Hydrogenic impurity states in quantum-well wires

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The binding energies for the bound states of a hydrogenic impurity placed on the axis of a quantum-well wire are calculated with the use of variational solutions to the effective-mass equation. The quantum-well wire is assumed to be a cylinder of GaAs surrounded by $Ga_{1-x}Al_xAs$. In a very small wire the electrons leak out of the wire and behave as three-dimensional electrons in $Ga_{1-x}Al_xAs$. An abrupt crossover to one-dimensional behavior occurs when the wire radius becomes greater than the radial spread of the bound state. In a very large wire the bound electrons no longer interact with the wire boundary and they behave as three-dimensional electrons in GaAs. In the quasi-one-dimensional regime, the binding energies are greatly enhanced and the wave functions are squeezed radially to fit the wire. In a small wire surrounded by an infinite barrier well, the electrons always behave as quasi-one-dimensional electrons and the binding energy of the $1s$ state becomes infinite when the wire radius vanishes. For a GaAs wire surrounded by $Ga_{0.6}Al_{0.4}As$, the maximum $1s$ binding energy is 6 times greater than the $1s$ binding energy in bulk GaAs and 2–3 times greater than those in comparable two-dimensional quantum wells. The implications of this enhanced binding for recent calculations of the effect of ionized impurity scattering on electron mobility in quantum-well wires are considered. Although scattering by charged impurities effectively limits the mobility in quasi-one-dimensional systems, the enhanced binding substantially reduces the number of available scattering centers.

I. INTRODUCTION

Stimulated by the interest in the physics and technological applications of two-dimensional quantum-well semiconductor structures and superlattices, researchers are now beginning to fabricate and investigate quasi-one-dimensional semiconductor structures. Quantum-well wires (QWW's) of GaAs surrounded by $Ga_{1-x}Al_xAs$ with dimensions as small as 20 nm$\times$10 nm in cross section have been made by Petroff *et al.*, using molecular-beam epitaxy and photolithography.[1] Fowler, Hartstein, and Webb[2] reduced the dimensionality of a two-dimensional quantum well by using a novel electrode configuration to constrict the electrons in the accumulation layer of a metal-oxide–silicon field-effect transistor to a quasi-one-dimensional channel. In theoretical studies,[3,4] the transport properties of GaAs quantum-well wires have been considered to determine whether quasi-one-dimensional wires have the high mobilities characteristic of the layered structures, and to assess the importance of size quantization.[5–7] In this paper a theoretical description of the bound states and the energy spectrum of a hydrogenic donor in a QWW that is made of GaAs, has a circular cross section, and is surrounded by $Ga_{1-x}Al_xAs$, is presented. This calculation is the first to be done for a quantum-well wire, although similar studies have been performed for impurity states and exciton levels in quasi-two-dimensional quantum wells and superlattices.[8–14]

An understanding of the nature of the impurity states in semiconductor structures is one of the crucial problems in semiconductor physics, and thus motivates this study for QWW structures. However, the problem is intrinsically appealing for the following reasons as well.

The QWW is an exciting system to study because the effective dimensionality of the wire can be changed by changing the wire radius. An electron bound to an impurity at the center of a QWW never encounters the boundary in a very large wire and behaves as a three-dimensional electron bound to an impurity in GaAs. For a wire with an intermediate radius, the electron confinement due to the potential well of the conduction-band discontinuity is greater than the confinement due to the impurity, and the electron behaves as a quasi-one-dimensional electron. For very small wires, the well cannot effectively confine the bound electrons, which leak out of the wire and behave as three-dimensional electrons in $Ga_{1-x}Al_xAs$ bound to the impurities and weakly perturbed by the potential well. Comparable changes in dimensionality occur in two-dimensional quantum wells when the thickness is varied.[8,9,13]

Moreover, the effective strength of the Coulomb interaction depends on the dimensionality of the problem and is greatly enhanced when the dimensionality is reduced. The binding energy for the ground state of a hydrogenic impurity in a three-dimensional semiconductor is

$$R_e = Rm_e/\epsilon^2 , \tag{1}$$

where $R=1$ Ry, m_e is the electron effective mass (in units of the electron mass), and ϵ is the static dielectric constant. In a strictly two-dimensional system the binding energy increases to $4R_e$, while in a quasi-two-dimensional quantum well with finite thickness the binding energy is between R_e and $4R_e$.[8–10] In quasi-one-dimensional systems,[15–21] such as the long-chain organic semiconductor polyacetylene[17,18] and hydrogen atoms in high magnetic

fields,[19–21] the binding energies can be much larger. For example, the donor states due to a point charge near a polyacetylene chain are bound by $10R_e$. Thus in QWW's the effective strength of the Coulomb interaction can be changed by varying the wire radius and changing the dimensionality of the wire. Conversely, dramatic changes in the binding energies serve as a blatant signature for changes in the dimensionality of the QWW. Similar effects occur in two-dimensional quantum wells. However, the effects are more striking in QWW's because the enhancement of the Coulomb interaction is much greater when the dimensionality is reduced from three to one, than when it is reduced from three to two.

