Exciton binding energy in a quantum-well wire

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A model calculation is performed of the ground-state energy of an exciton confined to a quantum-well-wire system as a function of the well's width and depth, using a variational approach. The variational wave functions used in the calculation are taken as the product of the appropriate confining Bessel functions and a hydrogenic (exponential) function. For an infinite confining potential well, the binding energy diverges as the well width decreases, while for a finite confining potential well, the binding energy reaches some peak value and then decreases to its value in the bulk material surrounding the wire. It is also shown that the optical absorption coefficient for a quantum-well wire diverges with decreasing wire size when using an infinite-confining-well model. However, for the finite-well model the coefficient reaches a peak value with decreasing wire size, and then drops to its bulk material value.

I. INTRODUCTION

With the development of new experimental crystal-growth techniques, semiconducting structures of dimensions comparable to the electronic de Broglie wavelength have been fabricated.[1-5] Such quantum-well structures alter by their very size the electronic and optical properties of the constituent semiconducting materials. For example, enhanced exciton binding energies[1] and very high electronic mobilities[3] have been reported for modulation-doped quantum-well layers of GaAs-$Ga_{1-x}Al_xAs$. Furthermore, calculations have been performed showing enhanced impurity binding energies in both layered quantum-well structures and quantum-well wires.[6-11]

Initial quantum-well research focused on quasi-two-dimensional (Q2D) systems.[4,12,13] Bastard *et al.*[12] calculated the binding energy of an exciton confined in an infinite potential well while Greene, Bajaj, and Phelps[13] calculated the exciton binding energy in a finite potential well. They found an enhancement of the binding energy which depended on the width and depth of the potential well. In a Q1D system, the enhancement in the binding energy of the exciton is expected to be greater than it is in a Q2D system, due to the additional confinement of the carriers in this kind of structure. In this paper, a model calculation of the ground-state binding energy of an exciton confined in a quantum-well wire by either infinite or finite cylindrical potentials will be performed using a variational approach. The variational wave function we use incorporates a hydrogenic part and appropriate Bessel functions to take into account the confinement of the carriers in a cylindrically symmetric wire. The variational wave function determined here is also used to calculate the intensity of the exciton peak in a quantum-well wire.

II. EXCITON BINDING ENERGY

The effective-mass approximation is used in constructing the Hamiltonian for the interacting electron-hole pair which forms the exciton. For a single electron-hole pair, the Hamiltonian of the system is given by

$$H=(p_1^2/2m_1)+(p_2^2/2m_2)+V_1(\boldsymbol{\rho}_1)+V_2(\boldsymbol{\rho}_2) -[e^2/\kappa(|\boldsymbol{\rho}_1-\boldsymbol{\rho}_2|^2+z^2)]^{1/2} . \quad (1)$$

Here, the subscripts 1 and 2 refer to quantities associated with the electron and the hole, respectively. The variable z gives the relative separation of the electron and the hole along the axis of the wire.

In our variational calculation using the infinite-well model, we take a trial wave function of the form

$$\Psi(\mathbf{r}_1,\mathbf{r}_2)=\begin{cases} NJ_0(k\rho_1)J_0(k\rho_2)\exp\{-\lambda[(\boldsymbol{\rho}_1-\boldsymbol{\rho}_2)^2+z^2]^{1/2}\}, & \rho_1 \text{ and } \rho_2 \le d \\ 0 \quad \rho_1 \text{ or } \rho_2 \ge d. \end{cases} \quad (2)$$

Here, the motion of the center of mass of the system has been neglected and λ is the variational parameter. In order to satisfy the boundary condition that $\Psi(\rho=d,\theta,z)=0$, kd is the first zero of $J_0(k\rho)$. The normalization constant N is given by $N^{-2}=-4\pi^2(dG_0/d\lambda)$, where

$$G_0=\int_0^d d\rho_1\rho_1 J_0^2(k\rho_1)\int_0^d d\rho_2\rho_2 J_0^2(k\rho_2)I_0(2\lambda\rho_<) \times K_0(2\lambda\rho_>) . \quad (3)$$

Equation (2) satisfies the boundary condition that the wave function vanish for either $\rho_1=d$ or $\rho_2=d$. It also approaches the exact solution to the Hamiltonian in the

1D and 3D limits where either $d \to 0$ or $d \to \infty$.

