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Exact solutions for hydrogenic donor states in a spherically rectangular quantum well

Jia-Lin Zhu

Center of Theoretical Physics, Chinese Center of Advanced Science and Technology (World Laboratory), Beijing, China and Department of Physics, Tsinghua University, Beijing, China

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Using different series forms in different regions of the radial equation, we have obtained exact solutions of donor states in a spherically rectangular quantum well by a numerical method. The calculated results show that there are stronger confinement and larger binding energy for a hydrogenic donor in the well of GaAs-$Ga_{1-x}Al_xAs$ than in quantum-well wires and two-dimensional quantum-well structures.

Stimulated by interest in the physics and technological applications of two-dimensional quantum-well semiconductor structures and superlattices, researchers are now beginning to fabricate and investigate GaAs-$Ga_{1-x}Al_xAs$ quantum-well wires (QWW's),[1,2] ribbons, and disks.[3] Understanding the impurity states in the structures is an important problem in semiconductor physics. The impurity levels and exciton states in quasi-two-dimensional quantum wells and superlattices have been well calculated.[4-18] Several calculations[19-22] have also been performed for the hydrogenic impurity levels of QWW's.

All of the calculations mentioned above have shown that the confinement and binding energy of an impurity electron in a quantum well depend on the barrier V_0 and the well size and shape, i.e., the well width for two-dimensional quantum-well structures (TDQW's) and the cross section and its shape for QWW's. The maximum of the binding energy also depends on V_0 and the well shape. For $V_0=40R^*$ (R^* is the effective Rydberg and equal to $m^*e^4/2\hbar\epsilon^2$, where m^* and ϵ are the electronic effective mass and the dielectric constant, respectively, of the semiconductor), the maxima of donor ground states in TDQW's (Ref. 23) and QWW's (Ref. 19) with circular cross section are respectively equal to $2.51R^*$ and $5.22R^*$, and for $V_0=80R^*$, $2.73R^*$ and $6.84R^*$. What about the confinement, binding energy, and its maximum for impurity states in spherically rectangular quantum wells (SRQW's)? In this Rapid Communication, we report for the first time the exact solutions of hydrogenic donor states in SRQW's and provide an answer to the question.

Because the transverse and longitudinal variables do not separate, the impurity states in TDQW's and QWW's cannot be solved exactly and approximation methods should be used. Therefore, it is interesting not only from a physical point of view but also from a mathematical point of view to find out the exact solutions of hydrogenic donor states in SRQW's.

Let us for definiteness consider a donor impurity atom at the center of a SRQW of radius R_0. The potential due to the discontinuity of the band edges at the GaAs-$Ga_{1-x}Al_xAs$ interface $r=R_0$ is as follows:

$$V(r)=\begin{cases}V_0 & \text{if } r\geq R_0,\\ 0 & \text{if } r<R_0,\end{cases} \tag{1}$$

where r is the electron-donor distance. The barrier height V_0 is obtained from a fixed ratio of the band-gap discontinuity. According to the hydrogenic-effective-mass theory, the Hamiltonian for the donor is

$$H=-\nabla^2-\frac{2w}{r}+V(r). \tag{2}$$

It is written in a dimensionless form so that all energies are measured in units of the effective Rydberg R^* and all distances are measured in units of effective Bohr radius a^*. w is equal to one.

