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Virial theorem and scaling of shallow-donor binding energy in quantum-sized semiconductor heterostructures

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Abstract

The variational and fractional-dimensional space approaches are used in a thorough 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 (QWs) and quantum-well wires (QWWs). In the case of the fractional-dimensional space approach, in which the three-dimensional actual anisotropic semiconductor heterostructure is modelled by a fractional-dimensional isotropic effective medium, we have shown that if the 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 Bohr radius is hyperbolic, both for GaAs/(Ga,Al)As 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. Moreover, calculations for the donor binding energies versus well widths or wire radii, within both the fractional-dimensional and the variational approaches, indicate that any general conclusion based on a given virial theorem value or donor energy versus Bohr radius scaling rule should be examined with caution.

1. Introduction

In the past two decades, there has been considerable interest in the study of the physics underlying various properties of low-dimensional semiconductor systems, due to their importance for potential applications in electronic and optoelectronic devices [1]. In particular, impurity and exciton states may be significantly modified by the barrier-potential confinement in quantum-sized semiconductor heterostructures, and much experimental and theoretical work has been devoted to the quantitative understanding of their properties in GaAs/$Ga_{1-x}Al_xAs$ quantum wells (QWs), quantum-well wires (QWWs), quantum dots (QDs) and semiconductor

heterostructures in general. Various approaches have been used to calculate the binding energies of Coulomb-bound states in quantum-sized low-dimensional heterostructures and, in this work, we are going to focus on both the variational procedure [2–11] and the fractional-dimensional space approach [12–18].

Recently, the scaling of the exciton binding energy in semiconductor QWs and QWWs was numerically investigated by Rossi *et al* [19], 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. These findings were attributed to the existence of a constant (shape- and/or size-independent) virial theorem value, respectively, for wires and wells, and that its value was larger for wires (=4) than for wells (=2). Zhang and Mascarenhas [20] re-examined 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 a constant or not is irrelevant. In particular, Zhang and Mascarenhas [20] found that the virial theorem value is not a constant for either wires or wells.

The purpose of this paper is to study, in the case of shallow donors, the scaling rule, if any, for the donor binding energies versus Bohr radius, and to investigate 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. The paper is organized as follows. In section 2 the theoretical basis of the study is summarized; results and discussion are given in section 3 and conclusions in section 4.

2. Theoretical framework

We consider the problem of a shallow donor at the position $\boldsymbol{r}_i$ 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, and with the Hamiltonian

$$H = \frac{p^2}{2m^*} - \frac{e^2}{\varepsilon\,|\boldsymbol{r} - \boldsymbol{r}_i|} + V_{\mathrm{b}}(\boldsymbol{r}) \tag{2.1}$$

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]. $V_{\mathrm{b}}(\boldsymbol{r})$ is the confining potential, which is taken as $V_{\mathrm{b}}(\boldsymbol{r}) = V_{\mathrm{b}}(z)$ for QWs or $V_{\mathrm{b}}(\boldsymbol{r}) = V_{\mathrm{b}}(\rho)$ for cylindrical QWWs. In the following sections 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 (2.1) may be taken as

$$\psi_{\mathrm{E}}(\boldsymbol{r}) = f(\boldsymbol{r})\phi_{\mathrm{E}}(\boldsymbol{r}) \tag{2.2}$$

where $f(\boldsymbol{r})$ is the ground-state solution of (2.1) in the absence of the Coulomb interaction. In the fractional-dimensional approach, one writes the Schrödinger equation [12–18] corresponding to (2.1) as

$$[H_D + W]\phi_{\mathrm{E}}(\boldsymbol{r}) = E\phi_{\mathrm{E}}(\boldsymbol{r}) \tag{2.3}$$

$$H_D = -\frac{\hbar^2}{2m^*}\nabla_D^2 - \frac{e^2}{\varepsilon r} \tag{2.4}$$

[3] The roles of r-dependence and mismatch of the dielectric constant are properly discussed in [6] and [7], respectively.