Subtracting the ground-state energy in the absence of the Coulomb interaction, the exciton binding energy is defined as

$$E_b(d) = [(\hbar k)^2/2\mu] - \varepsilon(d) = -(\hbar^2/2\mu)\lambda^2 - (2e^2/\kappa)[d(\ln G_0)/d\lambda]^{-1} \quad (4)$$

which is a positive quantity. Here $\varepsilon(d)$ is the expectation value of the energy. Maximizing Eq. (4) with respect to λ, we obtain the ground-state binding energy. The radial integrations and the maximization of the functions thereof are completed numerically. Our calculations are done for wires of circular cross section to minimize the numerical integrations involved. Figure 1 shows the exciton binding energy as a function of $y = d/a$. For $y \to 0$, the binding energy diverges because the electron and hole are being brought ever closer together by the infinite confining well, while for $y \to \infty$, the binding energy approaches R, where $R = e^2/2\kappa a$ is the exciton Rydberg unit in the well and $a = \kappa h^2/\mu e^2$ is the exciton Bohr radius. In the infinite-well model, the integrals can be expressed in a dimensionless form and it is found that the binding energy depends only upon the parameters of the wire and not those of the cladding.[14]

In a more realistic approximation, the confining potentials in the Hamiltonian are taken as zero for $\rho < d$, and some finite value for $\rho > d$. The confining well depths for the electron and hole are determined by the potential discontinuities between the conduction and valence bands of the well and the cladding which in turn depends upon the Al concentration x in the cladding.[15] In our calculations, we used the values $x = 0.1$, $Q_e/Q_h = 0.60/0.40$ for the light-hole exciton. Q_e is the fraction of potential discontinuity in the conduction band and Q_h is the fraction of the discontinuity in the valence band. The values of the effective masses are taken to be those of GaAs in an isotropic parabolic band model. All the other assumptions remain the same as those made in the infinite-well calculations.

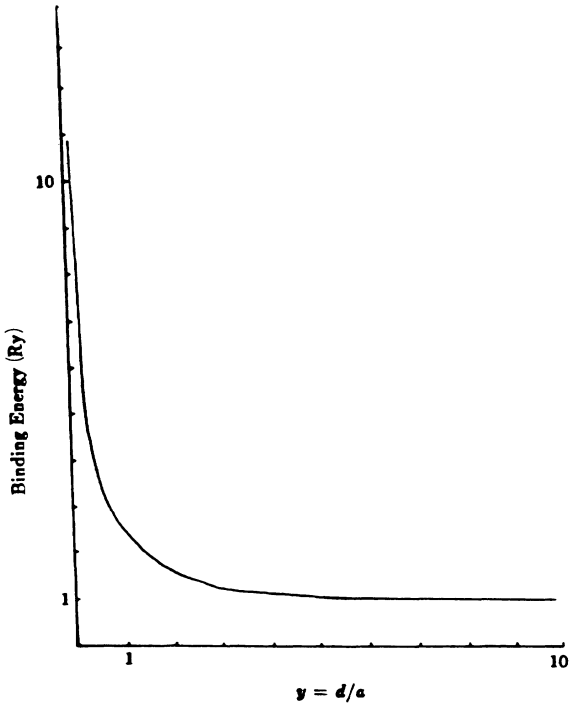


FIG. 1. Binding energy of excitons in a quantum-well wire as a function of the wire radius using an infinite potential well model.