In order to solve the Schrödinger-like equation

$$H\psi(r,\theta,\phi)=E\psi(r,\theta,\phi), \tag{3}$$

the wave functions of an electron with well-defined values of the orbital quantum number l and the magnetic one m in the spherically symmetric potential, which is the quantum well and Coulomb potential, are written in the form

$$\psi(r,\theta,\phi)=\psi(r)Y_{lm}(\theta,\phi), \tag{4}$$

where $Y_{lm}(\theta,\phi)$ and $\psi(r)$ are the spherical-harmonic and radial wave functions, respectively. Substituting (4) into (3), we find an equation for the function $\psi(r)$:

$$r^2\frac{d^2\psi(r)}{dr^2}+2r\frac{d\psi(r)}{dr}+\{[E(l)-V(r)]r^2-l(l+1)+2wr\}\psi(r)=0. \tag{5}$$

Using the method of series expansion, we can solve Eq. (5) exactly. It should be noted that zero and infinity are a regular and an irregular singular point of Eq. (5), respectively. In the region $0<r$, we have a series solution, which has a finite value at $r=0$, as follows:

$$\psi(r)=r^l\sum_{n=0}^{\infty}a_nr^n, \tag{6}$$

where

$$a_1=-a_0/(l+1), \tag{7}$$

and

$$a_n=-[2wa_{n-1}+E(l)a_{n-2}]/n(n+2l+1) \qquad n=2,3,4,\ldots; \tag{8}$$

a_0 is a constant. In the region $R_0 < r$, we can obtain a normal solution.[24] It approaches zero at $r = \infty$ and is found in the form

$$\psi(r) = e^{-Kr} r^{\rho} \sum_{n=0}^{N} b_n r^{-n}, \tag{9}$$

where

$$K = \sqrt{V_0 - E(l)}, \tag{10}$$

and

$$\rho = -1 + w/K, \tag{11}$$

$$b_{n+1} = -(\rho - n - l)(\rho - n + l + 1) b_n / 2K(n+1)$$

$$n = 0, 1, 2, \ldots; \tag{12}$$

b_0 is a constant. The series appear suitable for numerical computations for large r.[24] However, they are not suitable for R_0 if R_0 is small. In order to get an exact value at small R_0, we find a solution of uniformly convergent Taylor series in the region $R_0 < r \leq R_p$, where R_p is a proper point for using (9). It is as follows:

$$\psi(r) = \sum_{n=0}^{\infty} c_n (r - R_m)^n + \sum_{n=1}^{\infty} d_n (r - R_m)^n, \tag{13}$$

where R_m is in the region considered and c_0 and d_1 are constants. The other values of c_n and d_n can be determined by the recurrence relations.

Using the matching conditions that ψ and $\nabla\psi/m^*$ are continuous at the interface $r = R_0$ and R_p, we obtain the equation of the eigenenergies $E(l)$. It can be solved numerically. Once the nth eigenenergy $E(l)$ is known, the a_0, b_0, c_0, and d_1 [hence $\psi_n(r)$] are known with use of the normalized condition of $\psi_n(r)$. Thus, $\psi_n(r)$ depends on the value of l, the quantum well, the Coulomb potential, and the energy $E_n(l)$. We should point out that we have neglected the difference of the electronic effective masses between GaAs and $Ga_{1-x}Al_xAs$ in the Hamiltonian and the matching conditions. If the effective-mass difference is considered and the correct matching conditions are used, similar formulas to Eq. (10) are obtained with different values of K. Then, the binding energies become larger for GaAs-$Ga_{1-x}Al_xAs$ quantum wells.[23]

If there is no Coulomb potential in the Hamiltonian of Eq. (2), i.e., $w = 0$, using the same formulas, we can obtain wave functions $\psi_n(r, w = 0)$, and quantum levels $E_n(l, w = 0)$ of an electron in the quantum well. In fact, Eq. (6) and Eq. (9) become the lth-order spherical Bessel function and Hankel function of the first kind if $w = 0$. Therefore the same results are obtained if the wave functions and quantum levels are calculated with use of the Bessel and Hankel functions. Once $E_1(0)$ and $E_1(0, w = 0)$ are obtained, the binding energy of the ground-state of the donor in the quantum well is given by

$$E_B = E_1(0, w = 0) - E_1(0). \tag{14}$$

We have performed a numerical calculation for the GaAs-$Ga_{1-x}Al_xAs$ SRQW of the R_0 between 0 and $2.5a^*$ with different V_0. In Fig. 1, we show quantum levels of ground states in the SRQW of $V_0 = 40R^*$ with and without the Coulomb potential as a function of R_0. The first quantum level of $V_0 = \infty$ without the Coulomb potential is also shown in the figure to compare with that of $V_0 = 40R^*$. It is readily seen that the energy of $V_0 = \infty$ is increased quicker than one of $V_0 = 40R^*$ as R_0 is de-