This large enhancement of the effective Coulomb interaction that results from a reduction of the dimensionality can be understood with the following argument. In a quasi-one-dimensional system such as a QWW, the electron can move only a short distance in the other dimensions, and every path that takes an electron past the impurity must bring it close to the potential singularity. In a higher-dimensional system the electron has more paths that allow it to move around the impurity without passing close to it. Thus the binding of localized electrons should be much greater in lower-dimensional systems. In fact, when a quasi-one-dimensional system approaches the strictly one-dimensional limit, the binding energy of the lowest eigenstate approaches infinity and the state becomes very localized.[15–17] Formally, the strictly one-dimensional Coulomb problem can be solved by realizing that the one-dimensional Schrödinger equation is the same as the three-dimensional radial Schrödinger equation for an s state. Consequently, the binding energies of states in the strictly one-dimensional Coulomb problem should start at R_e and follow the Balmer series of the three-dimensional problem. This result is misleading.[15–17] The infinitely bound state, which occurs as a limit when the strictly one-dimensional case is approached from the quasi-one-dimensional case, is not a formal solution for the strictly one-dimensional case because infinitely bound states do not exist. However, this ambiguity does not change the results for quasi-one-dimensional systems: The binding energy of the lowest state is greatly enhanced and the other states occur at energies close to those of the Balmer series. Figure 1 shows the energy levels of the Coulomb problem and how they shift as the dimensionality is changed.

In this paper GaAs quantum-well wires surrounded by $Ga_{1-x}Al_xAs$ are considered. Petroff *et al.* made wires by using these materials, and most of the calculations for the two-dimensional layers have been done for this pair of materials. The binding energies and the spatial spread of donor states with different symmetry are calculated as a function of the wire size and the surrounding $Ga_{1-x}Al_xAs$ alloy composition. The results provide a useful indicator of the effective dimension of the QWW and of the onset of size quantization. For wires that are quasi-one-dimensional, the binding energies are enhanced and can be 2 to 3 times greater than those in comparable two-dimensional wells.

The consequences of the high binding energies in the quasi-one-dimensional regime should be apparent in the optical spectra of donors in QWW. Moreover, the high binding energies should affect the transport properties of QWW. Recent predictions[4] suggest that scattering from charged impurities inside the QWW will substantially reduce the electron mobility. However, the binding energies are sufficiently high that there may be too few charged impurities to have an effect.

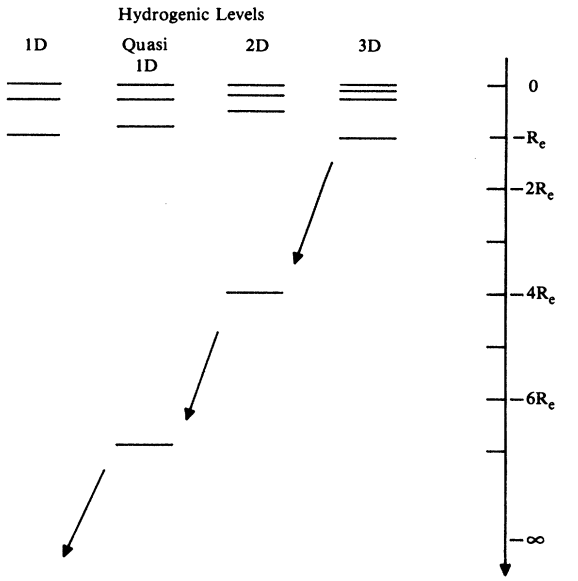

FIG. 1. Energy levels of the Coulomb problem for strictly one-dimensional (1D), quasi-one-dimensional, two-dimensional (2D), and three-dimensional (3D) systems. The arrows indicate how the levels shift as the dimensionality changes.

In Sec. II the model for the QWW and the methods used to find the eigenstates are presented, and the details of the numerical calculations that provide useful insight are discussed. The results are presented in Sec. III, and their relevance to the optical and transport properties of QWW's are discussed briefly in Sec. IV.

II. THEORY

Many choices could be made for the geometry and the composition of the QWW. Wires with rectangular[3] and circular cross sections[4] have been considered in transport calculations. Petroff *et al.* made wires with triangular cross sections.[1] For the calculations described here, the wires are assumed to have circular cross sections, are made of GaAs, and are surrounded by $Ga_{1-x}Al_xAs$. The choice of cylindrical symmetry was made because the calculations are much easier for that geometry. Other choices and the effect of geometry on the binding energies will be considered in future work.

The donor impurity is modeled as a point-charge impurity. For these calculations, the charge is located on the axis of the wire. Again, this assumption was made to simplify the calculation. Even so, a two-dimensional Schrödinger equation with a nonseparable Coulomb potential must be solved. To describe the dielectric screening of the point charge, the simplest approach was chosen. The example of the transport calculations[3,4] and most of

the calculations for the binding energies of point charges and excitons in two-dimensional layers[9–14] was followed, and it was assumed that the point charge is screened by the bulk static dielectric constant of GaAs. To date, only Mailhiot, Chang, and McGill have correctly treated the screening in a two-dimensional quantum well. The assumption made for the screening is motivated by the arguments that the electron is normally well confined to the GaAs wire and that, in any case, the static dielectric constant of GaAs ($\epsilon=13.1$) is not very different from that of $Ga_{1-x}Al_xAs$ [$\epsilon=13.1(1-x)+10.1x$].[8] This choice was made because the screened potential retains a simple form which can be treated analytically to simplify the ultimate numerical calculations. The effects of using a better model for the screening and of moving the impurity off the wire axis will also be considered later.

