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On the scaling of exciton and impurity binding energies and the virial theorem in semiconductor quantum wells and quantum-well wires

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ABSTRACT

We have used the variational and fractional-dimensional space approaches in a study of the virial theorem value and scaling of the shallow-donor binding energies versus donor Bohr radius in GaAs-(Ga,Al)As semiconductor quantum wells and quantum-well wires. A comparison is made with previous results with respect to exciton states. In the case the donor ground-state wave function may be approximated by a D-dimensional hydrogenic wave function, the virial theorem value equals 2 and the scaling rule for the donor binding energy versus quantum-sized Bohr radius is hyperbolic, both for quantum wells and wires. In contrast, calculations within the variational scheme show that the scaling of the donor binding energies with quantum-sized Bohr radius is in general nonhyperbolic and that the virial theorem value is nonconstant.

INTRODUCTION

Impurity and exciton states may be significantly modified by the barrier-potential confinement in quantum-sized semicondutor heterostructures, and much experimental and theoretical work have been devoted to the quantitative understanding of their properties in GaAs-$Ga_{1-x}Al_xAs$ quantum wells (QWs), quantum-well wires (QWWs), and semiconductor heterostructures in general. Recently, the scaling of the exciton binding energy in semiconductor QWs and QWWs was numerically investigated by Rossi et al [1], who found that in the strong confinement limit the same potential-to-kinetic energy ratio (virial theorem value) holds for quite different wire cross sections and compositions, and claimed that a universal parameter would govern the scaling of the exciton binding energy with size. Zhang and Mascarenhas [2] reexamined the subject by calculating the exciton binding energies and the corresponding virial theorem value in QWs and QWWs with infinite confinement barriers, and found that a shape-independent scaling rule does exist for QWWs, but argued that a virial theorem value being or not a constant is irrelevant. In particular, they found that the exciton virial theorem value is not a constant for either wires or wells. The purpose of this work is to investigate the scaling rule, if any, for the donor binding energies versus Bohr radius, and the virial theorem for shallow donors in quantum-sized semiconductor heterostructures, such as GaAs-$Ga_{1-x}Al_xAs$ cylindrical quantum wires or wells, both within the fractional-dimensional and variational approaches.

THEORETICAL FRAMEWORK

We consider a shallow donor at the position $\vec{\mathbf{r}}_i$ in a semiconductor GaAs-$Ga_{1-x}Al_xAs$ heterostructure such as a QW or a cylindrical QWW, within the effective-mass and non-degenerate-parabolic band approximations. The Hamiltonian is given by

$$H = \frac{p^2}{2m^*} - \frac{e^2}{\varepsilon\left|\vec{\mathbf{r}} - \vec{\mathbf{r}}_i\right|} + V_b(\vec{\mathbf{r}}), \qquad (1)$$

where m^* is the conduction-band effective mass and ε is the dielectric constant, which, for simplicity, are taken as the GaAs bulk values throughout the heterostructure [3]. $V_b(\vec{\mathbf{r}})$ is the confining potential, which is taken as $V_b(\vec{\mathbf{r}}) = V_b(z)$ for QWs or $V_b(\vec{\mathbf{r}}) = V_b(\rho)$ for cylindrical QWWs. In the following, we will limit ourselves to donors located at positions where cylindrical symmetry is preserved, i.e., at any position in QWs or at the wire axis in QWWs, and will focus on the impurity 1s-like ground state. The eigenfunctions of (1) may be taken as

$$\psi_E(\vec{\mathbf{r}}) = f(\vec{\mathbf{r}})\phi_E(\vec{\mathbf{r}}), \qquad (2)$$

where $f(\vec{\mathbf{r}})$ is the ground-state solution of (1) in the absence of the Coulomb interaction. In the fractional-dimensional approach, one finds that, for a given state, the "shallow donor + heterostructure" anisotropic system may be modeled by an effective isotropic hydrogenic system in a fractional D-dimensional space [4], a problem which may be solved analytically, with the D parameter chosen via the condition [5]

$$\int_0^\infty \int_0^\pi h\, r^2 \sin\theta\, \phi_E^*\, W\, \phi_j\, d\theta\, dr = 0 \qquad (3)$$

where the operator W in eq. (3) includes the effects of anisotropy. In the above equation, $\phi_E(\vec{\mathbf{r}})$ is the corresponding impurity eigenfunction, and ϕ_j (and E_j) are the exact eigenfunctions (and eigenvalues) of the D-dimensional Hamiltonian. If one is concerned with the ground-state donor binding energy, it follows [4] that

$$E_b = -E_{1s} = 4R_o/(D-1)^2 \qquad (4)$$

where $R_o = \frac{m^* e^4}{2\varepsilon^2\hbar^2}$ is the donor reduced Rydberg. If the ground-state wave function is chosen as $\phi^*_{E,1s} = e^{-\lambda r}$ with $\lambda = 2/[a_o(D-1)]$, the fractional-dimensional parameter is given [5] by