where H_D is the D fractional-dimensional space [12] Hamiltonian with $m = 0$ (m is the magnetic quantum number), and

$$W = -\frac{\hbar^2}{2m^*}\left[\left(\frac{\beta}{r} + \frac{1}{h}\frac{\partial h}{\partial r}\right)\frac{\partial}{\partial r} + \frac{1}{r^2}\left(\beta\cot\theta + \frac{1}{h}\frac{\partial h}{\partial\theta}\right)\frac{\partial}{\partial\theta}\right] \tag{2.5}$$

where $\beta = 3 - D$, $h = f^2(r\cos\theta + z_i)$ for QWs and $h = f^2(\rho)$ for QWWs (with $\rho = r\sin\theta$), and co-ordinates are taken with the origin at the impurity position. Following previous works [16–18], one finds that, for a given state, the 'shallow donor and heterostructure' anisotropic system may be modelled by an effective isotropic hydrogenic system in a fractional D-dimensional space, a problem which may be solved analytically, with the D parameter chosen via the condition

$$\int_0^\infty\int_0^\pi hr^2\sin\theta\,\phi_{\mathrm{E}}^* W\phi_j\,\mathrm{d}\theta\,\mathrm{d}r = 0 \tag{2.6}$$

where the operator W in (2.5) includes the effects of anisotropy. In the above equation, $\phi_{\mathrm{E}}(\boldsymbol{r})$ 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 [12–15] that

$$E_{\mathrm{b}} = -E_{1\mathrm{s}} = \frac{4R_0}{(D-1)^2} \tag{2.7}$$

where $R_0 = \frac{m^*e^4}{2\varepsilon^2\hbar^2}$ is the donor reduced Rydberg. As shown in appendix A, if the ground-state wave function is approximated by $\phi_{\mathrm{E,1s}}^* = \mathrm{e}^{-\lambda r}$ with $\lambda = 2/[a_0(D-1)]$, the fractional-dimensional parameter may be given by

$$D = 1 + 2\sqrt{\frac{a_{\mathrm{I}}}{a_0}} \tag{2.8}$$

where $a_0 = \frac{\hbar^2\varepsilon}{m^*e^2}$ is the reduced Bohr radius, and we have followed Rossi *et al* [19] and Zhang and Mascarenhas [20] and defined a *quantum-confined impurity Bohr radius* as

$$a_{\mathrm{I}} = \langle\psi_{\mathrm{E,1s}}|\frac{1}{r}|\psi_{\mathrm{E,1s}}\rangle^{-1} \tag{2.9}$$

with co-ordinates taken with the origin at the impurity position. From (2.7)–(2.9), one obtains the hyperbolic dependence of the donor binding energy on the impurity Bohr radius

$$E_{\mathrm{b}} = R_0\left(\frac{a_0}{a_{\mathrm{I}}}\right) = \frac{e^2}{2\varepsilon a_{\mathrm{I}}}. \tag{2.10}$$

Notice that (2.8) 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 (2.9). Also, it is straightforward to demonstrate that (2.8) and (2.9) give the exact results corresponding to the two- and three-dimensional limits.

The above (2.10) result should be compared with (see appendix B)

$$E_{\mathrm{b}} = -\langle V_{\mathrm{c}}\rangle\left(1 + \frac{\langle\hat{t}\rangle}{\langle V_{\mathrm{c}}\rangle}\right) = \frac{e^2}{\varepsilon a_{\mathrm{I}}}\left(1 - \frac{1}{\beta}\right) \tag{2.11}$$

which relates the donor binding energy to the virial theorem value $\beta = -\langle V_{\mathrm{c}}\rangle/\langle\hat{t}\rangle$. It is clear, therefore, that one finds 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 $\phi_{\mathrm{E}}(\boldsymbol{r})$ envelope wave function, and minimize the impurity energy with respect to the

variational parameters [2–11]. Although one may choose a two- or three-parameter hydrogenic variational wave function [3–5] 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 [8] for the variational wave function. We choose, therefore, $\phi_{\rm E}(\boldsymbol{r}) = \phi_{1{\rm s}}(\boldsymbol{r}) = {\rm e}^{-\lambda r}$ for the ground-state wave function, where λ is a variational parameter, and write

$$E_{\rm b}(\lambda) = \frac{e^2}{\varepsilon a_{\rm I}(\lambda)} - \frac{\hbar^2\lambda^2}{2m^*} = \frac{e^2}{\varepsilon a_{\rm I}(\lambda)}\left(1 - \frac{1}{\beta(\lambda)}\right). \tag{2.12}$$