The electron bound states and their binding energies are found by solving the effective-mass equation.[8–14] Normally, the effective-mass equation is reliable only for weakly bound states, and one might worry that the effective-mass equation is inappropriate when the binding energy is greatly enhanced in quasi-one-dimensional systems. However, the band gap of GaAs is 1.4 eV, while the effective Rydberg $R_e=5.3$ meV. Thus roughly a hundredfold enhancement of the binding energy is necessary before the effective-mass equation becomes inapplicable. This difference is much greater than the enhancement seen in the cases considered here.

The solutions of the Schrödinger equation will be cylindrically symmetric because the point charge is on the wire axis. Thus the envelope wave function is an eigenfunction of the angular momentum L_z along the wire axis, and the wave function can be written as a product

$$\Psi_{nL}(r,z,\theta)=\psi_{nL}(r,z)\exp(iL\theta) , \tag{2}$$

where r, z, and θ are the cylindrical coordinates. The Schrödinger equation to be solved is

$$-\frac{\hbar^2}{2m_1}\nabla^2\Psi_{nL}-\frac{e^2}{\epsilon(r^2+z^2)^{1/2}}\Psi_{nL}=E_{nL}\Psi_{nL} \quad (r<d) \tag{3a}$$

and

$$-\frac{\hbar^2}{2m_2}\nabla^2\Psi_{nL}-\frac{e^2}{\epsilon(r^2+z^2)^{1/2}}\Psi_{nL}+V_0\Psi_{nL}=E_{nL}\Psi_{nL} \quad (r>d) , \tag{3b}$$

where d is the wire radius, V_0 is the discontinuity in the conduction-band edge, m_1 is the electron effective mass in GaAs, and m_2 is the effective mass in $Ga_{1-x}Al_xAs$ (m_0 is the electron mass):

$$V_0=1.06x \text{ eV} , \tag{4a}$$

$$m_1=0.067m_0 , \tag{4b}$$

and

$$m_2=(0.067+0.083x)m_0 . \tag{4c}$$

Equations (3a) and (3b) are solved for bound states subject to the boundary conditions[8,22] at $r=d$, that the envelope wave function and the radial particle current (velocity operator in the radial direction) be continuous. This choice ensures that the Hamiltonian defined by Eqs. (3a) and (3b) is Hermitian on the space of functions which satisfy the boundary conditions.

Equations (3a) and (3b) are solved by expanding the envelope function in terms of products of basis functions of z and r,

$$\psi_{nL}(r,z)=\sum_{i,j}C_{ij}^{(n,L)}f_i^{(L)}(r)g_j(z) . \tag{5}$$

The basis set $\{f_i^{(L)}\}$ is chosen so that each function satisfies the boundary conditions. However, neither the basis set of radial functions $\{f_i^{(L)}\}$ nor the set of z-basis functions $\{g_j\}$ is necessarily an orthonormal set. Eigenstates with different symmetries are investigated by using basis sets with different symmetries. With these basis functions the Hamitonian matrix $\langle ij\,|\,H\,|\,st\rangle$ and the overlap matrix $\langle ij\,|\,st\rangle$ are determined [where $\langle r,z\,|\,ij\rangle \equiv f_i^{(L)}(r)g_j(z)$] and the generalized eigenvalue problem is solved for the energies E_{nL}:

$$\sum_{st}\{\langle ij\,|\,H\,|\,st\rangle-E_{nL}\langle ij\,|\,st\rangle\}C_{st}^{(n,L)}=0 . \tag{6}$$

The energies are minimized by adjusting the parameters that describe the basis functions and by increasing the number of functions used. The binding energies are found by taking the difference between E_{nL} and the subband energy when no impurity is present. For a given symmetry only the eigenstate with the lowest energy is reliably determined because the variational approach is used to obtain a best estimate for the energies.

The z-basis functions $g_j(z)$ were chosen to be Gaussian,

$$g_j(z)=z^q\exp(-\tfrac{1}{2}\xi_j z^2) , \tag{7}$$

where $q=0$ or 1 determines the parity of the state relative to the point charge. Calculations were done, typically, with five Gaussian functions for even states ($q=0$) and seven for odd states. A reliable set of ξ_j was determined by solving the strictly one-dimensional Coulomb problem using the even-parity Gaussian functions. The binding energy could be predicted with less than 0.1% error using the set $\{\xi_j a_e^2\}=\{0.17,0.47,1.4,5.6,39.0\}$, where $a_e=\epsilon(m_0/m_e)a_0$ is a scale factor, the effective Bohr radius, which accounts for the dielectric response ϵ and the effective mass of the material m_e/m_0, and a_0 is the Bohr radius. For bulk GaAs, $a_e=196a_0=10.3$ nm. Solutions with odd z parity have lower binding energy and are more extended along the wire. For these eigenstates the basis set was augmented to include $\xi_j a_e^2=0.02$ and 0.1, which provide more extended basis functions. Most of the results presented here were found with the use of these parameters. Not much additional minimization was obtained by varying them.

