Pramana – J. Phys. (2018) 90:7
https://doi.org/10.1007/s12043-017-1497-6

Perturbation method for calculating impurity binding energy in an inhomogeneous cylindrical quantum dot with dielectric mismatch

NILANJAN SIL[1,*], NIBEDITA DARIPA[2], ACHINT KAPOOR[3] and SANJAY KUMAR DEY[3]

[1]Department of Physics, Silli Polytechnic, Ranchi 835 102, India
[2]Department of Physics, Delhi Public School, Ranchi 834 004, India
[3]University Department of Physics, Ranchi University, Ranchi 834 008, India
*Corresponding author. E-mail: nilanjansil@gmail.com

MS received 3 June 2016; revised 7 June 2017; accepted 1 August 2017; published online 18 December 2017

Abstract. In the present paper, we have studied the binding energy of the shallow donor hydrogenic impurity, which is confined in an inhomogeneous cylindrical quantum dot (CQD) of GaAs-$Al_xGa_{1-x}As$. Perturbation method is used to calculate the binding energy within the framework of effective mass approximation and taking into account the effect of dielectric mismatch between the dot and the barrier material. The ground-state binding energy of the donor is computed as a function of dot size for finite confinement. The result shows that the ground-state binding energy decreases with the increase in dot size. The result is compared with infinite dielectric mismatch as a limiting case. The binding energy of the hydrogenic impurity is maximum for an on-axis donor impurity.

Keywords. Cylindrical quantum dots; shallow hydrogenic impurity; effective mass boundary conditions.

PACS Nos 81.07.Ta; 78.67.Hc; 73.63.Kv

1. Introduction

The physics of semiconductor low-dimensional heterostructure systems, such as quantum wells (QWs), quantum wires (QWWs) and quantum dots (QDs) have been studied intensively for the last few decades. These structures are important because they chiefly attribute to transport properties associated with carrier confinement. Quantum dots have been the subject of intensive experimental and theoretical investigations. QDs are semiconductor inclusions with dimensions in nanometer scale showing quantum size effects due to complete confinement in zero-dimensional structures [1–7]. In the recent past, a new class of quantum dots called quantum dot–quantum well or inhomogeneous quantum dots has been made possible, which is composed of two semiconductor materials having different band gaps [8]. The study of hydrogenic impurity is chiefly attributed to low-dimensional semiconductor heterostructures because the presence of impurity in such structures influences the electronic and optical properties [9–14].

Quantum dots (QDs) are low-dimensional nanostructures which exhibit exotic behaviours distinct from their bulk counterparts chiefly due to size quantization effect, which is typical of a quantum confined system. In such nanoheterostructures, whenever the de Broglie wavelength of electron exceeds the appropriate dimensions of the device structure, the quantum nature dictates the physical properties in them. As a result, the energy of the electrons in the confined directions become quantized and forms a discrete energy spectrum. For such size-quantized electrons, the scattering probability is drastically suppressed [15].

The donor impurity in semiconductor nanoheterostructures introduces bound state in the forbidden energy gap which strongly affects both the optical and transport properties of semiconductor heterostructures. Therefore, understanding the impurity states in semiconductor heterostructures is of utmost importance. Although the impurity states within bulk semiconductors had been exhaustively studied, the same within the quantum well (QW) structures was initiated only in the last decade [10, 16–18]. Recently, similar studies have been extended to quasi-one-dimensional and quasi-zero-dimensional structures like quantum well wires (QWWs) [19,20] and quantum dots (QDs) [11,21]. The effect of the geometry of QDs [22] and that of the cross-sectional forms of QWWs [23] on the impurity binding energy have also been investigated. However, the investigators have so far only concentrated their interests on the impurity ground

state, using variational techniques mostly in spherical quantum dots under the effective mass approximation [24–30]. In the present analysis, a perturbation method has been employed to calculate the shallow donor hydrogenic impurity state in cylindrical QDs having a square potential well of finite barrier. The impurity binding energies are theoretically estimated for QDs of wide-gap semiconductors and computed for GaAs-$Al_xGa_{1-x}As$ as a typical representative.

The reason for the choice of quantum dot with cylindrical geometry is that this type of structure is naturally conceived and mathematically more suitable to exploit with the use of Bessel functions in cylindrical structures [31,32].