By imposing the condition $\frac{\partial E_{\rm b}(\lambda)}{\partial\lambda} = 0$, one obtains the following trancendental equation for λ

$$\lambda = \frac{2}{a_{\rm I}}\left(\frac{\langle r\rangle}{a_0} - \frac{a_{\rm I}}{a_0}\right) \tag{2.13}$$

with

$$E_{\rm b} = \frac{e^2}{\varepsilon a_{\rm I}}\left(1 - \frac{1}{\beta}\right) \tag{2.14}$$

and

$$\beta = \frac{\frac{a_{\rm I}}{a_0}}{2\left[\frac{\langle r\rangle}{a_0} - \frac{a_{\rm I}}{a_0}\right]^2} \tag{2.15}$$

where the quantities in (2.14) and (2.15) are now evaluated at the values of λ given by (2.13). Notice that, in the absence of a barrier-confining potential and if one evaluates the above expectation values for the exact D-dimensional wave function, one recovers the fractional-dimensional results $\lambda = \frac{2}{a_0(D-1)}$ and $D = 1 + 2\sqrt{\frac{a_{\rm I}}{a_0}}$ (cf equation (2.8)), as expected.

3. 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 $\Delta E_{\rm g}$ (eV) $= 1.247\ x$, where x is the Al concentration. Results are presented with energies and lengths expressed in units of the impurity reduced Rydberg (R_0) and reduced Bohr radius (a_0), respectively.

In figure 1(a) we compare the theoretical fractional-dimensional calculations of the binding energies for on-centre donors in GaAs/$Ga_{0.7}Al_{0.3}$As QWs with the corresponding results using a variational 1s-like hydrogenic envelope wave function [8]. Results are also shown for an infinite-barrier potential. Notice that the on-centre donor binding energies of both fractional-dimensional and variational calculations are in excellent agreement. Although not shown here, the fractional dimension goes from two to three, for an infinite-barrier potential, as the well width goes from 0 to ∞, and the binding energy varies from 4 R_0 to 1 R_0, respectively, as expected (see figure 1(a)). For finite-barrier potentials one finds that the fractional dimension (not shown here) goes to three as the well width goes to zero, because the donor wave function becomes essentially immersed in the $Ga_{1-x}Al_x$As layer and, as expected, the fractional dimension has the limiting value of three as the well width increases, as the QW approaches the bulk limit. The fractional-dimensional and variational results for the quantum-confined donor Bohr radii (see equation (2.9)) are shown in figure 1(b) as functions of the well width in GaAs/$Ga_{1-x}Al_x$As QWs, both for $x = 0.30$ and infinite-barrier potentials.

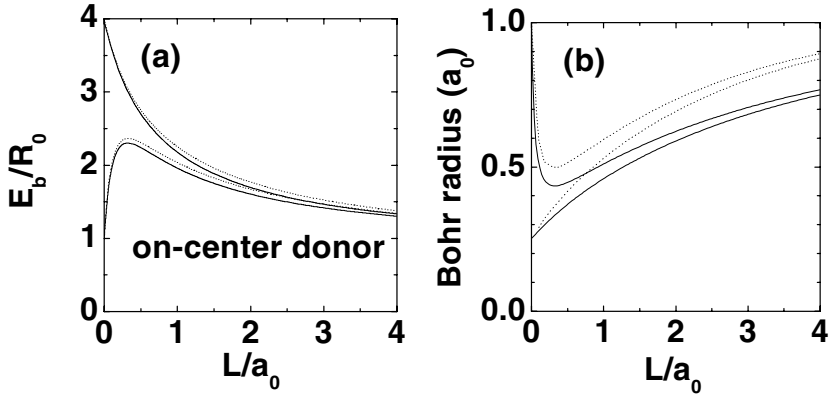

Figure 1. On-centre donor binding energies (a) and corresponding quantum-confined donor Bohr radii (b) as functions of the well width in GaAs/$Ga_{1-x}Al_xAs$ QWs, both for $x = 0.30$ and infinite-barrier potentials. Solid curves correspond to fractional-dimensional results whereas dotted lines are calculated using a variational procedure. Energies and well widths are expressed in units of the impurity reduced Rydberg (R_0) and reduced Bohr radius (a_0), respectively.