$$D = 1 + 2\sqrt{\frac{a_L}{a_o}}, \qquad (5)$$

where $a_o = \frac{\hbar^2\varepsilon}{m^* e^2}$ is the reduced Bohr radius, and we have followed Rossi et al [1] and Zhang and Mascarenhas [2] and defined a *"quantum-confined impurity Bohr radius"* as

$$a_I = \left\langle \psi_{E,1s} \left| \frac{1}{r} \right| \psi_{E,1s} \right\rangle^{-1}, \qquad (6)$$

with coordinates taken with the origin at the impurity position. Notice that (5) provides a simple relation between the fractional dimension of the effective isotropic medium and the localization of the ground-state wave function through the donor Bohr radius (6). Also, it is straightforward to demonstrate that (5) and (6) give the exact results corresponding to the 2D and 3D limits. One then obtains [5] the hyperbolic dependence of the donor binding energy on the impurity Bohr radius,

$$E_b = R_o \left(\frac{a_o}{a_I} \right) = \frac{e^2}{2\varepsilon\, a_I}, \qquad (7)$$

and a virial theorem value of $\beta = 2$ within the fractional-dimensional space approach, for donors either in QWs or QWWs.

Alternatively, in the variational procedure, one may introduce a variational function for the donor $\phi_E(\mathbf{r})$ envelope wave function, and minimize the impurity energy with respect to the variational parameters [3]. Although one may choose a two- or three-parameter hydrogenic variational wave function for a shallow donor in a QW, the comparison between results using the fractional-dimensional space approach and the variational scheme is probably best illustrated with the simplest one-parameter hydrogenic choice [3] for the variational wave function. We choose therefore $\phi_E(\mathbf{r}) = \phi_{1s}(\mathbf{r}) = e^{-\lambda r}$ for the ground-state wave function, where λ is a variational parameter, and write

$$E_b(\lambda) = \frac{e^2}{\varepsilon\, a_I(\lambda)} - \frac{\hbar^2 \lambda^2}{2m^*} = \frac{e^2}{\varepsilon\, a_I(\lambda)} \left(1 - \frac{1}{\beta(\lambda)} \right). \qquad (8)$$

By imposing the condition $\frac{\partial E_b(\lambda)}{\partial \lambda} = 0$, one obtains a transcendental equation for λ, and

$$\beta(\lambda) = \frac{\frac{a_I}{a_o}}{2\left[\frac{\langle r \rangle}{a_o} - \frac{a_I}{a_o} \right]^2} \qquad (9)$$

for the virial theorem value within the variational approach.

RESULTS AND DISCUSSION

In the following, we have used a GaAs conduction-band effective mass $m^* = 0.0665\, m_0$, where m_0 is the free – electron mass, and a 60% (40%) rule for the conduction (valence) – barrier potential with respect to the total band-gap offset, with the band gap discontinuity taken

as ΔE_g (eV) = 1.247 x, where x is the Al concentration. Results are presented with energies and lengths expressed in reduced units of the impurity Rydberg (R_o) and radius (a_o), respectively.

In Fig. 1(a) we compare the theoretical fractional-dimensional calculations of the binding energies for on-center donors in GaAs-$Ga_{0.7}Al_{0.3}As$ QWs with the corresponding results using a variational 1s-like hydrogenic envelope wave function [3]. Results are also shown for an infinite-barrier potential. Notice that the on-center donor binding energies of both fractional-dimensional and variational calculations are in excellent agreement. Figs. 1(b) and (c) show the on-center donor binding energy and corresponding virial theorem value β versus the quantum-confined donor Bohr radius [see eq. (6)], calculated in the variational [3] and fractional-dimensional [5] approaches, for GaAs-$Ga_{1-x}Al_xAs$ QWs, both for x = 0.30, and infinite-barrier potentials. We notice that the fractional-dimensional approach leads to the hyperbolic dependence of the donor binding energy on the impurity Bohr radius, and to a virial theorem value of $\beta = 2$. In contrast, within the variational procedure, the virial theorem value has a strong dependence on the donor Bohr radius, and approaches the exact bulk value of 2 from above as the width of the well approaches infinite, both in the case of infinite-confining and finite-barrier potentials. One should point out that variational results for finite barriers may exhibit two different virial theorem values for a given donor Bohr radius, as a donor radius may correspond to two well widths. In the case of infinite-potential barrier in the variational scheme, the virial theorem value also approaches the exact 2D value of 2 for vanishing QW width. The above variational results for the virial theorem value in the case of shallow donors in QWs are quite similar to the results for excitons reported by Zhang and Mascarenhas [2].

The fractional-dimensional and variational results for the binding energies of donors at the axis of a cylindrical GaAs-$Ga_{1-x}Al_xAs$ wire are presented in Fig. 2(a). A comparison between fractional-dimensional results and a donor variational calculation indicates good agreement for the binding energies in the cases of moderate and large values of the wire radius. The on-axis donor binding energy and virial theorem value are shown in Figs. 2(b) and (c) versus the quantum-confined donor Bohr radius, calculated in the variational and fractional-dimensional approaches, for both x = 0.30 and infinite-barrier potential GaAs-$Ga_{1-x}Al_xAs$ QWWs. As before, the fractional-dimensional approach leads to the hyperbolic dependence of the impurity binding energy on the donor Bohr radius, and to a virial theorem value of $\beta = 2$. As in the work on excitons by Zhang and Mascarenhas [2], the virial theorem value, obtained within the variational procedure, has a significant dependence on the donor Bohr radius, and approaches the exact bulk value of 2 from above as the radius of the well approaches infinite, both in the case of infinite-confining and finite-barrier potentials, similar to the results for donors in QWs in Fig. 1. Also, in the case of infinite potential in the variational scheme, the virial theorem value approaches the exact 1D value of 2 for a vanishing QWW radius.