A theoretical work is presented in this paper for cylindrical quantum dot within the framework of effective mass Schrödinger equation for investigating binding energy of the impurity state for finite confinement in transverse plane and infinite in the axial direction. An electron as impurity is assumed to be confined in a cylindrical quantum dot formed by GaAs semiconductor surrounded by a barrier semiconductor material $Al_xGa_{1-x}As$ having finite band gap as compared to the well material constituting inhomogeneous quantum dots. In the structures under consideration, the boundary conditions to be satisfied across the well–barrier interface are the effective mass boundary conditions (EMBC) which are also referred to as Bastard boundary conditions [33–35]. In the present work, the result of perturbation method yields the first-order correction as the second-order correction seemed to be insignificant [36].

2. Theory

The CQD under study is embedded in a matrix of lower dielectric constant (ε_{out}). Our theoretical investigation presents a simplified approach, wherein the electron–phonon interaction and ion–phonon coupling have been ignored.

In the effective mass approximation, the Hamiltonian of a single hydrogenic impurity in a CQD can be expressed as

$$\hat{H} = \frac{\hat{p}^2}{2m^*} + V_C - \frac{e^2}{4\pi\varepsilon r} = \hat{H}_0 + \hat{H}' \tag{1}$$

where

$$\hat{H}_0 = \frac{\hat{p}^2}{2m^*} + V_C$$

and

$$\hat{H}' = -\frac{e^2}{4\pi\varepsilon r}$$

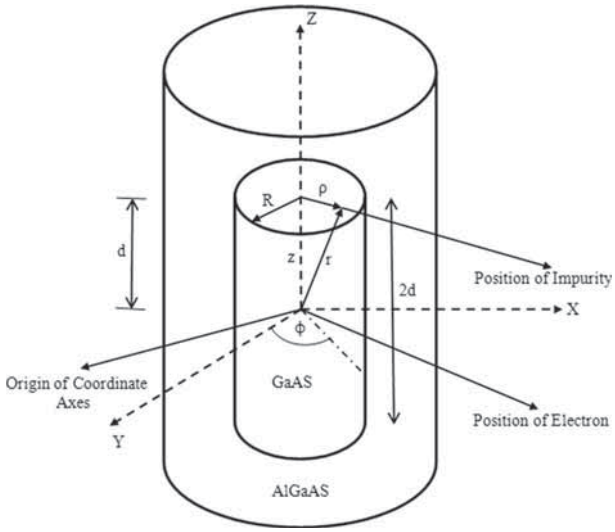

Figure 1. Geometry of CQD.

with e and m^* represent respectively, the charge and effective mass of the electron, p is the momentum, ε is the dielectric constant of the cylindrical dot material and r gives the location of the impurity with respect to the centre of the cylindrical dot as illustrated in figure 1. V_C describes the confining potential and its profile is given as

$$V_C = \begin{cases} 0; & \rho \le R \\ V_0; & rho > R \end{cases} \tag{2}$$

and

$$V_C = \begin{cases} 0; & |z| \le d \\ \infty; & |z| > d. \end{cases} \tag{3}$$

The effective mass and the dielectric constant of the CQD vary as

$$m^*, \varepsilon = \begin{cases} m_1^*, \varepsilon_{\text{in}}; & \rho \le R \text{ and } |z| \le d \\ m_2^*, \varepsilon_{\text{out}}; & \rho > R \text{ and } |z| > d, \end{cases} \tag{4}$$

where R is the radius of the cylindrical dot, $2d$ is the height of the dot and ρ is the distance of the impurity from the axis of the CQD in transverse plane. The last term in eq. (1) is the Coulomb interaction term due to the presence of hydrogenic impurity which acts as perturbation over the original Hamiltonian.

The eigenfunction of the Hamiltonian in the absence of the impurity in CQD is given by

$$\psi(\rho, z) = A_0 f(\rho) g(z), \tag{5}$$

where $f(\rho)$ is the ground-state solution of the effective mass Schrödinger equation in the transverse plane assuming the azimuth angle ϕ to be invariant in that plane and $g(z)$ is its solution in z-direction of the dot respectively with A_0 as the normalisation constant.

