QUASI-STATIONARY ELECTRON STATES IN SPHERICAL ANTI-DOT WITH DONOR IMPURITY*

V. HOLOVATSKY, O. MAKHANETS, I. FRANKIV

Chernivtsi National University, Chernivtsi, 58012, Ukraine, E-mail: ktf@chnu.edu.ua

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The electron energy spectrum in $Al_xGa_{1-x}As/GaAs$ semiconductor quantum anti-dot with donor impurity, placed into the center of a nanostructure is studied. The energies and semi-widths of the quasi-stationary states are defined within the distribution of the probability density of electron residence in quantum anti-dot.

Key words: quantum anti-dot, quasi-stationary state, electron energy spectrum.

1. INTRODUCTION

The investigation of quantum effects arising in artificial potential wells, created at the base of semiconductors attracts the attention of scientists studying the properties of nanostructures more than twenty years. The majority of investigations concern the so-called closed nano-systems with stationary energy spectra for the quasi-particles. Among them, the quantum dots, quantum wires and nano-films are the most researched [1-2].

Recently, it is observed the increasing interest to the open nano-systems or resonance tunnel semiconductor structures, where the quasi-particles can penetrate the potential barrier and move into infinity. The open nano-systems are distinguished due to the spatial confinement and dimension. In the number of papers the open quantum dots, radial and axial open quantum wires and resonance tunnel plane nanostructures are studied. All these nano-systems are characterized by quasi-stationary energy spectra of quasi-particles and have the unique perspectives of utilization for the creation of field transistors, diodes and quantum cascade lasers [3-4].

In paper [5], the possibility of the creation of open nano-system as quantum anti-dot (QAD) with donor impurity is discussed. Here, the stationary states of electron bound by donor impurity, placed into the center of $ZnS/Cd_xZn_{1-x}S$ QAD

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are studied. The energies of stationary states and distribution of probability density of electron residence in nanostructure are calculated. It is proven that depending on the potential barrier height and energy the electron can be localized in deep or shallow potential well, created by Coulomb and QAD potentials. The electron, having the bigger energies, can tunnel through the potential barrier and move into infinity. The resonance states, manifesting themselves in scattering processes, are observed at the energies higher than the potential barrier.

In this paper we study the quasi-stationary and resonance states of electron in semiconductor spherical nanostructure ($Al_xGa_{1-x}As/GaAs$) with central donor impurity. The investigation of electron energy spectra is performed using the method of limit transition from the open nanostructure to the respective closed spherical core-shell one with unpenetrable outer interface, increasing GaAs-shell sizes till the macroscopic ones. The detailed approbation of the method for open spherical systems is given in [4], where it is shown that the basic properties of an electron in a simple open spherical quantum dot can be reproduced to any specified accuracy in the model of a closed two-well spherical quantum dot with a sufficiently large width of the outer well.

2. HAMILTONIAN OF ELECTRON AND SOLUTION OF SCHRODINGER EQUATION

The nanostructure: spherical semiconductor core (0) with radius r_0, embedded into the semiconductor shell (1) with radius r_1 (Fig.1) is under study. The hydrogen-like donor impurity, placed into the center of nanostructure, creates the Coulomb potential for the electron. The electron spectrum is obtained within the effective masses approximation with its

$$m(r) = \begin{cases} m_0, & r < r_0, \\ m_1, & r_0 \le r \le r_1. \end{cases} \tag{1}$$

The Hamiltonian of the electron is written as

$$H = -\nabla \frac{\hbar^2}{2m(r)} \nabla + V(r) - \frac{Ze^2}{\varepsilon\ r}, \tag{2}$$

where

$$V(r) = \begin{cases} V_0, & r < r_{0,} \\ 0, & r_0 \le r < r_1, \\ \infty, & r = r_1 \end{cases} \tag{3}$$

and ε - dielectric constant of QAD.

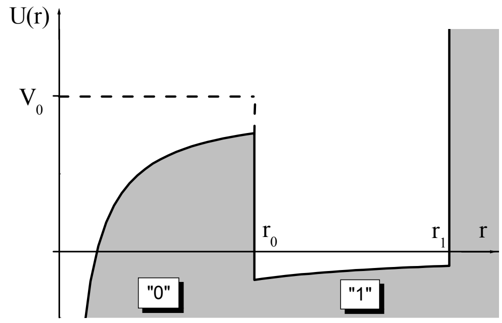

Fig. 1 – Scheme of potential energy for electron in the nanostructure with impurity.