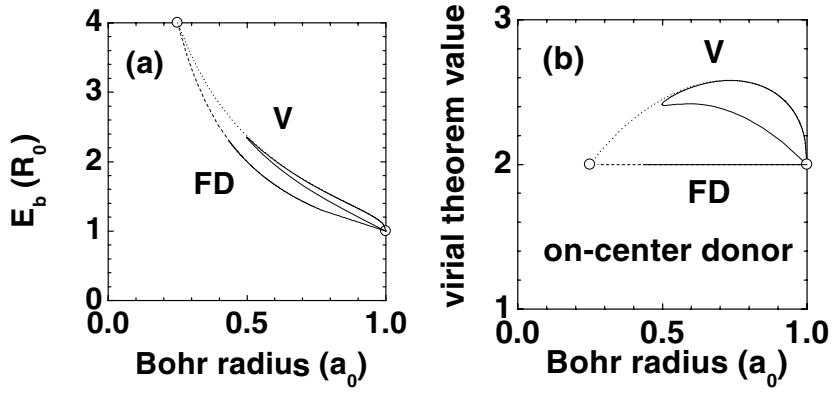

Figure 2. On-centre donor binding energies (a) and virial theorem value (b) as functions of the quantum-confined donor Bohr radius in GaAs/$Ga_{1-x}Al_xAs$ QWs, both for $x = 0.30$ (full curves) and infinite-barrier potentials, with calculations within the variational (V) or fractional-dimensional (FD) approaches. In the cases of infinite-barrier potentials, the dotted (dashed) curve is for results using the variational (fractional-dimensional) approach. Open dots correspond to exact results.

Notice that, for a given QW width, the variational procedure leads to larger donor Bohr radii in comparison with the fractional-dimensional results, although, as noticed before, the two approaches give essentially the same results for the donor binding energy as function of the well width.

Figure 2 shows the on-centre donor binding energy and corresponding virial theorem value $\beta = -\langle V_c\rangle/\langle\hat{t}\rangle$ versus the quantum-confined donor Bohr radius, calculated in the variational [8] and fractional-dimensional 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, in the approximation outlined in appendix A, 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

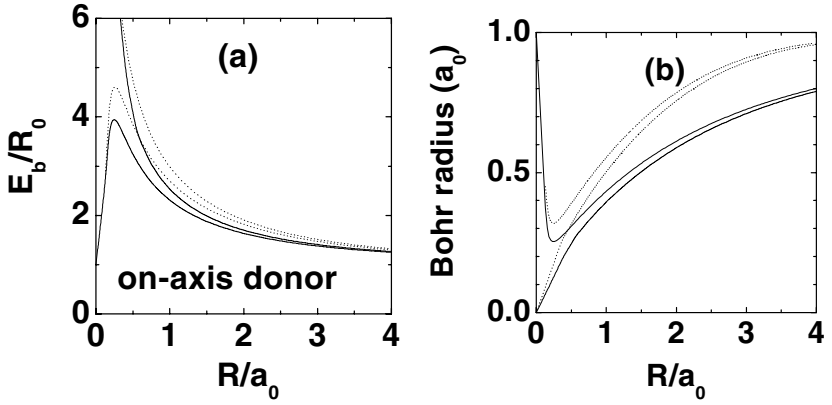

Figure 3. On-axis donor binding energies (a) and corresponding quantum-confined donor Bohr radii (b) as functions of the wire radius in GaAs/$Ga_{1-x}Al_x$As cylindrical QWWs, both for $x = 0.30$ and infinite-barrier potentials. Solid curves correspond to fractional-dimensional results whereas dotted lines are calculated using a variational procedure. Energies and wire radii are expressed in units of the impurity reduced Rydberg (R_0) and reduced Bohr radius (a_0), respectively.

the donor Bohr radius, and approaches the exact bulk value of two 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, which may be understood by the results in figure 1(b), as a given Bohr radius corresponds to two well widths. In the case of an infinite-potential barrier in the variational scheme, the virial theorem value also approaches the exact two-dimensional value of two 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 [20].