The boundary conditions are that the constituent wave function and its first derivative normal to the potential boundary are continuous at the potential boundaries. The ground-state variational wave function is taken as

$$\Psi(\mathbf{r}_1,\mathbf{r}_2) = \begin{cases} (NJ_0(g\rho_1)J_0(h\rho_2)\exp\{-\lambda[(\boldsymbol{\rho}_1-\boldsymbol{\rho}_2)^2+z^2]^{1/2}\}, & \rho_1 \text{ and } \rho_2 \le d \\ N[J_0(gd)/K_0(jd)]K_0(j\rho_1)J_0(h\rho_2)\exp\{-\lambda[(\boldsymbol{\rho}_1-\boldsymbol{\rho}_2)^2+z^2]^{1/2}\}, & \rho_1 \ge d \text{ and } rh_2 \le d \\ N[J_0(hd)/K_0(md)]J_0(g\rho_1)K_0(m\rho_2)\exp\{-\lambda[(\boldsymbol{\rho}_1-\boldsymbol{\rho}_2)^2+z^2]^{1/2}\}, & \rho_1 \le d \text{ and } \rho_2 \ge d \\ N[J_0(jd)J_0(hd)/K_0(md)K_0(jd)]K_0(j\rho_1)K_0(m\rho_2)\exp\{-\lambda[(\boldsymbol{\rho}_1-\boldsymbol{\rho}_2)^2+z^2]^{1/2}\}, & \rho_1 \text{ and } \rho_2 \ge d, \end{cases} \quad (5)$$

where the parameters g,j,h and m are determined by the boundary conditions. The normalization factor N is given by $N^{-2} = -4\pi^2(d/d\lambda)[G_0+G_1+G_2+G_3]$, with

$$G_1 = [J_0(gd)/K_0(jd)]^2 \int_d^\infty d\rho_1\rho_1 K_0^2(j\rho_1)K_0(2\lambda\rho_1) \int_0^d d\rho_2\rho_2 J_0^2(h\rho_2)I_0(2\lambda\rho_2) , \quad (6)$$

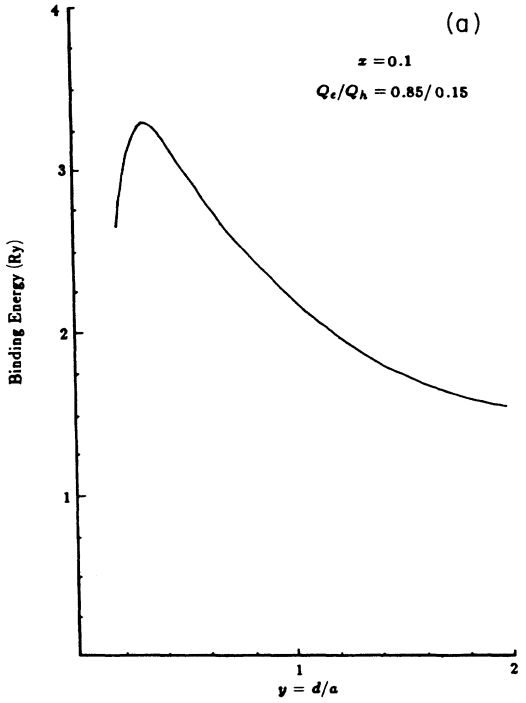
$$G_2 = [J_0(hd)/K_0(md)]^2 \int_0^d d\rho_1\rho_1 J_0^2(g\rho_1)I_0(2\lambda\rho_1) \int_d^\infty d\rho_2\rho_2 K_0^2(m\rho_2)K_0(2\lambda\rho_2) , \quad (7)$$

and

$$G_3 = [J_0(jd)J_0(hd)/K_0(md)K_0(jd)]^2 \int_d^\infty d\rho_1\rho_1 K_0^2(j\rho_1) \int_d^\infty d\rho_2\rho_2 K_0^2(m\rho_2)I_0(2\lambda\rho_<)K_0(2\lambda\rho_>) . \quad (8)$$

Defining the exciton binding energy as before, we have

$$E_b(d) = (\hbar^2/2)(g^2/m_1 + h^2/m_2) - \varepsilon(d) = -(\hbar^2/2\mu)\lambda^2 - (2e^2/\kappa)[(d/d\lambda)\ln(G_0+G_1+G_2+G_3)]^{-1} . \quad (9)$$