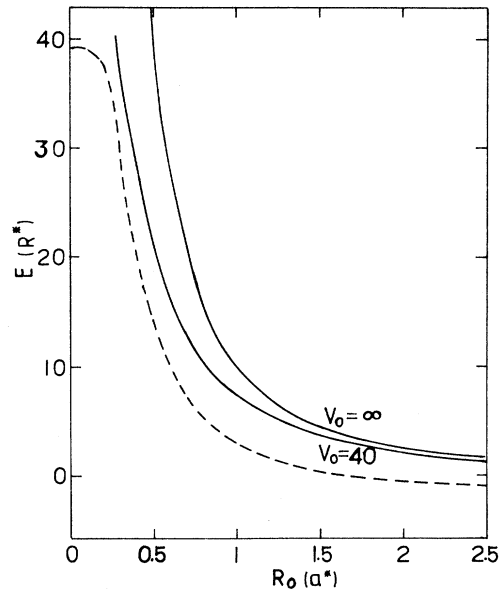

FIG. 1. Ground-state energy level E of an electron in a SRQW vs the well radius R_0. The top and middle curves represent the levels of the wells of $V_0 = \infty$ and $40R^*$, respectively. The dashed curve represents the ground state of a donor in the SRQW of $V_0 = 40R^*$. All energies are expressed in terms of the effective Rydberg (R^*) and all distances are expressed in terms of the effective Bohr radius (a^*). Same units are used in all of the following figures.

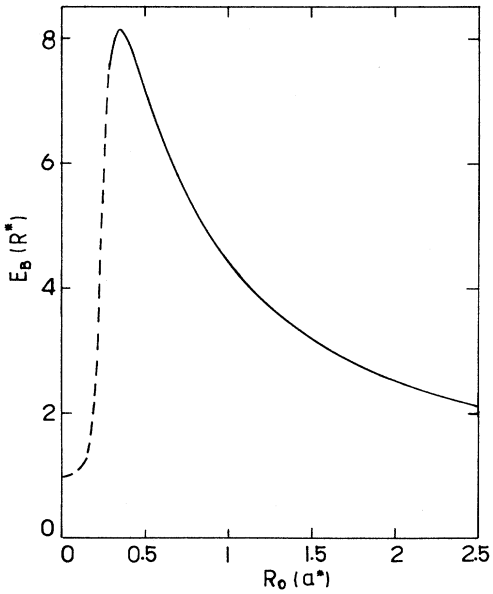

FIG. 2. Binding energy E_B of a donor ground state in the SRQW of $V_0 = 40R^*$ vs the well radius R_0.

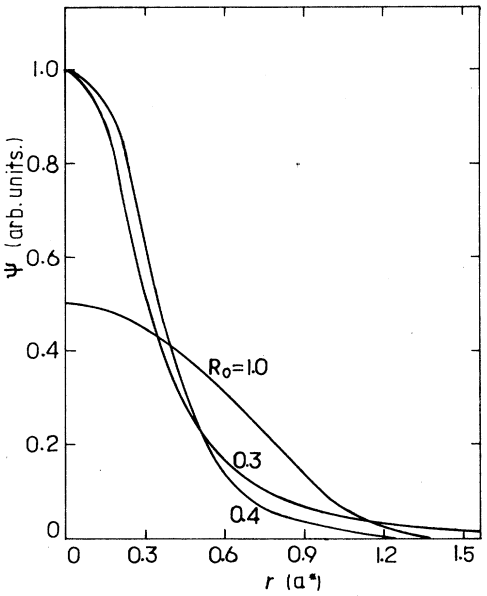

FIG. 3. Wave functions of ground states in the SRQW of $V_0=40R^*$ with $R_0=0.3a^*$, $0.4a^*$, and $1.0a^*$ vs position along the radial axis. The wave functions are in arbitrary units.