The exact forms of wave functions in the ground state on solving the effective mass Schrödinger equation in the two regions $\rho < R, |z| < d$ and $\rho > R, |z| > d$ respectively are given by

$$\psi_i(\rho, z) = A_0 J_0(\Re_1 \rho) \cos \Re_1 z;\ \rho < R, |z| < d \tag{6}$$

and

$$\psi_0(\rho, z) = \frac{A_0 J_0(\Re_1 R)}{K_0(\Re_2 R)} K_0(\Re_2 \rho) \times \cos \Re_1 d \mathrm{e}^{-\Re_2(z-d)};\ \rho > R, |z| > d, \tag{7}$$

where

$$f(\rho)\alpha \begin{cases} J_0(\Re_1 \rho); & \rho \le R \text{ and } |z| \le d \\ \dfrac{J_0(\Re_1 R)}{K_0(\Re_2 R)} K_0(\Re_2 \rho); & \rho > R \text{ and } |z| > d \end{cases} \tag{8}$$

and

$$g(z)\alpha \begin{cases} \cos \Re_1 z; & \rho \le R \text{ and } |z| \le d \\ \cos \Re_1 d\, \mathrm{e}^{-\Re_2(z-d)}; & \rho > R \text{ and } |z| > d \end{cases} \tag{9}$$

with

$$\Re_1 = \sqrt{\frac{2m_1^* E}{\hbar^2}}$$

and

$$\Re_2 = \sqrt{\frac{2m_2^* (V_0 - E)}{\hbar^2}}$$

wherein E is the energy of the electron and V_0 is the confining potential.

The binding energy of the hydrogenic impurity is defined as the difference between the energy states without and with the impurity in a particular level. Thus, the impurity binding energies are given by the correction term obtained from the perturbation method.

Now the impurity binding energy inside the CQD is given by

$$\Delta E_{\text{in}}^{(1)} = \langle \psi_i^* | \hat{H}' | \psi_i \rangle = \int \psi_i^* \hat{H}' \psi_i \mathrm{d}\tau \tag{10}$$

$$\Delta E_{\text{in}}^{(1)} = \int \psi_i^* \hat{H}' \psi_i \mathrm{d}\tau = \int A_0 J_0(\Re_1 \rho) \cos \Re_1 z \left(-\frac{e^2}{4\pi \varepsilon_{\text{in}} r} \right) \times A_0 J_0(\Re_1 \rho) \cos \Re_1 z \mathrm{d}\tau, \tag{11}$$

where

$$\mathrm{d}\tau = \rho \mathrm{d}\rho \mathrm{d}\phi \mathrm{d}z$$

in cylindrical coordinate system and

$$r = (\rho^2 + z^2)^{1/2}.$$

Hence eq. (11) becomes

$$\Delta E_{\text{in}}^{(1)} = -\frac{A_0^2 e^2}{4\pi \varepsilon_{\text{in}}} \int J_0^2(\Re_1 \rho) \cos^2 \Re_1 z \times \frac{\rho}{\sqrt{\rho^2 + z^2}} \mathrm{d}\rho \mathrm{d}\phi \mathrm{d}z \tag{12}$$

for the CQD, it is assumed that $(z/\rho) \cong 1$ [37]. Hence eq. (12) becomes

$$\Delta E_{\text{in}}^{(1)} = -\frac{A_0^2 e^2}{4\pi \varepsilon_{\text{in}} \sqrt{2}} \int_0^R J_0^2(\Re_1 \rho) \mathrm{d}\rho \times \int_{-d}^{d} \cos^2 \Re_1 z \mathrm{d}z \int_0^{2\pi} \mathrm{d}\phi. \tag{13}$$

The solution of eq. (13) after simplification yields

$$\Delta E_{\text{in}}^{(1)} = -\frac{A_0^2 e^2}{4\pi \varepsilon_i \sqrt{2}} 2\pi R \left(d + \frac{1}{2\Re_1} \sin 2\Re_1 d \right). \tag{14}$$

On solving for the normalization constant A_0, we get the value of normalization constant as

$$A_0^2 = \frac{2}{2\pi R^2 (d + (1/2\Re_1) \sin 2\Re_1 d)}.$$

Now putting the value of normalization constant A_0^2 in eq. (14), we get

$$\Delta E_{\text{in}}^{(1)} = -\frac{2e^2}{4\pi \varepsilon_{\text{in}} \sqrt{2} R}. \tag{15a}$$

Negative sign signifies that binding energy is attractive in nature.

$$|\Delta E_{\text{in}}^{(1)}| = \frac{2e^2}{4\pi \varepsilon_{\text{in}} \sqrt{2} R}. \tag{15}$$

Equation (15) gives the ground-state binding energy of the hydrogenic impurity inside a CQD with square well potential.