Solving the Schrodinger equation in spherical coordinate system, it is clear that the radial ones have the form

$$\frac{\hbar^2}{2m_0}\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{\ell(\ell+1)}{r^2}\right]R_{nl}(r)+(E_{nl}-V_0+\frac{e^2}{\varepsilon r})\,R_{nl}(r)=0\,,\ r<r_0 \quad (4)$$

$$\frac{\hbar^2}{2m_1}\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}-\frac{\ell(\ell+1)}{r^2}\right]R_{nl}(r)+(E_{nl}+\frac{e^2}{\varepsilon r})\,R_{nl}(r)=0\,,\ r_0<r<r_1 \quad (5)$$

Using the convenient parameters

$$\xi_0=\frac{\sqrt{8m_0(V_0\text{-}E_{nl})}}{\hbar},\quad \xi_1=\frac{\sqrt{8m_1\ E_{nl}}}{\hbar},\quad \eta_{0,1}=\frac{2\ \ m_{0,1}e^2}{\varepsilon\ \ \xi_{0,1}\hbar^2} \quad (6)$$

and radial wave function written as

$$R_{nl}(r)=\begin{cases}\dfrac{\chi_0(\xi_0 r)}{r}, & r<r_0,\\ \dfrac{\chi_1(\xi_1 r)}{r}, & r_0\le r<r_1,\\ 0, & r=r_1\end{cases} \quad (7)$$

the differential equations are obtained

$$\frac{1}{\xi_0^2}\frac{\partial^2\chi_0(\xi_0 r)}{\partial^2 r}-\left(\frac{1}{4}+\frac{\eta_0}{\xi_0 r}-\frac{1/4-(\ell+1/2)^2}{\xi_0^2 r^2}\right)\chi_0(\xi_0 r)=0,\ \ r<r_0 \quad (8)$$

$$\frac{1}{\xi_1^2}\frac{\partial^2\chi_1(\xi_1 r)}{\partial^2 r}-\left(\frac{1}{4}+\frac{\eta_1}{\xi_1 r}-\frac{1/4-(\ell+1/2)^2}{\xi_1^2 r^2}\right)\chi_1(\xi_1 r)=0,\ \ r>r_0\,. \quad (9)$$

Their general solution can be written within Whittaker functions [6],

$$\chi_0(\xi_0 r) = A_0 M(\eta_0,\ \ell + 1/2,\ \xi_0 r) + B_0 W(\eta_0,\ \ell + 1/2,\ \xi_0 r), \quad (10)$$

$$\chi_1(\xi_1 r) = A_1 M(\eta_1, \ell + 1/2,\ \xi_1 r) + B_1 W(\eta_1, \ell + 1/2,\ \xi_1 r). \quad (11)$$

As far as $W(z)$ function is singular at z = 0, it is obtained $B_0 = 0$ from the condition that the wave function must be finite.

From the condition of the radial wave functions and their densities of currents continuity at the interface

$$R_{n\ell}^{(0)}(r)\Big|_{r=r_0} = R_{n\ell}^{(1)}(r)\Big|_{r=r_0}, \quad (12)$$

$$\frac{1}{m_0}\frac{\partial R_{n\ell}^{(0)}(r)}{\partial r}\Bigg|_{r=r_0} = \frac{1}{m_1}\frac{\partial R_{n\ell}^{(1)}(r)}{\partial r}\Bigg|_{r=r_0}, \quad (13)$$

$$R_{n\ell}^{(1)}(r)\Big|_{r=r_1} = 0, \quad (14)$$

the discrete energy spectrum (E_{nl}) of electron in spherical nanostructure with central donor impurity is obtained. The normality condition for the wave function

$$\int_0^{r_1} \left|R_{nl}(r)\right|^2 r^2 \mathrm{d}r = 1. \quad (15)$$

fixes the normality coefficient. Now the electron energy spectrum (E_{nl}) and its radial wave functions ($R_{nl}(r)$) for the closed spherical core-shell nanostructure are completely defined.

