Available online at www.sciencedirect.com

SciVerse ScienceDirect

Physics Procedia 28 (2012) 44 – 47

Physics Procedia

15th Brazilian Workshop on Semiconductor Physics

Impurity Donor in a Quantum Disk

P. C. M. Machado[a,*], A. B. A. Marques[a], F. A. P. Osório[b,c] and A. N. Borges[b,c]

[a]*Escola de Engenharia Elétrica e de Computação, UFG, CP 131, Goiânia – GO, 74001-970, Brazil*
[b]*Instituto de Física, UFG, CP 131, Goiânia – GO, 74001-970, Brazil*
[c]*Núcleo de Pesquisa em Física, PUC-GO, Goiânia – GO, 74605-220, Brazil*

Abstract

The donor binding energy of a hydrogenic donor impurity located in the center of a GaAs-$Al_xGa_{1-x}As$ circular quantum dot is calculated by solving analytically the Schrödinger equation. The electron wave functions and the impurity energy levels are determined in the standard manner through the solution of the transcendental equations obtained from the boundary conditions imposed at the interfaces of the quantum disk. The roots of the transcendental equations were numerically found for quantum disks with finite height of the confinement potential.

Keywords: Binding energy; quantum disk; donor impurity.

1. Introduction

Quasi-zero dimensional electron systems (QZD) occurring in semiconductor quantum dots have attracted much attention in the last few years, due to their potential applications in the electronic and optoelectronic devices fabrication. In these QZD electron systems the presence of donor impurities plays an important role, because the effective strength of the Coulomb interaction is greatly enhanced due to the electron confinement. Also the impurity binding energies show a strong dependence on the geometry and dimensionality of the system.

In the present work we report a theoretical calculation of the electron energy levels of a shallow impurity located at the center of a GaAs-AlGaAs circular quantum dot called a quantum disk (QD). The electron wave functions are obtained analytically by solving the Schrödinger equation and the impurity energy levels are determined through the solution of the transcendental equation obtained from the boundary condition imposed in the interfaces of the QD. This transcendental equation includes the first and second solutions of the confluent hypergeometric functions (CHF) and their first derivatives. Thus for one to find the roots of this equation is a complicated task due to the complex behavior of the CHF mainly in the positive energy region (QD with small radius) where the arguments become imaginary. Frequently such numerical difficulties to find the transcendental equation roots lead authors to calculate the impurity energy levels through variational methods [1-5]. Here we solve the transcendental equation

* Corresponding author. Tel.: +55-62-3209-6400; fax: +55-62-3209-6292.
E-mail address: pcmmachado@gmail.com.

1875-3892 © 2012 Published by Elsevier B.V. Selection and/or peer-review under responsibility of Universidade Federal de Juiz de Fora, Brazil. Open access under CC BY-NC-ND license. doi:10.1016/j.phpro.2012.03.668

and we calculate the impurity energies of the ground state and first excited state and the electron binding energies as a function of the QD radius, for different confinement potential barriers. We also show how to calculate the same energies for spherical quantum dots (SQD) from the QD equations.

2. Theory

Let us consider an impurity donor located in the center of a QD, with radius R, composed of GaAs surrounded by $Al_xGa_{1-x}As$, where x is the aluminum concentration in the barrier material. Within the framework of the effective mass approximation and in polar coordinate system the dimensionless Schrödinger equation can be written as,

$$\delta(r)H_1\Psi(r,\theta)+V(r)\Psi(r,\theta)-\frac{2}{r}\Psi(r,\theta)=E\Psi(r,\theta) \tag{1}$$

Where,

$$H_1=-\left\{\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\right\} \tag{2}$$

The electron effective mass depends on the electron position and this fact is taken into account in equation (1) by the $\delta(r)$ step function, which is equal to the unity for $r<R$ and assumes the value $\delta = m_1/m_2$ for $r>R$, where m_1 and m_2 are the electron conduction band effective mass, in GaAs and AlGaAs respectively. The electron-confinement potential $V(r)$ is assumed as zero for $r<R$ and $V(r)=V_o$ for $r>R$, where $V_0 = 0.6[1047x + 470\,x^2]$ meV [6].