Now the Hamiltonian outside the CQD ($\rho > R$) is given by

$$\hat{H} = \frac{\hat{p}^2}{2m_2^*} + V_C - \frac{e^2}{4\pi \varepsilon_{\text{out}} r} = \hat{H}_0 + \hat{H}', \tag{16}$$

where

$$\hat{H}_0 = \frac{\hat{p}^2}{2m_2^*} + V_C$$

and

$$\hat{H}' = -\frac{e^2}{4\pi\varepsilon_{\text{out}} r}$$

for $\rho > R$, $V_C = V_0$ and for $|z| > d$, $V_C = \infty$.

The wave function outside the CQD is given as

$$\psi_0(\rho, z) = \frac{A_0 J_0(\Re_1 R)}{K_0(\Re_2 R)} \times K_0(\Re_2 \rho)\cos\Re_1 d\, \mathrm{e}^{-\Re_2(z-d)} \quad (17)$$

$$= C_0 K_0(\Re_2\rho)\,\mathrm{e}^{-\Re_2 z} \quad (18)$$

where

$$C_0 = \frac{A_0 J_0(\Re_1 R)}{K_0(\Re_2 R)}\cos\Re_1 d\,\mathrm{e}^{\Re_2 d}.$$

Now the impurity binding energy outside the CQD is given by

$$\Delta E^{(1)}_{\text{out}} = \langle\psi_0^*|\hat{H}'|\psi_0\rangle = \langle\psi_0^*|-\frac{e^2}{4\pi\varepsilon_{\text{out}} r}|\psi_0\rangle \quad (19)$$

$$\Delta E^{(1)}_{\text{out}} = \int \psi_0^*\hat{H}'\psi_0 \mathrm{d}\tau = -\int C_0 K_0(\Re_2\rho)\,\mathrm{e}^{-\Re_2 z}\frac{e^2}{4\pi\varepsilon_{\text{out}} r} \times C_0 K_0(\Re_2\rho)\,\mathrm{e}^{-\Re_2 z}\rho\mathrm{d}\rho\mathrm{d}\phi\mathrm{d}z. \quad (20)$$

Equation (20) implies

$$\Delta E^{(1)}_{\text{out}} = -\frac{C_0^2 e^2}{4\pi\varepsilon_{\text{out}}}\int \frac{K_0^2(\Re_2\rho)}{\sqrt{\rho^2+z^2}}\mathrm{e}^{-2\Re_2 z} \times \rho\mathrm{d}\rho\mathrm{d}\phi\mathrm{d}z \quad (21)$$

for the CQD, it is assumed that $(z/\rho) \cong 1$ [37]. Hence eq. (21) becomes

$$\Delta E^{(1)}_{\text{out}} = -\frac{C_0^2 e^2}{4\pi\varepsilon_{\text{out}}\sqrt{2}}\int_R^\infty K_0^2(\Re_2\rho) \times \int_{-d}^{d}\mathrm{e}^{-2\Re_2 z}\mathrm{d}z\int_0^{2\pi}\mathrm{d}\phi. \quad (22)$$

The solution of eq. (22) after simplification yields

$$\Delta E^{(1)}_{\text{out}} = -\frac{C_0^2 e^2 2\pi}{4\pi\varepsilon_{\text{out}}\sqrt{2}}\frac{\mathrm{e}^{-2\Re_2 R}}{\pi\Re_2^2 R}\left[\frac{1}{\Re_2}\sinh(2\Re_2 d)\right]. \quad (23)$$

The value of C_0 is written as

$$C_0^2 = \frac{1}{2\pi(\mathrm{e}^{-2\Re_2 R}/\pi\Re_2^2)\,((1/\Re_2)\sinh(2\Re_2 d))}. \quad (24)$$

Now putting the value of C_0^2, we get $\Delta E^{(1)}_{\text{out}}$ as

$$\Delta E^{(1)}_{\text{out}} = -\frac{e^2}{4\pi\varepsilon_{\text{out}}\sqrt{2}}\frac{1}{R} \quad (25a)$$

$$|\Delta E^{(1)}_{\text{out}}| = \frac{e^2}{4\pi\varepsilon_{\text{out}}\sqrt{2}}\frac{1}{R}. \quad (25)$$