3. RESULTS OF CALCULATIONS AND DISCUSSION

3.1. ELECTRON ENERGY SPECTRUM AND WAVE FUNCTIONS FOR THE CLOSED NANOSTRUCTURE WITH IMPURITY

Computer calculations of the electron energies and wave functions were performed for $Al_xGa_{1-x}As/GaAs$ nanostructure with physical parameters: $V_0 = 0.57(1155\ x + 370\ x^2)$ meV – the height of potential barrier, $m(x) = (0.067+0.083x)\ m_e$ – electron effective mass, m_e – pure electron mass, ε=11.71 – dielectric constant of QAD, a_{GaAs}= 5.65(Å) – GaAs lattice constant. The dependences of electron energy spectrum on the shell radius (r_1) at different values of core radius (r_0) and Al concentration (x) are presented in Fig. 2 for the QAD with_and hydrogen-like donor impurity in the center. It is clear that electron energy spectrum consists of the energy states where the electron is localized in the core (0) and in the shell (1). At the increases of the shell radius (r_1), the width of the potential well becomes bigger. It brings to the weaker effect of size quantization and the energy levels, corresponding to the states of electron localized in the shell (1) are shifting into the range of lower energies. The energies of electron localized in the core (0) do not depend on shell radius (r_1). As a result, the effect of anti-crossing of electron energy levels is observed in Fig.2.

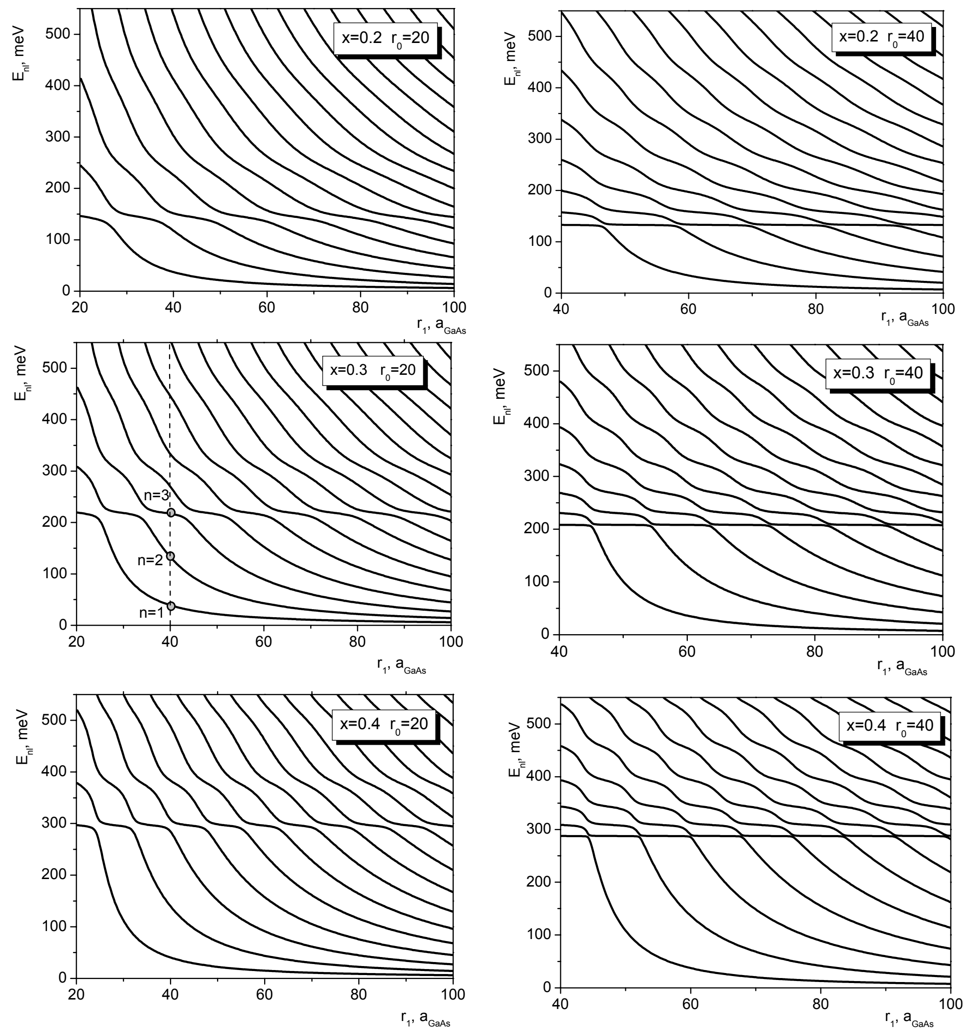

Fig. 2 – Evolution of electron energy spectrum as function of shell radius (r_1) for the nanostructure with the central donor impurity at core radius: $r_0 = 20\ a_{GaAs}$; $40\ a_{GaAs}$, and Al concentration: $x = 0.2, 0.3, 0.4$.