Two basis sets were used for the radial basis functions, with each choice best suited for different ranges of the wire radius. For large wires ($d\gtrsim 100a_0$), radial solutions for the free electron in the quantum well were used as basis functions. These solutions are oscillatory Bessel functions of integer order L inside the wire matched at the boundary to decaying Bessel functions of order L.

Typically, qualitatively accurate binding energies could be obtained by using only the lowest subband state. Other subband states were included to obtain more accurate binding energies.

In a small wire with a finite well constraining the electrons to the wire, the electrons leak sufficiently far from the wire that their behavior becomes three dimensional. In these small wires the Bessel function basis set is inappropriate either because only one subband level exists and it cannot accurately describe the three-dimensional nature of the bound state, or because no subband state exists. Instead, for small wires, Gaussian functions were used for the radial basis functions,

$$f_i^{(L)}(r)=r^L\exp(-\tfrac{1}{2}\alpha_i^{(L)}r^2) \quad (r<d) , \tag{8a}$$

$$=Ar^L\exp(-\tfrac{1}{2}\beta_i^{(L)}r^2) \quad (r>d) . \tag{8b}$$

A was chosen to make $f_i^{(L)}$ continuous at the wire boundary, and $\alpha_i^{(L)}$ and $\beta_i^{(L)}$ were chosen to make the particle current continuous,

$$\alpha_i^{(L)}=\beta_i^{(L)}\frac{m_1}{m_2}+\left[\frac{m_2-m_1}{m_2}\right]\frac{L}{d^2} . \tag{8c}$$

In practice, $\beta_i^{(L)}$ takes on values comparable to those used for the z basis set and $\alpha_i^{(L)}$ is determined by Eq. (8c). This procedure ensures that the basis functions are chosen to best describe the three-dimensional Coulomb problem outside the wire when the wire is small and the potential well is a weak perturbation to the Coulomb problem. The calculated binding energies are sensitive to the choices made for the $\beta_i^{(L)}$. Thus the $\beta_i^{(L)}$ were varied extensively, and the size of the basis set was increased to nine or ten functions to obtain accurate results. For most cases the $\{\beta_i^{(L)}\}$ used for the radial basis functions was the set of ξ_i used for the z-basis functions augmented with larger $\beta_i^{(L)}$ to properly describe the extra confinement due to the potential well. Gaussian functions were not used for large radius wires because too many were needed to describe the effects of the potential well even with no impurity present. For large wires the Bessel function basis was better because it already contained the effects of the potential well on the eigenstate.

The overlap integrals and the matrix elements for the kinetic energy and potential well can be evaluated analytically with these basis functions. The z integration for the Coulomb matrix elements can also be done analytically, but the remaining radial integration must be obtained numerically. Attempts to perform the radial integration analytically were frustrated because the radial basis functions change form at the wire boundary.

III. RESULTS

The results for the binding energies and for the root-mean-square spread of the bound states both parallel and perpendicular to the wire are discussed in this section. Calculations were made for three choices of the alloy composition of $Ga_{1-x}Al_xAs$ ($x=0.1$, 0.2, or 0.4) to illustrate how the changeover in dimensionality is affected by the well depth. Calculations were also performed with the assumption that an infinite barrier prevents the electron from leaving the wire.[23] The difference between the results for the infinite- and finite-well wires is striking when the wires become small and the finite-well wire changes from being one dimensional to being three dimensional. A similar dimensional crossover and similar differences between results for infinite and finite wells occur when the wells are two dimensional.[8,9,13] A comparison of these results for QWW's points out the limitations of the infinite-barrier model and the danger of using the model for small wires[3–7] to which it no longer applies.

When the impurity is on the wire axis, the symmetry of a bound state is defined by its even or odd z parity ($q=0$ or 1) and its angular momentum L in the z direction. The lowest-energy states with the symmetries $L=0$, $q=0$; $L=0$, $q=1$; $L=1$, $q=0$; and $L=1$, $q=1$ were studied. They correspond, respectively, to $1s$, $2p_z$, $2p_x$ and $2p_y$, and $3d_{xz}$ and $3d_{yz}$ states. The excited states with these symmetries (e.g., the $2s$, $3p_x$, $3p_z$, and $3p_y$ states) are determined less reliably by the variational method, and will not be discussed.

One of the features apparent in all the results to be presented is the changeover in the effective dimension of the wire as the wire radius changes. This crossover from one-dimensional to three-dimensional behavior, when the wire radius becomes small, is made more obvious when the results for finite-well wires are compared with those for an infinite-well model. In the latter case, the wires remain quasi-one-dimensional no matter how small the wire. A similar result occurs for two-dimensional wells with infinite barriers.[8–14] Moreover, the binding energy of the $1s$ state in the infinite-well model approaches infinity as the wire radius becomes very small, while the binding energy in a finite-well QWW approaches that of the $1s$ state in bulk $Ga_{1-x}Al_xAs$.