The ground-state binding energy of the hydrogenic impurity in a CQD is given by

$$E_b = |\Delta E^{(1)}_{\text{in}}| + |\Delta E^{(1)}_{\text{out}}|$$

$$\boxed{E_b = \frac{e^2}{4\pi\sqrt{2}}\left(\frac{2}{\varepsilon_{\text{in}}} + \frac{1}{\varepsilon_{\text{out}}}\right)\frac{1}{R}}. \quad (26)$$

Limiting Case

In the limit when dielectric mismatch becomes infinitely high, i.e. $\varepsilon_{\text{out}} \to \infty$, the expression for binding energy is

$$E_b = |\Delta E^{(1)}_{\text{in}}| = \frac{2e^2}{4\pi\varepsilon_{\text{in}}\sqrt{2}R}. \quad (27)$$

This is the situation when the shallow hydrogenic impurity is totally confined within the CQD. This is akin to infinite potential confinement where the band offset is assumed to be infinitely high. It is thus seen that result of the binding energy under the limiting condition of infinite dielectric mismatch for $\varepsilon_{\text{out}} \to \infty$ leads to the same result of binding energy already obtained by others [38] under infinite potential confinement.

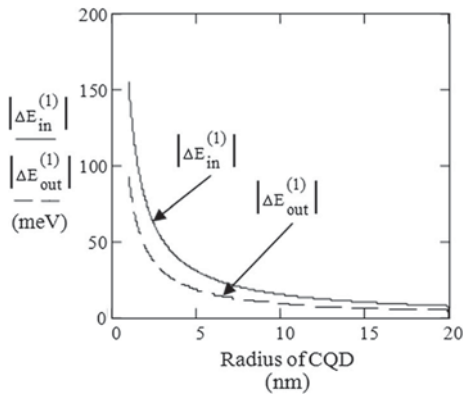

Figure 2. Variation of impurity binding energy with radius of the CQD for impurity lying inside and outside the dot.

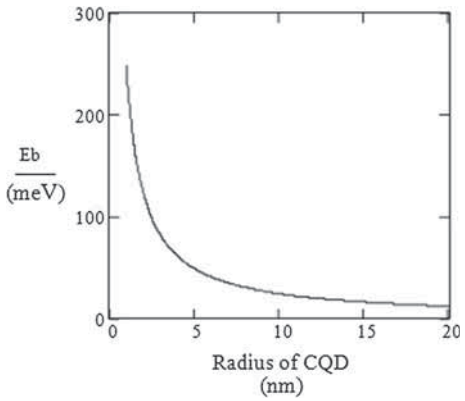

Figure 3. Variation of total binding energy of the impurity with radius of the CQD.

3. Results and discussion

To compute the impurity binding energy, the parameters used for GaAs and $Al_xGa_{1-x}As$ with $x = 0.7$, rel. dielectric constants $\varepsilon_{in} = 13.18$ and $\varepsilon_{out} = 10.996$ respectively (where, $\varepsilon_{out} = 13.18 - 3.12x$) [39] gives the Bohr radius as 10.4 nm. For the perturbation calculation to be valid, the quantized energy should be greater than the Coulombic interaction between the electron and the impurity. This implies that the radius of the QD must be sufficiently smaller than the Bohr radius. The perturbation calculation even for QDs of radius larger than twice the Bohr radius with error remaining within 1% is sufficiently accurate [40]. In the present analysis, we have restricted our calculation for CQD with dot radius upto 20 nm. In this paper, figure 2 shows the variation of impurity binding energy with dot radius for impurity lying inside and outside the dot and figure 3 shows the variation of total binding energy of the impurity with dot radius.

4. Conclusion

In this paper, the impurity binding energy has been calculated by following perturbation method for a shallow hydrogenic impurity in inhomogeneous cylindrical quantum dots having finite dielectric mismatch in the structure. The computed results show that the impurity binding energy is quite sensitive to the dot size, i.e. the binding energy of the impurity decreases with the increase in dot size. It is seen that result of the binding energy under the limiting condition of infinite dielectric mismatch ($\varepsilon_{out} \to \infty$) in the heterostructure leads to the result already obtained for infinite potential confinement by others. The binding energy of the hydrogenic impurity becomes maximum for an on-axis impurity, i.e. when the radius of the CQD tends to zero.

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