The fractional-dimensional and variational results [11] for the binding energies of donors at the axis of a cylindrical GaAs/$Ga_{1-x}Al_x$As wire are presented in figure 3(a). We notice that, for infinite-barrier potentials, the fractional dimension (not shown here) goes from one to three as the wire radius goes from zero to infinite, and the donor binding energy varies from infinite (the 1s state has infinite binding energy in a strictly one-dimensional hydrogenic system [22, 23]) to a bulk-like 1 R_0, respectively, as one would expect. A decrease of the barrier potential (or decrease of the Al concentration) leads to a smaller donor binding energy, with the fractional dimension reducing to about two with decreasing wire radius and then going up to three when the radius size reaches some critical value with the donor wave function leaking into the barrier $Ga_{1-x}Al_x$As material. A comparison between fractional-dimensional results and a donor variational [11] calculation indicates good agreement for the binding energies in the cases of moderate and large values of the wire radius. Results for the quantum-confined donor Bohr radii are shown in figure 3(b) as functions of the wire radii in GaAs/$Ga_{1-x}Al_x$As QWWs, both for $x = 0.30$ and infinite-barrier potentials. As in the QW case, the variational procedure leads to larger donor Bohr radii in comparison with the fractional-dimensional results.

The on-axis donor binding energy and virial theorem value are shown in figure 4 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/$Ga_{1-x}Al_x$As QWWs. As before, the fractional-dimensional approach leads approximately (see appendices A and B and

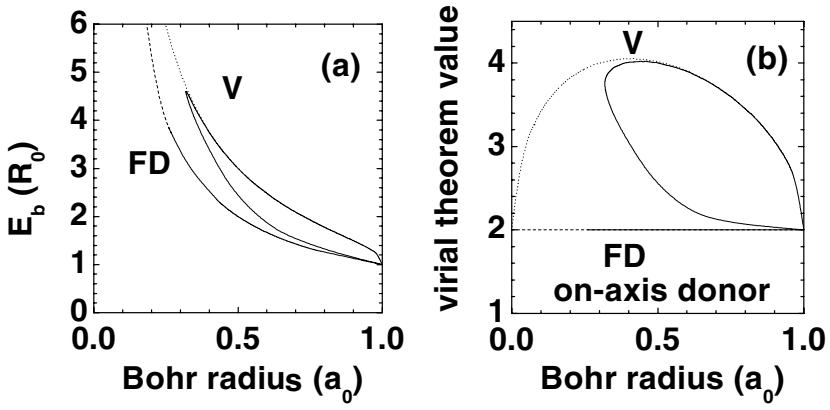

Figure 4. On-axis donor binding energies (a) and virial theorem value (b) as functions of the quantum-confined donor Bohr radius in GaAs/$Ga_{1-x}Al_xAs$ QWWs, both for $x = 0.30$ (full curves) and infinite-barrier potentials, with calculations within the variational (V) or fractional-dimensional (FD) approaches. In the cases of infinite-barrier potentials, the dotted (dashed) curve is for results using the variational (fractional-dimensional) approach.

equations (2.10) and (2.11)) 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 [20], 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 two 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 figure 2. Also, in the case of infinite potential in the variational scheme, the virial theorem value approaches the exact [20] one-dimensional value of two for a vanishing QWW radius.

4. Conclusions

We have presented a detailed 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, we have analytically demonstrated that if the three-dimensional actual anisotropic semiconductor heterostructure may be substituted by a fractional-dimensional effective medium with a ground-state wave function given approximately by $\phi^*_{\mathrm{E},1\mathrm{s}} = \mathrm{e}^{-\lambda \mathrm{r}}$ 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.