The results for the infinite-barrier wire are shown in Fig. 2. The binding energies increase monotonically and the wire becomes more strictly one dimensional as the radius decreases. The centrifugal potential lowers the binding energy when the wire has a finite radius. However, as the wire becomes more strictly one dimensional, the binding energies become insensitive to the angular momentum L. The binding energy of the lowest-energy even-parity state for each L approaches infinity while that of the lowest odd state for each L approaches R_e. At large d the behavior should be three dimensional. Although this conclusion is not completely obvious in Fig. 2, the binding energy of the $2p_x$ state does drop below R_e when $d\gtrsim 600a_0$ and begins to approach that of the $2p_z$ state. Also, for large d the $2p_z$ and $3d_{yz}$ states have different energies. However, even at $1000a_0$ the binding energy of the $1s$ state is $1.15R_e$ and the binding energy of the $2p_x$ state is 50% greater than that of the $2p_z$ state. Thus quasi-one-dimensional effects persist to large radii.

For realistic $GaAs/Ga_{1-x}Al_xAs$ QWW's, the binding energies of the $1s$ and $2p_x$ states are shown in Fig. 3, and the binding energies of the $2p_x$ and $3d_{xz}$ states are shown in Fig. 4. The enhancement of the binding energy by the one-dimensional confinement is clearly the dominant effect. The finite-well results closely follow those for the quasi-one-dimensional infinite-well wire, except for small wires. The bound states in the finite-well wires have

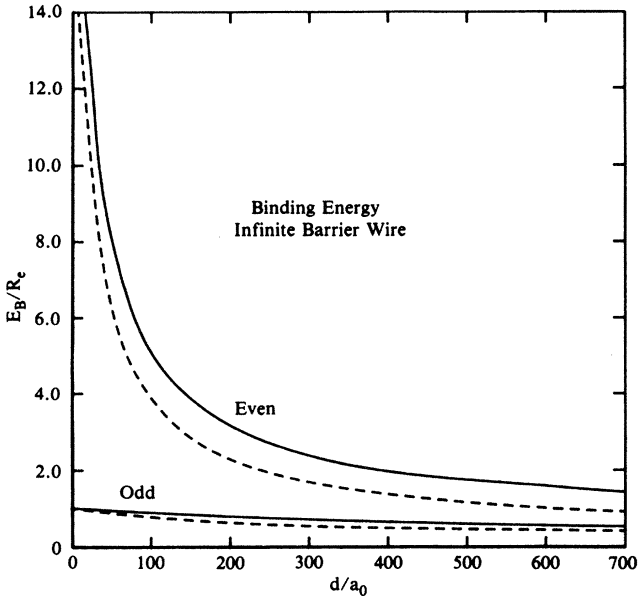

FIG. 2. Binding energy E_B of an electron bound to a hydrogenic impurity on the axis of an infinite-barrier GaAs wire of radius d. The radius is normalized by the Bohr radius a_0, and E_B is normalized by the effective Rydberg R_e in GaAs [see Eq. (1)]. The binding energies for the lowest-energy states with even and odd z parity and with $L=0$ (solid curve) and $L=1$ (dashed) are shown.

slightly lower binding energies because the finite-well wires are less one dimensional. Only the $2p_z$ binding energy in an $x=0.4$ well wire of radius $d\sim 25a_0$ is larger than the corresponding binding energy in the infinite-well wire. The reason for this is not clear. Electrons in realistic QWW's should behave as three-dimensional electrons for $d \gtrsim 1000a_0$, because the results for finite- and infinite-well wires are nearly identical at these d. For all wires the binding energy increases as the Al content x increases. This change occurs because the confining well depth increases as x increases, making the wires more one-dimensional, and because the electron effective mass in $Ga_{1-x}Al_xAs$ increases as x increases, making the electrons easier to bind.

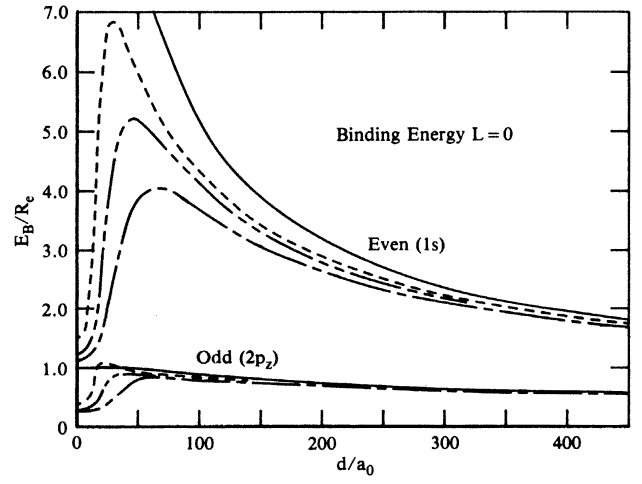

FIG. 3. Binding energies of $L=0$, even- and odd-parity bound states for GaAs wires of radius d surrounded by an infinite barrier (solid curve) and by $Ga_{1-x}Al_xAs$ with $x=0.1$ (dotted-dashed), 0.2 (dashed-double dotted), and 0.4 (dotted).