The distribution of probability density of electron residence in nanostructure (x = 0.3, r_0 = 20 a_{GaAs}, r_1 = 40 a_{GaAs}) is presented at Fig. 3 for the first three states (*n* = 1, 2, 3). The calculations were performed only for spherically symmetric states (*l*=0) but analogous ones can be fulfilled for $l \neq 0$. Fig. 3 proves that in the states *n* = 1 and *n* = 2 the electron is localized in outer well and in the state *n* = 3 – in inner one.

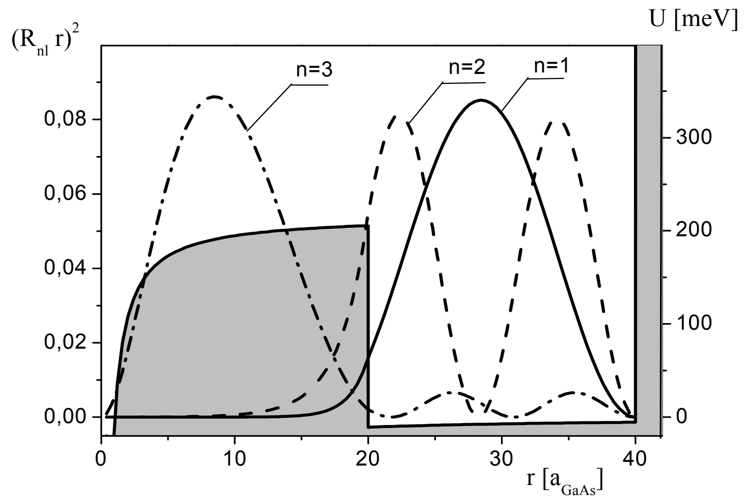

Fig. 3 – Distribution of probability density of electron location in nanostructure with central donor impurity

At r_1 > 50000 a_{GaAs} the distance between the neighbour energy levels is less than 0.1 meV, since, such spectrum can be assumed as quasi-continuous. Thus, at $r_1 \to \infty$ the shell (1) becomes a macroscopic medium and the nanostructure reforms into the open QAD with central impurity.

3.2. THE QUASI-STATIONARY ENERGY SPECTRUM OF ELECTRON IN QAD WITH CENTRAL IMPURITY

The quasi-stationary electron spectrum is calculated within the distribution of probability density of its residence in the space of QAD ($0 < r < r_0$)

$$W(E_{nl}) = \int_0^{r_0} \left|R_{nl}(r)\right|^2 r^2 \mathrm{d}r \,. \qquad (16)$$

The set of energies (E_{nl}), at which the probability of electron location inside of QAD reach the maxima, defines the position of quasi-stationary energy levels. All of them are characterized by their own radial and orbital quantum numbers. The radial quantum number for every quasi-stationary level is fixed by its ordinal number in energy scale and the orbital one is fixed by that l value, at which the calculation of energy spectra (E_{nl}) for the respective closed nanostructure was performed.

The semi-width of every quasi-stationary level is defined by the distance between the points located at the half of the height of $W(E)$ function peak. The quasi-stationary electron spectrum in QAD with central impurity is shown in Fig. 4 at different magnitudes of Al concentration (x) and core radius (r_0).