Acknowledgments

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Appendix A

The fractional-dimensional parameter D may be obtained through equation (2.6),

$$\int_0^\infty \int_0^\pi hr^2 \sin\theta\, \phi_{\rm E}^* W \phi_j \,{\rm d}\theta\, {\rm d}r = 0 \tag{A.1}$$

which is a transcendental equation for D, by choosing ϕ_j as the ground-state solution of the D-dimensional problem, i.e., $\phi_{j=0} = {\rm e}^{-\lambda r}$ with $\lambda = 2/[a_0(D-1)]$, where $a_0 = \frac{\hbar^2 \varepsilon}{m^* e^2}$ is the reduced Bohr radius. One obtains, by using (2.5) for the W operator,

$$\int_0^\infty \int_0^\pi hr^2 \sin\theta \phi_{\rm E,1s}^* \left(\frac{\beta}{r} + \frac{1}{h}\frac{\partial h}{\partial r}\right) {\rm e}^{-\lambda r} \,{\rm d}\theta\, {\rm d}r = 0 \tag{A.2}$$

where we are now concerned with the 1s-like ground-state eigensolution of (2.1). After some tedious although straightforward transformations, one obtains

$$(\beta - 2)\int_0^\infty \int_0^\pi r^2 \sin\theta \left(\frac{h}{r}\right) \phi_{\rm E,1s}^* {\rm e}^{-\lambda r} \,{\rm d}\theta\, {\rm d}r + \int_0^\infty \int_0^\pi r^2 \sin\theta h {\rm e}^{-\lambda r} \left(\lambda \phi_{\rm E,1s}^* - \frac{\partial \phi_{\rm E,1s}^*}{\partial r}\right) {\rm d}\theta\, {\rm d}r = 0 \tag{A.3}$$

which, in the effective-mass approximation, is an exact equation for determining the D parameter associated with the fractional-dimensional effective isotropic environment. As the exact $\phi_{\rm E,1s}(\boldsymbol{r})$ 1s-like wave function is not known, we assume that the approximation $\phi_{\rm E,1s}^* \approx {\rm e}^{-\lambda r}$ would be valid, provided the anisotropy of the actual semiconductor system is not too strong, and obtain

$$D = 1 + 2\sqrt{\frac{a_{\rm I}}{a_0}} \tag{A.4}$$

where we have defined a *quantum-confined impurity Bohr radius* as [19, 20]

$$a_{\rm I} = \langle \psi_{\rm E,1s} | \frac{1}{r} | \psi_{\rm E,1s} \rangle^{-1} \tag{A.5}$$

with co-ordinates taken with the origin at the impurity position.

Appendix B

The potential energy in (2.1) may be written as the sum of the $V_{\rm c}$ Coulomb potential and the $V_{\rm b}$ barrier potential, i.e., $V = V_{\rm c} + V_{\rm b}$. The generalized virial theorem allows one to write [21]

$$2\langle \hat{T} \rangle = -\langle V_{\rm c} \rangle + \langle \boldsymbol{r} \cdot \nabla V_{\rm b} \rangle \tag{B.1}$$

where $\hat{T}$ is the kinetic-energy operator. The donor state energy E is then given by

$$E = \langle \hat{T} \rangle + \langle V_{\rm b} \rangle + \langle V_{\rm c} \rangle = \tfrac{1}{2}\langle V_{\rm c} \rangle + \langle V_{\rm b} \rangle + \tfrac{1}{2}\langle \boldsymbol{r} \cdot \nabla V_{\rm b} \rangle \tag{B.2}$$

and the binding energy $E_{\rm b} = \varepsilon_{\rm c} - E$, where $\varepsilon_{\rm c}$ is the energy of the bottom of the first conduction subband, may be written as

$$E_{\rm b} = -\tfrac{1}{2}\langle V_{\rm c} \rangle \left[1 - \frac{\varepsilon_{\rm c} - \langle V_{\rm b} \rangle - \frac{1}{2}\langle \boldsymbol{r} \cdot \nabla V_{\rm b} \rangle}{\frac{1}{2}\langle V_{\rm c} \rangle}\right]. \tag{B.3}$$