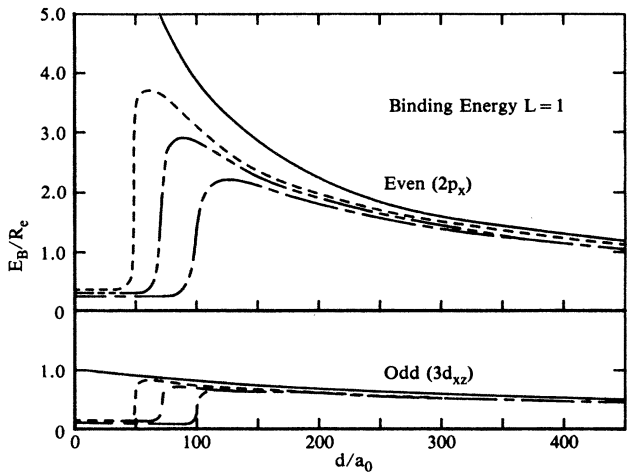

FIG. 4. Binding energy of $L=1$, even- and odd-parity bound states for GaAs wires of radius d surrounded by an infinite barrier (solid curve) and by $Ga_{1-x}Al_xAs$ with $x=0.1$ (dotted-dashed), 0.2 (dashed-double dotted) and 0.4 (dotted).

For a small finite-well QWW the electron behaves as a three-dimensional electron in $Ga_{1-x}Al_xAs$. The crossover from three-dimensional to one-dimensional behavior at small d is dramatic and rapid. The crossover occurs as d changes by $(10-25)a_0$ when $L=0$. When L is finite, the electron is pushed partly out of the wire and this crossover occurs as d changes by only $5a_0$, corresponding to one-half of an atomic layer. One would expect the crossover to be broader if an atomistic model were used for the calculations. When this crossover occurs and the electrons can leak out of the wire, the binding energies become more sensitive to the composition of the $Ga_{1-x}Al_xAs$. For very small wires the binding energy increases proportionally to the area of the wire (d^2), as predicted by lowest-order perturbation theory, because the confining potential is a weak perturbation to the three-dimensional impurity problem. The limiting value of the binding energy for small d is that for bulk $Ga_{1-x}Al_xAs$.

A comparison of the binding energies for the $1s$, $2p_x$, $2p_z$, and $3d_{yz}$ states for one alloy composition is shown in Fig. 5. The crossover from three-dimensional to one-dimensional behavior is obvious in a comparison of the $2p_x$ and $2p_z$ binding energies. When d is large or small the results for the two states are similar. When the wires are quasi-one-dimensional the results are very different. The $2p_x$ state is much more tightly bound than the $2p_z$ state because the $2p_x$ state has even z parity while the $2p_z$ state has odd parity. This increase in binding occurs even though the $2p_x$ state has finite angular momentum and the centrifugal potential tries to push the state from the wire. The centrifugal potential is able to expel the electron only from very small wires, for which the $2p_z$ state has a lower binding energy.

Also shown in Fig. 5 are the results found by assuming

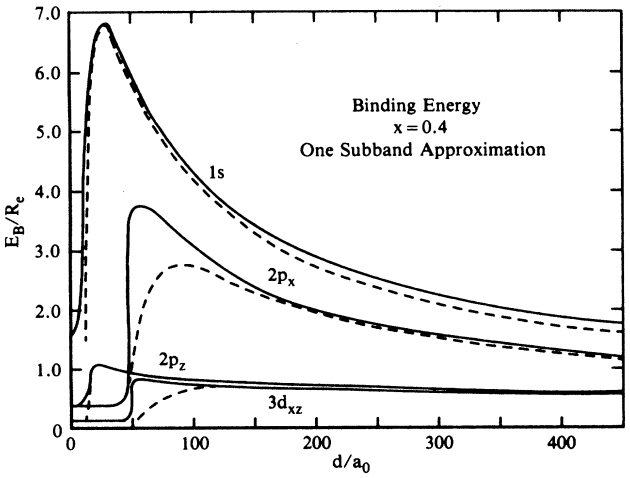

FIG. 5. Comparison of the binding energies of different states for GaAs surrounded by $Ga_{0.6}Al_{0.4}As$. The dashed curves give the binding energies calculated by assuming that the electron is in the lowest subband. The dashed curves end at small d when no subbands exist. For the $2p_z$ and $3d_{xz}$ states, the approximate results are indistinguishable from the solid curves for large radii and are not shown.