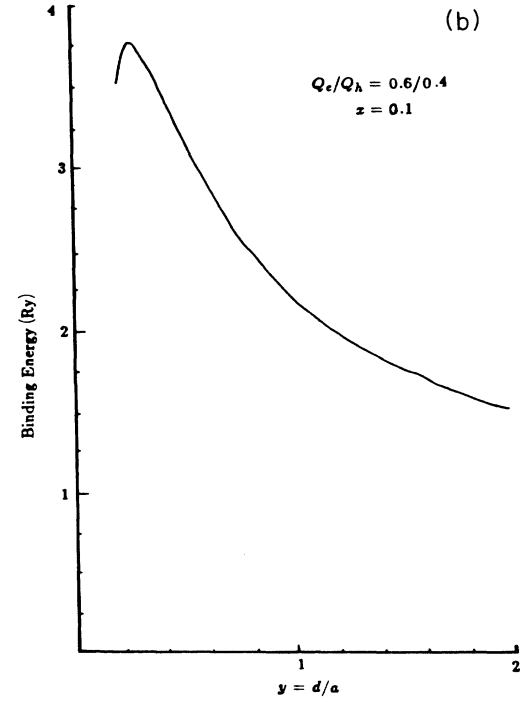
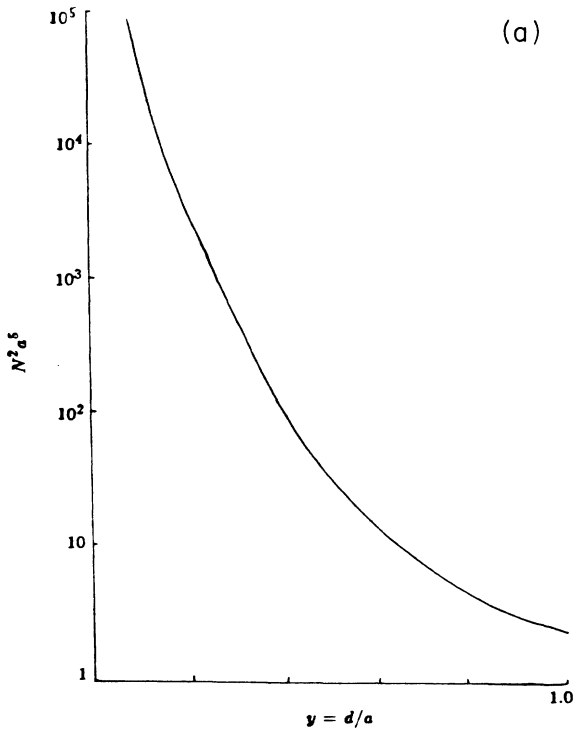


FIG. 2. (a) Binding energy of the heavy-hole exciton as a function of the wire radius using a finite potential well model. The parameters used in the calculation are characteristic of GaAs surrounded by a $Ga_{0.0}Al_{0.1}As$ cladding with the value of the ratio $Q_e/Q_h = 0.85/0.15$. (b) Binding energy of the light-hole exciton as a function of the wire radius using a finite potential well model. The parameters used in the calculation are the same as in (a) except that the value of the ratio $Q_e/Q_h = 0.60/0.40$ is used.



