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Screening of Donors in GaAs/$Ga_{1-x}Al_xAs$ as Quantum Dots.

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We have carried out variational model calculations of the binding energy of a screened donor in a spherical GaAs/$Ga_{1-x}Al_xAs$ quantum dot as a function of the quantum dot radius. We have found that the effect of screening on the binding energy of the donor becomes more pronounced as the radius of the quantum dot decreases. This behavior is similar to that obtained earlier in model calculations of the binding energy of a donor in a quantum well, or in a quantum-well wire.

INTRODUCTION

Reduced dimensionality systems, such as a quantum well (QW), a quantum-well wire (QWW), or a quantum dot (QD), have received much attention in the last few years. Due to the small size of these structures, a physical property, such as the binding energy of a donor, proved to be different from that in the bulk semiconductor.

The binding energy of a hydrogenic donor in a $Ga_{1-x}Al_xAs$/GaAs/$Ga_{1-x}Al_xAs$ QW has been calculated by Bastard[1,2] who applied a variational approach. The screening of a donor ion in a QW by the valence electrons of GaAs has been considered by Csavinszky and Elabsy,[3] who used a screening function of Resta.[4] The binding energy of a hydrogenic donor in a GaAs/$Ga_{1-x}Al_xAs$ QWW of circular cross section has been calculated by Brown and Spector[5] using a variational approach. The screening

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of a donor ion by the valence electrons of GaAs in a QWW has been considered by Csavinszky and Oyoko[6,7] who used the screening function of Resta.[4] These calculations revealed that the screening of the donor ion leads to a significant effect on the binding energy of the donor electron. It was found that the screening effect becomes more pronounced with the reduction of the width of the QW, and the reduction of the radius of the QWW. Recently, the binding energy of hydrogenic impurities in a GaAs/$Ga_{1-x}Al_xAs$ QD of radius R has been investigated by Porras-Montenegro and Pérez-Merchancano.[8] These authors have performed variational calculations both for an infinite confining potential, and for a finite confining potential.

In this paper, we restrict ourselves to the case of a screened donor located at the center of a GaAs/$Ga_{1-x}Al_xAs$ QD and, for the purpose of a model calculation, we assume an infinite confining potential betweeen the two materials. Our approach is a variational approach and our units are atomic units, (the unit of energy is the hartree, unit of length is the bohr, unit of charge is the magnitude of the electron charge).

THEORY

The Hamiltonian for a screened donor in the center of a spherical QD of radius R is given by

$$H = -\frac{1}{2m^*}\nabla^2 + V_l(r_l) + V_b(r), \tag{1}$$

where

$$V_l(r) = -\frac{1}{\epsilon_l(r)r} \tag{2}$$

and

$$V_b(r) = \begin{cases} 0 & r \le R \\ \infty & r \ge R \end{cases} \tag{3}$$

In Eq. (1), $m^* = 0.0665$ is the scalar effective mass of an electron bound to a singly charged donor ion in GaAs. In Eq. (2), $\epsilon_l(r)$ is the screening function of Resta,[4] given by

$$\epsilon_l(r) = \begin{cases} \epsilon_0 \quad qR_l/\{\sinh[q(R_l - r)] + qr\} & r \le R_l \\ \epsilon_0 & r \ge R_l \end{cases} \tag{4}$$

In Eq. (3), $V_b(r)$ is the confining potential. In Eqs. (2) and (4), the subscript l on $V_l(r)$, $\epsilon_l(r)$, and the screening radius R_l, refers to the word *linearized*. These quantities have been obtained by Resta[4] who linearized a nonlinear Thomas-Fermi equation.

In Eq. (4), $\epsilon_o = 12.58$ denotes the static dielectric constant of GaAs. The screening radius R_1 is obtained by Resta[4] from the relation

$$\sinh (qR_1) / qR_1 = \epsilon_o . \tag{5}$$

For GaAs, $R_1 = 4.428$ a.u.

In Eqs. (4) and (5), the quntitiy q is defined by

$$q = (4\ \kappa_F/\pi)^{1/2} \tag{6}$$

where

$$\kappa_F = (3\ \pi^2 n)^{1/3} . \tag{7}$$

In Eq. (6), κ_F denotes the Fermi wave vector, while in Eq. (7), n denotes the electron concentration in GaAs. The calculation of n has been described in detail by Csavinszky and Elabsy.[3]