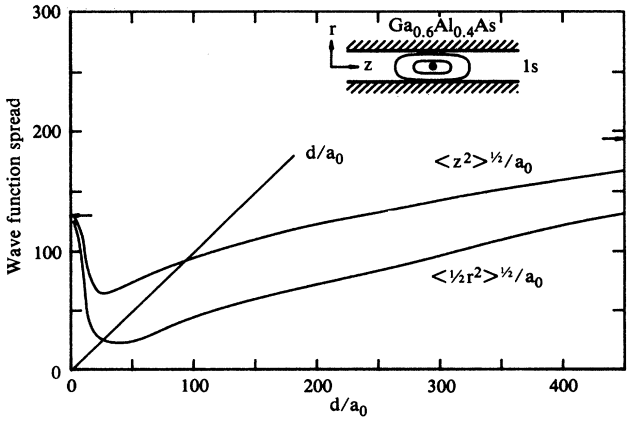

FIG. 6. Spread of the $1s$ bound state for GaAs surrounded by $Ga_{0.6}Al_{0.4}As$. The arrows indicate the $d=0$ and infinity limits. All distances are normalized by the Bohr radius a_0. The effective Bohr radius in GaAs is $196a_0$; in $Ga_{0.6}Al_{0.4}As$, $131a_0$. The inset illustrates the distortion of the wave function.

that the electron is confined to the lowest subband. The surprising accuracy of the approximation over such a large range of d is another indication of the quasi-one-dimensional nature of the wires. This approximation should not describe the three-dimensional nature of the bound state in large wires which is apparent for the $1s$ state. The approximation becomes worse for larger wires, although the error is still only 10%. For states less tightly bound by the impurity, the well confinement is an even more important effect and the approximation is much better. For small d the Coulomb effects dominate the effect of the potential well and the approximation again breaks down. This deficiency is more obvious when $L=1$ because the dimensional crossover occurs at larger d for these states. For very small d the approximation cannot be made because no subband states exist. The Gaussian basis must be used in this case.

The binding energy of the $1s$ state never reaches infinity for the realistic finite-well QWW. However, for small wires it can be substantially larger than the binding energies in three-dimensional ($E_B=R_e$) and strictly two-dimensional ($E_B=4R_e$) systems. The $1s$ binding energies are less than $4R_e$ when the wires are large. However, they are still typically a factor of 2 larger than those calculated by Mailhiot[8] for comparable realistic quasi-two-dimensional GaAs wells in $Ga_{1-x}Al_xAs$.

The spread of the wave function is plotted in Fig. 6 for the $1s$ state, in Fig. 7 for the $2p_x$ and $2p_z$ states, and in Fig. 8 for the $3d_{xz}$ state for a GaAs wire in $Ga_{0.6}Al_{0.4}As$. Results for $x=0.1$ and 0.2 are similar and will not be presented. The quantities plotted are the spread along the wire axis, $\langle z^2\rangle^{1/2}/a_0$, and the radial spread, $\langle \frac{1}{2}r^2\rangle^{1/2}/a_0$. The brackets denote the expectation value for the particular state. The radial spread is defined with a factor of $\sqrt{1/2}$ so that the radial and z spread will be equal for the $1s$ state in the three-dimensional limit. When the wires are quasi-one-dimensional, the enhanced binding constricts the bound state in both the z and radial directions. In addition, the bound states are distorted so that they are cigar-shaped and conform to the geometry of the wire. For example, the radial and z spread of the $1s$ state are much smaller than in bulk GaAs. The state is not spherical in the wire except for small or large d because the radial spread is much smaller than the z spread. Of the states considered, only the $2p_x$ state has a larger radial spread than z spread when the bound state is three dimensional. However, even this state becomes cigar-shaped when it is one dimensional.

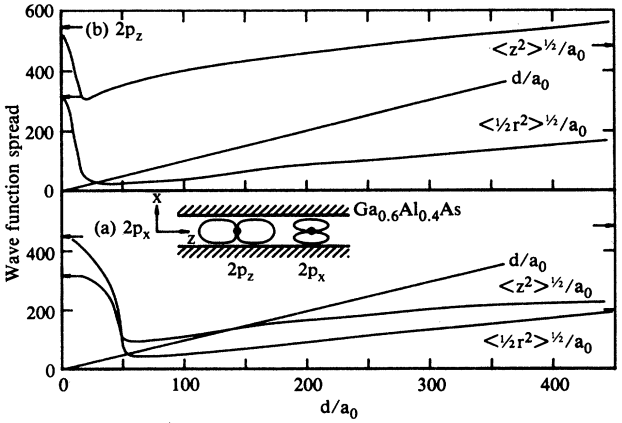

FIG. 7. Spread of the (a) $2p_x$ and (b) $2p_z$ bound states for GaAs surrounded by $Ga_{0.6}Al_{0.4}As$. The $d=0$ limits are indicated by arrows. For the $2p_z$ state the limit when d becomes infinite is indicated by the arrow for the radial spread and is $830a_0$ for the z spread. For the $2p_x$ state the limit for the radial spread is $677a_0$ and the limit for the z spread is indicated by the arrow.