CONCLUSIONS

We have presented a study, within the fractional-dimensional and variational approaches, of the virial theorem value and results for the scaling of the shallow-donor binding energies versus donor Bohr radius in GaAs-(Ga,Al)As QW and QWW quantum-sized semiconductor heterostructures. In the case of the fractional-dimensional space approach, if the 3D actual anisotropic semiconductor heterostructure may be substituted by a fractional-dimensional

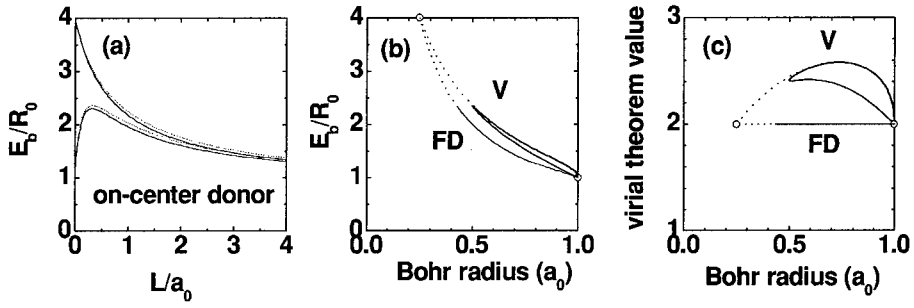

Figure 1. On-center donor binding energies as functions of the well width (a) and quantum-confined donor Bohr radius (b) in GaAs-$Ga_{1-x}Al_xAs$ QWs, both for x = 0.30 and infinite-barrier potentials. The corresponding virial theorem value is shown in (c). In (a) solid curves correspond to fractional-dimensional results whereas dotted lines are calculated using a variational procedure. In (b) and (c), x = 0.30 results using the variational - V or fractional-dimensional - FD approaches are given as full curves, and dotted curves are in the cases of infinite-barrier potentials. Open dots correspond to exact results. Energies and lengths are expressed in reduced units of the impurity Rydberg (R_o) and radius (a_o), respectively.

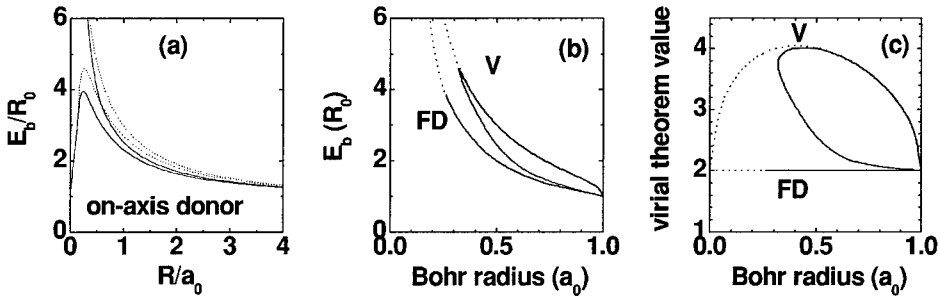

Figure 2. On-axis donor binding energies as functions of the wire radius (a) and quantum-confined donor Bohr radius (b) in GaAs-$Ga_{1-x}Al_xAs$ cylindrical QWWs, both for x = 0.30 and infinite-barrier potentials. The corresponding virial theorem value is shown in (c). In (a) solid curves correspond to fractional-dimensional results whereas dotted lines are calculated using a variational procedure. In (b) and (c), x = 0.30 results using the variational - V or fractional-dimensional - FD approaches are given as full curves, whereas results for infinite-barrier potentials are given by dotted curves. Energies and lengths are expressed in reduced units of the impurity Rydberg (R_o) and radius (a_o), respectively.

effective medium with a ground-state wave function given by $\phi^{*}_{E,1s} = e^{-\lambda r}$ with $\lambda = 2/[a_0(D-1)]$, the virial theorem value equals 2 and the scaling rule for the donor binding energy versus Bohr radius is hyperbolic, both for GaAs-(Ga,Al)As QWs and QWWs. In contrast, calculations within the variational scheme unambiguously show that the scaling of the donor binding energies with Bohr radius is, in general, nonhyperbolic and that the virial theorem value is nonconstant. Moreover, calculations for the donor binding energies versus QW widths or QWW radii, within both the fractional-dimensional and variational approaches, result in essentially the same binding energies with quite different virial theorem values or Bohr radii. This indicates that any general conclusion based on a given virial theorem value or donor energy versus Bohr radius scaling rule should be examined with due caution.

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