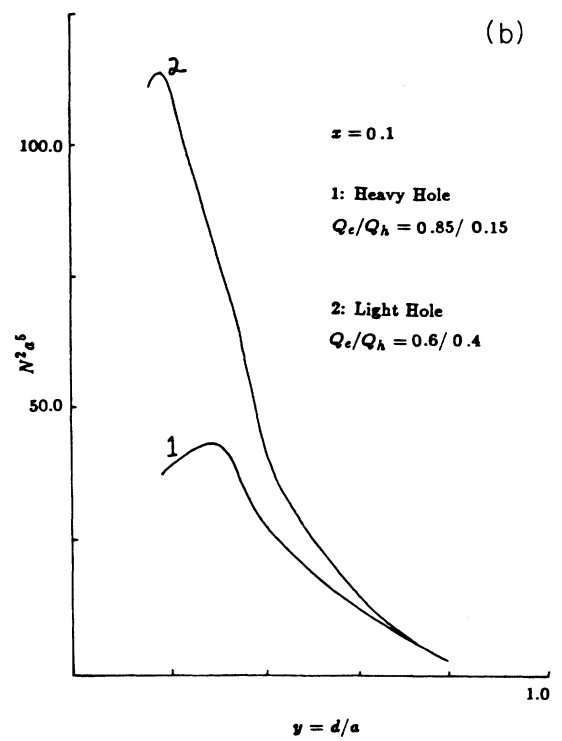


FIG. 3. (a) The normalized optical absorption due to excitons in a quantum-well wire is shown as a function of wire radius in the infinite potential well model. (b) The normalized optical absorption due to excitons in a quantum-well wire is shown as a function of wire radius using the finite potential well model. The parameters used are as given in Fig. 2.

As in the infinite-well case, one can express the binding energy in a dimensionless form. However, the Rydberg-normalized binding energies depend upon the materials chosen for the wire and its cladding, through the potentials V_1 and V_2, unlike the case for the infinite potential well.[14] The maximization of the equation for the binding energy given by Eq. (9), as well as the integrations, were completed numerically. Because of the large amount of computer time needed for the numerical integrations, the binding energy was only evaluated for y values in the range $0.2 < y < 2.0$. The heavy-hole exciton binding energy as a function of y is shown in Figure 2a. For increasing y the binding energy approaches the value of the Rydberg unit in the well, while for $y \rightarrow 0$, the binding energy approaches the value of the Rydberg unit in the cladding. The peak in the binding energy occurs for the smallest value of y for which the probability of the electron or hole being found outside the well is not significant. Figure 2(b) shows the light-hole exciton binding energy. The same general behavior is observed as for the case of the heavy-hole exciton.

Elliot[16] has shown that the intensity at the exciton peak in a bulk semiconducting crystal is proportional to the associated density of states of the electron-hole pair and to the magnitude squared of the exciton wave function for vanishing relative separation between the electron and the hole. Lederman and Dow[17] have studied the optical absorption due to a strictly two-dimensional exciton in a uniform electric field and found similar behavior except that the density of states of the electron-hole pair is two dimensional in this case. In the problem considered here, the density of states is one dimensional because of the two-dimensional confinement of the electron-hole pair in the wire. For the variational wave function used here, the value of the wave function for vanishing separation between the electron and the hole is directly proportional to the normalization coefficient. Thus, the optical absorption coefficient is proportional to the square of the normalization coefficient, N^2. Figure 3(a) shows the dimensionless quantity N^2a^5 as a function of the wire size y using the infinite-well model. In this figure, one sees that the optical absorption coefficient drops to its bulk material value for $y \rightarrow \infty$ and diverges for $y \rightarrow 0$. Figure 3(b) shows the quantity N^2a^5, as a function of y of both light- and heavy-hole excitons using the finite-well model. Again, this quantity approaches its $3D$ value as $y \rightarrow \infty$ but as $y \rightarrow 0$, it reaches a peak value and then decreases.

III. DISCUSSION

We have used a variational approach to determine the ground-state binding energy of an exciton in a quantum-well wire. The exciton binding energy is found to be enhanced using both the infinite and finite potential well models as is the intensity at the exciton peak in a quantum-well wire. The enhancement in both the binding energy and the intensity occur because the confining potential is forcing the electron and hole closer together.

The models used in our calculations are deficient in that they neglect the anisotropy of the carrier masses in GaAs and the change in the effective masses between the GaAs quantum well and its $GaAs_{1-x}Al_xAs$ cladding. However, we believe that the model used here should yield a good zeroth-order approximation to the dependence of the exciton binding energies and the intensity of the optical absorption at the exciton peak on the radius of the quantum-well wire in real quantum-well wires.

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