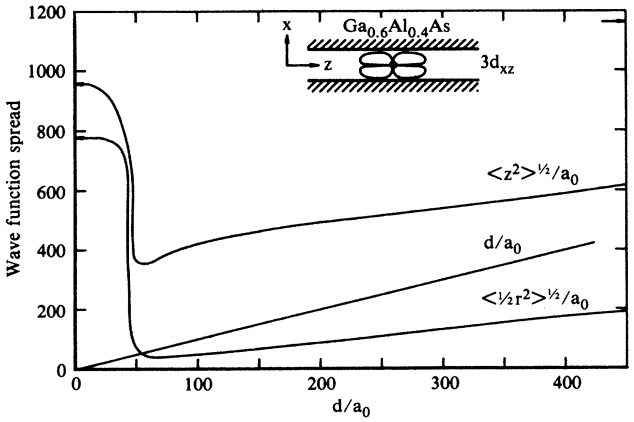

FIG. 8. Spread of the $3d_{xz}$ state for GaAs surrounded by $Ga_{0.6}Al_{0.4}As$. The arrows indicate the $d=0$ and d very large (radial spread only) limits. The limit for the z spread for large d is $1440a_0$.

The crossover from three-dimensional to one-dimensional behavior of the wire is directly correlated to the abrupt change in the way the radial spread varies with the wire radius. This crossover occurs for each of the states when the radial spread equals the wire radius. The wire is one dimensional when the radial spread is less than d and the electrons are confined to the wire, and three dimensional when the radial spread is greater than d.

IV. DISCUSSION AND SUMMARY

The binding energies for the bound states of a hydrogenic impurity placed on the axis of a quantum-well wire have been calculated. The QWW is a cylinder of GaAs surrounded by $Ga_{1-x}Al_xAs$. For very small wires, the electrons leak out of the wire and behave as three-dimensional electrons in $Ga_{1-x}Al_xAs$. As the wire size increases, an abrupt crossover from three-dimensional to one-dimensional behavior occurs when the radial spread of the wave function becomes smaller than the wire radius and the electron no longer leaks out of the wire. The strong enhancement of the binding energy is a dramatic signature of this crossover. Moreover, the wire remains quasi-one-dimensional out to the largest radii ($1000a_0$) studied here. Similar effects occur in two-dimensional wells.

This strong enhancement of the binding energy should have important consequences for optical studies and for transport measurements on QWW's. For example, Petroff[1] has observed cathodoluminescence in QWW's which he attributes to transitions involving exciton states. The observed transitions occur at (8—10)-meV higher binding energy than those in two-dimensional quantum wells, and the lines are much broader. These results for excitons are consistent with the results for hydrogenic impurities. The $1s$ binding energies of hydrogenic impurities in QWW's can be 10 meV greater than those in comparable two-dimensional wells.[8] Thus the increased binding observed by Petroff *et al.* is consistent with the enhancement of the Coulomb interaction expected when the system is quasi-one-dimensional. Moreover, one might expect broader luminescence for QWW's than for two-dimensional wells. The binding energy is more enhanced in quasi-one-dimensional systems and is more sensitive to the location of the impurity or exciton relative to the well boundary.

Recent calculations of the carrier mobility in QWW's have considered the contributions of charged impurity scattering by impurities outside[3,4] and inside[4] the wire. It was suggested[4] that the enhanced scattering by charged impurities inside the quasi-one-dimensional wire should greatly reduce the electron mobility in small wires. The results presented here show that the binding energy also increases rapidly as the QWW becomes smaller, thus reducing the number of ionized impurities. In addition, for very small wires the crossover to three-dimensional behavior occurs and the scattering is no longer enhanced by one-dimensional confinement. Thus a large reduction in mobility from scattering by impurities inside the wire need not occur.

Boundary effects should have a major influence on the physics of electrons in small structures any time that the electron wavelength is comparable to the device dimension. The quasi-one-dimensional nature of the impurity levels in QWW's and the abrupt crossover behavior are dramatic evidence of the importance of boundary effects in QWW structures. These results have been illustrated qualitatively using the specific example of a cylindrical wire and an impurity on the wire axis. In small semiconductor structures the actual shape of the wire and the location of the impurity should strongly influence the quantitative results because the influence of the boundary is so important.

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[22]Continuity of the envelope function and the particle current is not the only set of boundary conditions that can be chosen [see T. Ando and S. Mori, Surf. Sci. 113, 124 (1982)]. They suggest boundary conditions for $GaAs/Ga_{1-x}Al_xAs$ interfaces with small discontinuities in the envelope function and the particle current. The discontinuities are chosen so that the Hamiltonian remains Hermitian. I have also performed calculations for QWW's by assuming that the envelope function and its derivative are continuous. However, in this case the boundary conditions do not guarantee that the Hamiltonian is Hermitian. The binding energies can be found only after the Hamiltonian is forced to be Hermitian by arbitrarily adjusting the off-diagonal elements below the main diagonal to satisfy the Hermitian condition. The binding energies found by using these boundary conditions are qualitatively similar to those found by assuming that the particle current is continuous. The results should be insensitive to other possible choices of similar boundary conditions. This is understandable, since a first-order change in a variational wave function causes a second-order change in the energy.
[23]For an infinite-barrier well a basis set of Bessel functions can be used for each wire radius because a complete set of subband states exists for each wire radius.