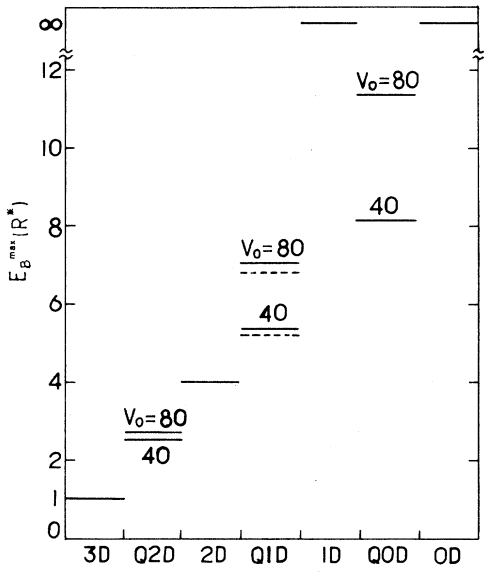

FIG. 4. Maximum binding energy E_B^{max} of a donor ground state in a quantum well vs the well dimensionality and barrier height V_0. For the Q1D case, the dashed lines represent the maximum binding energies (Ref. 19) and the solid lines represent the mean values of the maxima of the TDQW's and the SRQW's.

creased. There are no bound states for the finite quantum well if $R_0<0.31a^*$. However, the bound states do exist for the donor in the SRQW with an arbitrary R_0 as shown in Fig. 1. The binding energy of the ground state is shown in Fig. 2 as a function of the R_0. It is seen that the binding energy goes through a maximum as the well size is reduced from $2.5a^*$. Then, it is decreased as the well size is reduced continuously. The maximum of the binding energy is equal to $8.13R^*$. The value is much larger than those in TDQW's and QWW's with the same V_0. It can be understood if it is noted that the effect of the Coulomb interaction is enhanced by the electron confinement. The wave functions have been well calculated for electrons in both TDQW's and QWW's. In Fig. 3, we have plotted the wave functions of an electron in the SRQW of $V_0=40R^*$ with different R_0 in the absence of the Coulomb potential ($w=0$). As seen in the figure, the electron in a SRQW is confined strongly compared with electrons in TDQW's and QWW's with the same V_0. When V_0 is increased, the enhancement of the maximum binding energy, shown in Fig. 4, is greater in SRQW's (quasi-zero-dimensional) than in QWW's (Q1D) and TDQW's (Q2D). This is because of the enhancement of the electron confinement in three dimensions in SRQW's. In Figs. 2 and 3, it is readily seen that the binding energy is larger as the confinement is stronger. In Fig. 4, the mean values of the maxima of the TDQW's and the SRQW's have also been shown by solid lines. It is interesting to note that the mean values are very close to (slightly larger than) the maxima for the QWW's.

In conclusion, we have used the method of series expansion to solve the radial Eq. (5). The exact solutions of donor states in the SRQW have been obtained numerically. Then, the numerical results reveal that the confinement and binding energy of hydrogenic donor states in quantum wells of GaAs-$Ga_{1-x}Al_xAs$ are strongly dependent on the dimensionality of the wells, and that there are larger confinement and binding energies of donor states in the SRQW's than in the QWW's and TDQW's. Finally, we should point out that, based on the exact solutions obtained, the quantum levels and wave functions of donors located out of the center of SRQW's can be obtained by use of a variation method, and that the exact solutions are also useful for the calculation of exciton states in SRQW's. They are in progress.

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