Alternatively, one may write the eigenfunction of (2.1) as $\psi_{\rm E}(\boldsymbol{r}) = f(\boldsymbol{r})\phi_{\rm E}(\boldsymbol{r})$ (cf (2.2)), and obtain

$$\langle \hat{T} \rangle = \varepsilon_{\rm c} + \langle \hat{t} \rangle - \langle V_{\rm b} \rangle \tag{B.4}$$

$$\langle \hat{t} \rangle = -\frac{\hbar^2}{2m^*} \int d^3 r h \phi_{\rm E}^* \left(\nabla^2 \phi_{\rm E} + \frac{\nabla h}{h} \cdot \nabla \phi_{\rm E} \right) \tag{B.5}$$

and, therefore,

$$E = \varepsilon_{\rm c} + \langle \hat{t} \rangle + \langle V_{\rm c} \rangle \tag{B.6}$$

$$E_{\rm b} = -\langle V_{\rm c} \rangle \left(1 + \frac{\langle \hat{t} \rangle}{\langle V_{\rm c} \rangle} \right) = \frac{e^2}{\varepsilon a_{\rm I}} \left(1 - \frac{1}{\beta} \right) \tag{B.7}$$

which relates the donor binding energy to the quantum-confined impurity Bohr radius (cf (A.5)) and to the virial theorem value $\beta = -\langle V_{\rm c} \rangle / \langle \hat{t} \rangle$.

References

[1] Kelly M J 1995 *Low-Dimensional Semiconductors: Materials, Physics Technology, Devices* (Oxford: Clarendon) and references therein
[2] Bastard G 1981 *Phys. Rev.* B **24** 4714
[3] Mailhiot C, Chang Y-C and McGill T C 1982 *Phys. Rev.* B **26** 4449
[4] Greene R L and Bajaj K K 1983 *Solid State Commun.* **45** 825
[5] Greene R L and Bajaj K K 1985 *Phys. Rev.* B **31** 913
[6] Oliveira L E and Falicov L M 1986 *Phys. Rev.* B **34** 8676
[7] Fraizzoli S, Bassani F and Buczko R 1990 *Phys. Rev.* B **41** 5096
[8] Oliveira L E 1988 *Phys. Rev.* B **38** 10641
[9] Bryant G W 1985 *Phys. Rev.* B **31** 7812
[10] Brown J W and Spector H N 1986 *J. Appl. Phys.* **59** 1179
[11] Porras-Montenegro N and Pérez-Merchancano S T 1992 *Phys. Rev.* B **46** 9780
[12] Stillinger F H 1977 *J. Math. Phys.* **18** 1224
[13] He X-F 1991 *Phys. Rev.* B **43** 2063
[14] Christol P, Lefebvre P and Mathieu H 1993 *J. Appl. Phys.* **74** 5626
[15] Thilagam A 1999 *Phys. Rev.* B **59** 3027
[16] Matos-Abiague A, Oliveira L E and de Dios-Leyva M 1998 *Phys. Rev.* B **58** 4072
[17] Reyes-Gómez E, Oliveira L E and de Dios-Leyva M 1999 *J. Appl. Phys.* **85** 4045
[18] Reyes-Gómez E, Matos-Abiague A, Perdomo-Leiva C A, de Dios-Leyva M and Oliveira L E 2000 *Phys. Rev.* B **61** 13104
[19] Rossi F, Goldoni G and Molinari E 1997 *Phys. Rev. Lett.* **78** 3527
[20] Zhang Y and Mascarenhas A 1999 *Phys. Rev.* B **59** 2040
[21] Merzbacher E 1961 *Quantum Mechanics* (New York: Wiley) p 162
[22] Haines L K and Roberts D H 1969 *Am. J. Phys.* **37** 1145
[23] Moss R E 1987 *Am. J. Phys.* **55** 397