The wave function for the system given by equation (1) can be written as $\Psi(r,\theta)=\psi(r)e^{im\theta}$, where $m=0,\pm1\ldots$. Then the electron wave function for the bound states with negative energies values ($E < 0$) is given by,

$$\Psi(r,\theta)=\begin{cases}A\xi^{|m|}\exp(im\theta-\xi/2)M(a,b;\xi), & r\le R\\ B\zeta^{|m|}\exp(im\theta-\zeta/2)U(a_1,b;\zeta), & r\ge R\end{cases} \tag{3}$$

where A and B are the normalization constants, $M(a,b;x)$ and $U(a,b;x)$ are the first and second solutions of the CHF respectively. The parameters of the CHF are given by: $a=(|m|+0.5-\lambda)$, $a_1=(|m|+0.5-\lambda_1)$, $b=(2|m|+1)$. The parameters λ and λ_1 are calculated by solving the transcendental equation obtained from the wave function continuity condition and current conservation at the QD interface ($r = R$) given by,

$$\frac{M'}{M}-\frac{\lambda}{\lambda_1}\frac{U'}{U}-\frac{1}{2}\left(1-\frac{\lambda}{\lambda_1}\right)+|m|\left(\frac{1}{\xi}-\frac{\lambda}{\lambda_1\zeta}\right)=0 \tag{4}$$

and they are related by,

$$\frac{1}{\lambda^2}=\frac{1}{\delta\lambda_1^2}-V_0 \tag{5}$$

where M' and U' denote the first derivative of M and U respectively.

The electron wave function in the region of positive energy values (E > 0) that occurs for QD with small radius, can be obtained simply by the substitution of $\lambda\to i\eta$ and $\xi\to -i\xi$ in equation (3). The transcendental equations for negative and positive energy values are similar but finding the solutions in the last case is more complicated due to the complex arguments of the CHF. In order to calculate the binding energy we also have solved the Schrödinger equation without the presence of the donor impurity in the QD.

The solutions of the problem of a donor impurity placed in the center of a spherical quantum dot (SQD) can be obtained from that for QD equations simply making in the previous equations the following changes in indices:

$$\left(|m|+\frac{1}{2}\right) \rightarrow \left(|L|+1\right) \tag{6}$$

where $L=0,1,2\ldots$ is an integer.

3. Results and Discussion

Our numerical calculations for the energies are for a donor impurity located in the center of a QD compound of GaAs surrounded by $Al_xGa_{1-x}As$ where x is the aluminum concentration, with x=0.1 and x=0.3 corresponding to confining potential barrier heights of V_0 =66 meV and V_0 =214 meV, respectively. Here we consider the values for the electron conduction band mass as $m_1=0.067m_0$ for the GaAs and $m_2=(0.067+0.083x)m_0$ for the AlGaAs, where m_0 is the free electron mass. Other GaAs physical parameters used in the calculations were the effective Bohr radius, a_0 = 98.69 Å, and the effective Rydberg, R_y^* = 5.85 meV.

The results for the ground state energy ($m=0$) for an electron confined in a QD with (dotted line) and without (dashed line) the presence of the center-donor impurity as a function of the QD radius for V_0 =214 meV and V_0 =66 meV are plotted in Fig.1 and Fig.2 respectively. As one can note, the energy increases with decreasing disk radius for both QD. In these figures the impurity energy (dotted line) for QD increases from -4 R_y^*, the value of the ground state energy for a two-dimensional hydrogen atom [7]. The energy value is zero at the points R_o = 51 Å (Fig.1) and R_o = 38 Å (Fig.2) and become positive for smaller radius of the QD.

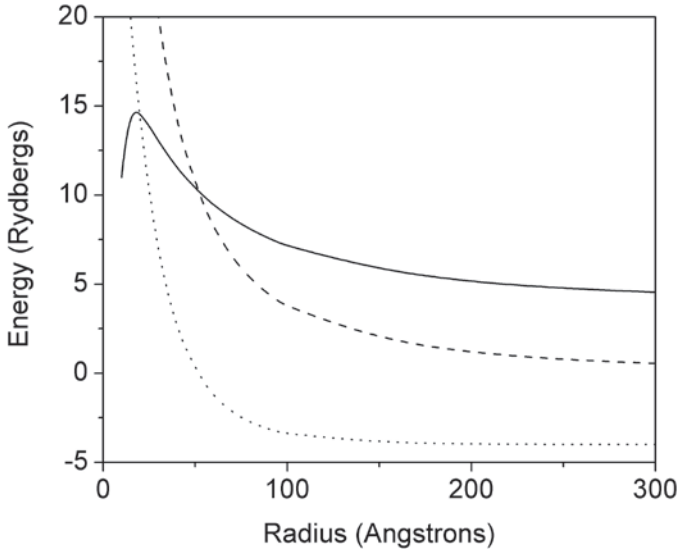

Figure 1: Ground state binding energy (solid line), impurity energy (dotted line) and electron energy (dashed line) as a function of the radius for a QD for V_0 =214 meV.

