sweep method). It permits to avoid tedious calculations to obtain, with high accuracy, the donor binding energy in any heterostructure once the probability density of the free electron is known.

We have calculated the ground-state binding energies for a donor confined in a QW, cylindrical QWW, and a spherical QD with a square-well potential. Our results are in a good agreement with those obtained previously by using more rigorous methods such as the Monte Carlo[11] and the series expansion.[7,22] Moreover, we apply the fractal-dimension method to the problems of donors in coaxial QWW's and cylindrical GaAs-(Ga,Al)As QWW's with a smooth variation of the Al concentration within the transition region of the heterostructure junction. Similarly, the problem can be treated in more complex heterostructures such as T- shaped[23] and V- shaped[24] quantum wires.

Finally, we can argue that it is possible to reduce any problem for a few-particle system confined in semiconductor heterostructures to a similar one in an isotropic space with a variable fractal dimension by using the variational principle. In this way, our method might be applied to study properties of any carriers bounded states (neutral and negatively charged donors, acceptors, exciton, biexcitons, trions, and so on) in different types of heterostructures such as SL's, QW's, QWW's, QD's, rings, etc. in the presence of any external perturbation, and it may even exhibit practical advantages like in the cases considered in this work.

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