The expectation value of $V_l(r)$ can be written as

$$\langle V_l(r)\rangle = -\frac{4\pi N^2}{\epsilon_0}\left[\frac{1}{4R_l}X + \frac{1}{qR_l}Y + Z\right] \tag{8}$$

where

$$X = \frac{1}{\lambda(\lambda^2 + \kappa_{l0}^2)}\left\{\kappa_{l0}^2 (1 - e^{-2\lambda R_l}) - 2\lambda \sin(\kappa_{l0}R_l)\, e^{-2\lambda R_l}\left[\lambda \sin(\kappa_{l0}R_l) + \kappa_{l0}\cos(\kappa_{l0}R_l)\right]\right\} \tag{9}$$

$$Y = \int_{r=0}^{R_l} dr\, \frac{1}{r} \sin^2(\kappa_{l0}r) \sinh[q(R_l - r)]\, e^{-2\lambda r_l} \tag{10}$$

and

$$Z = \int_{r=R_l}^{R} dr\, \frac{1}{r} \sin^2(\kappa_{10}\, r)\, e^{-2\lambda r} . \tag{11}$$

In Eqs. (9), (10), and (11), the quantity λ is a variational parameter in our trial function, chosen as

$$\Psi(r) = \begin{cases} N \dfrac{\sin(\kappa_{l0}\, r)\, e^{-\lambda r}}{r} & r \le R \\ 0 & r \ge R . \end{cases} \tag{12}$$

This function is the same as that used for the unscreened case by Porras-Montenegro and Pérez-Merchancano.[8] In Eq. (12), N is the normalization constant given by; in the work of Porras-Montenegro and Pérez-Merchancano[8] there is an omission. In the expression for N^2, Eq. (13) in the present paper, the factor κ_{l0}^2 in the denominator does not appear.

$$N^2 = \frac{\lambda(\lambda^2 + \kappa_{l0}^2)}{\pi (1 - e^{-2\lambda R})\, \kappa_{l0}^2} \tag{13}$$

where, in Eqs. (9) – (13),

$$\kappa_{10} = \frac{\pi}{R} \tag{14}$$

The next step is the finding of the binding energy, $E_b(R)$, of the donor placed at the center of the QD of radius R. This quantity is defined as the ground state-energy, $\kappa^2_{10}/2m^*$, of the system without the impurity present, minus the impurity ground state energy $\xi(R)$. We can then write

$$E_b(R) = \frac{\kappa^2_{10}}{2m^*} - \xi(R) \tag{15}$$

where

$$\xi(R) = <T> + <V_l(r)> \tag{16}$$

In Eq. (16), $< T >$ denotes the expectation value of the kinetic energy calculated from Eq. (1) with Eq. (12).

DISCUSSION

Our results for the binding energy, based on the extremalization of Eq. (16) with respect to λ, for a series of R values, are presented in Figure 1. Note that in Figure 1 the binding energy E_b is given in meV, and the QD radius R is given in Å. It is seen from Figure 1 that the effect of screening becomes more pronounced as the radius of the QD decreases. This finding is similar to that for a QW, or for a QWW. In the case of a QW, it has been found by Csavinszky and Elabsy[3] that the screening effect is enhanced when the width of the QW is reduced. In the case of QWW, it has been found by Csavinszky and Oyoko[6,7] that the screening effect is enhanced when the radius of the QWW is reduced.

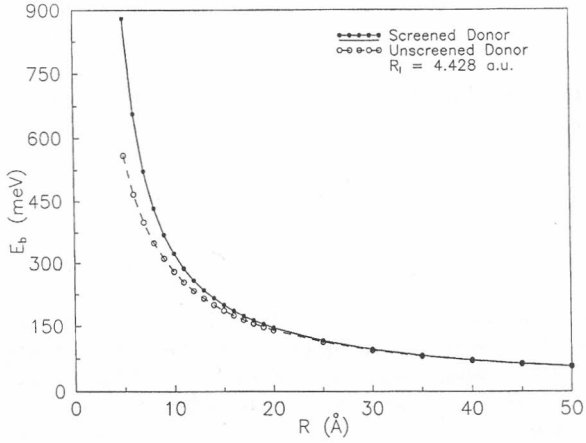

Figure 1. Binding energies (in meV) of screened and unscreened donors in a GaAs/$Ga_{1-x}Al_xAs$ QD of radius R (in Å).

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SAŽETAK

Zasjenjenje donora u kvatnim točkama GaAs/$Ga_{1-x}Al_xAs$

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Provedeni su varijacijski modelni računi za energiju vezivanja zasjenjenog donora u sfernoj kvantnoj točki GaAs/$Ga_{1-x}Al_xAs$ u ovisnosti o njezinu polumjeru. Nađeno je da učinak zasjenjenja na energiju vezivanja donora postaje to izrazitiji što je polumjer kvantne točke manji. To je ponašanje slično onome nađenom ranije za eneriju vezivanja donora u kvatnom loncu i kvantnoj žici.