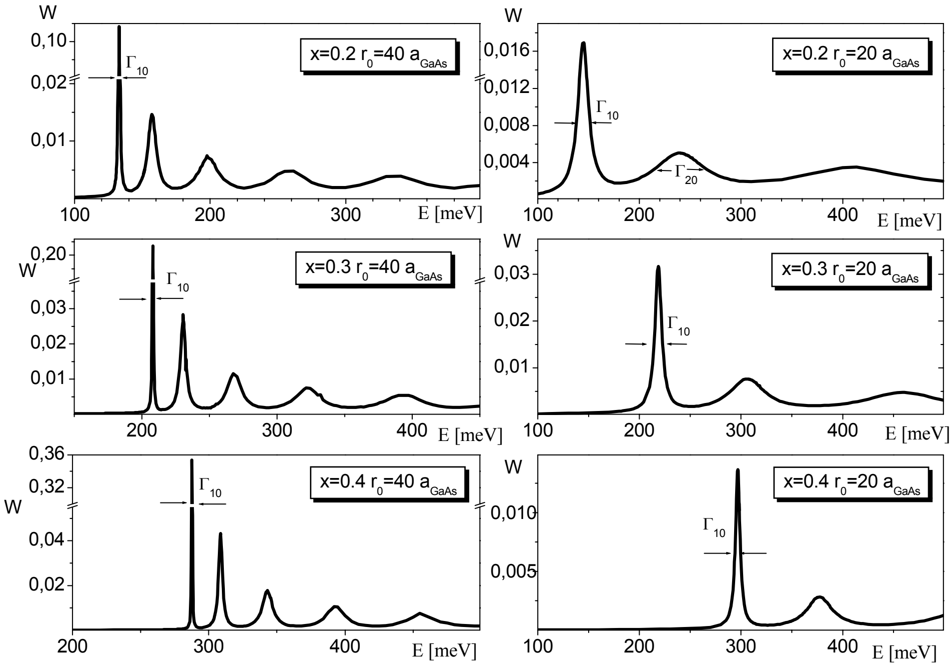

Fig. 4 – Quasi-stationary energy spectrum of electron in QAD with donor impurity at x = 0.2, 0.3, 0.4; $r_0 = 20\ a_{GaAs}$, $40\ a_{GaAs}$.

Numerical value of the energies, semi-width and the life-times of the lowest quasi-stationary sates are shown in Table 1.

Table 1

Energy E_{10} and semi-width Γ_{10} of the quasi-stationary states and life-time τ_{10}

Parameters	E_{10} [meV]	Γ_{10} [meV]	τ_{10} [ps]
x=0.2, r_0=40 a_{GaAs}	132.9	0.8	0.8
x=0.3, r_0=40 a_{GaAs}	280.1	0.5	1.3
x=0.4, r_0=40 a_{GaAs}	287.7	0.3	2.2
x=0.2, r_0=20 a_{GaAs}	145.1	12.1	0.05
x=0.3, r_0=20 a_{GaAs}	218.6	8.1	0.08
x=0.4, r_0=20 a_{GaAs}	296.7	5.3	0.12

Fig. 4 proves that when Al concentration (x) becomes bigger, the height of the potential barrier increases and the quasi-stationary levels shift into the region of higher energies. The increasing QAD radius causes the shift of quasi-stationary levels into the region of lower energies. Herein, the probability of electron tunneling through the barrier decreases, thus, the semi-width becomes smaller too and the distance between quasi-stationary levels also decreases. The lower is the quasi-stationary level in the energy scale, the smaller is its width and, consequently, the bigger is the life time of electron in this state. It is explained by the increasing width of the barrier through which the electron tunnels. The resonance levels with the energies bigger than the barrier height are characterized by the big semi-width and small life-time, respectively.

4. SUMMARY

The electron energy spectrum in QAD with central donor impurity is obtained within the limit transition from open nano-system to the closed one at $r_1 \to \infty$. The exact solutions of the Schrodinger equation for spherical core-shell nanostructure with hydrogen-like donor impurity placed into its center are obtained for the electron. The electron energies and the semi-widths of quasi-stationary states are defined by the distribution of the probability density of its residence inside the QAD. Within the used method of limit transition, the dependences of quasi-stationary states parameters on the core radius are obtained. It is shown that at the increasing QAD radius the energies of quasi-stationary states of the electron bound by central donor impurity are shifting into the low-energy range of spectrum. Herein, their semi-widths are decreasing. The quasi-stationary states can manifest themselves in the processes of electron scattering through the array of QADs with impurities inside.

REFERENCES

1. U.Woggon, *Optical properties of semiconductor Quantum Dots*, Springer, Berlin, 1996.
2. P.Harrison, *Quantum wells*, *wires, and dots*: *theoretical and computational physics of semiconductor nanostructures*. Wiley, Chichester, 2009.
3. M.Tkach, V.Holovatsky, O.Voitsekhivska, Electron and hole quasistationary states in opened cylindrical quantum wire. Physica E: Low dimensional systems and Nanostructures. **11**, 17–26 (2001).
4. M.Tkach, Yu. A. Sety, Properties of the electron spectrum of a closed two-well spherical quantum dot and evolution of the spectrum with the outer-well width. Semiconductors. **40**, 1083–1092 (2006), translated from russian Fizika i Tekhnika Poluprovodnikov. **40**, 1111–1119 (2006).
5. V.Holovatsky, O.Makhanets, O.Voitsekhivska, Oscillator strengths of electron quantum transitions in spherical nanosystems with donor impurity in the center, Physica E. **41,** 1522–1526 (2009).
6. A. Abramowitz and I. Stegun, *Handbook of Mathematical Function with Formulae, Graphs and Mathematical Tables*, Washington, 1964.