As one can see from these figures the qualitative behavior of the binding energy as a function of the QD radius is the same as observed in quantum wells [8] and quantum wires [9,10]: the binding energy increases as the QD radius decreases, reaches a maximum value and finally decreases for smaller QD radius. In Fig.1 and Fig. 2 the binding energy peaks near 15Ry* and 9Ry* respectively. In the limit of the QD radius going to zero, the binding energy goes to the value 5,48 Ry*, the ground state energy for a two-dimensional hydrogen atom placed in the barrier material (AlGaAs) [7]. As one can see when the QD radius decreases, smaller the potential confinement barrier height faster is the convergence of the binding energy to this value.

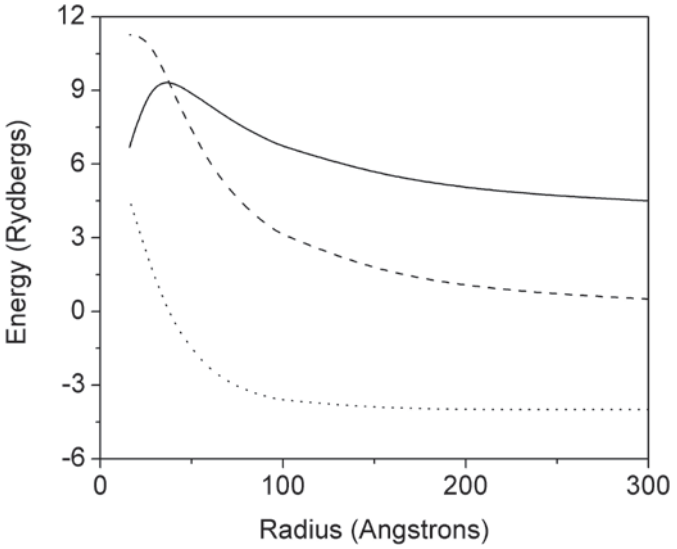

Figure 2: Ground state binding energy (solid line), impurity energy (dotted line) and electron energy (dashed line) as a function of the radius for a QD for V_0 =66 meV.

4. Conclusions

We have studied the ground-state binding energies of a donor impurity placed in the center of a GaAs/AlGaAs quantum disk as a function of the QD radius and the confinement potential barrier height. The bound electron wave functions are obtained analytically by solving the Schrödinger equation and the impurity energy levels are determined through the solution of the transcendental equation obtained from the boundary condition imposed at the interfaces of the QD. The limit for large and small values of the quantum disk dimensionality is satisfied by the obtained energy spectra. Our results show that the binding energy increases with decreasing QD radius and increasing confining potential barrier height. Unfortunately for the best of our knowledge there is no experimental data available to the problem of a donor impurity in a circular (cylindrical) quantum dot so we can compare with our theoretical results. However, when compared with the variational results of [1] our analytical results present a significant difference of 10%.

Acknowledgements

We thank to the Fundação de Apoio à Pesquisa (FUNAPE – UFG), Fundação de Apoio à Pesquisa do Estado de Goiás (FAPEG) and Pró-Reitoria de Pesquisa e Pós-Graduação da PUC Goiás (PROPE) for financial support.

References

[1] F.A.P. Osório, O. Hipólito and F. M. Peeters, Mater. Res. Soc. Proc. **281** (1993) 79-83.
[2] F.A.P. Osório, A.B. Marques, P.C.M. Machado and A.N.Borges,Microelectronics Journal 36 (2005) 244-7
[3] Jin-liang Zheng, Phys. E 40 (2008) 2879-83.
[4] C. M. Hsiao, W. N. Mei and D. S. Chuu, Solid State Commun. 81 (1992) 807-810.
[5] H. Akbas, C. Dane, A. Guleroglu, S. Minez, Phys. E 41 (2009) 605-8.
[6] E. Sadeghi, Phys.E 41 (2009) 365-7.
[7] S. Yngve, Am. J. Phys. 54, 1103 (1986).
[8] C. Mailhiot, Yia-Chung Chang, and T. C. McGill, Phys. Rev. B 26 (1982) 4449-57.
[9] F. A. P. Osório, M.H.Degani and O. Hipólito, Phys. Rev. B37 (1988) 1402-5; Superl. and Micros. 6 (1989) 111-3.
[10] G. W. Bryant Phys. Rev. B29 (1984) 6632-9; Phys. Rev. B31 (1985) 7812-8.