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STATIONARY AND QUASI-STATIONARY ELECTRON SPECTRUM IN QUANTUM WIRE AND QUANTUM ANTI-DOT WITH IMPURITY

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The quasi-stationary electron states in open semiconductor cylindrical quantum dot embedded into quantum wire and in spherical anti-dot with donor impurity are studied. The problems are solved using the probability distribution function of electron location in the respective closed nano-systems. The method verified for the first nano-system allowed the investigation of quasi-stationary spectrum of electron interacting with donor impurity in quantum anti-dot without using the S-matrix method.

Key words: electron spectrum, quantum dot, impurity.

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I. INTRODUCTION

The number of investigations concerning open or resonance-tunnel semiconductor structures has essentially increased. This is caused by the unique perspectives of their utilization for the creation of field transistors, diodes and quantum cascade lasers [1–3].

In the series of theoretical papers the calculation of resonance energies and resonance widths of electron quasi-stationary states (QSSs) in nano-systems have been performed using the permeability coefficient or S-matrix methods [4]. Both of them allow obtaining the dependences of energy spectra and quasi-particles life times on geometrical parameters of resonance-tunnel structure. However, the S-matrix method is rather cumbrous or principally impossible for the establishing of the exciton spectrum theory or study interaction between electron and impurity in open nano-systems.

In Ref. [5] it is shown that the electron QSSs in single spherical quantum dot can be found using the respective parameters of distribution function W (over the energy) of probability density of electron location in a nano-system. Just this function makes possible to get the limit transition from closed to open nano-systems. It is very important for the establishment of the exciton theory and electron — impurity interaction in open nano-systems.

In the paper, using the probability distribution function of quasi-particle location in a nano-system, the electron QSSs are investigated for:

1. Open semiconductor cylindrical quantum dot (CQD) embedded into the cylindrical quantum wire (CQW).
2. Quantum anti-dot (QAD) with donor impurity in the center.

II. EVOLUTION OF ELECTRON ENERGY SPECTRUM IN THREE-WELL CLOSED CQD EMBEDDED INTO CQW

The combined CQW containing three quantum dots of the same material (medium “0”) separated by the shell of the other material (medium “1”) is under study. The radius of CQW (ρ_0), quantum dots heights (h_0, h_1, h_2) and different barrier thicknesses (Δ_1, Δ_2) separating quantum dots are fixed and shown in Fig.1b. It is clear that such a nano-system is the closed one and quasi-particle energy spectrum is stationary.

From Fig. 1 it is also clear that at $h_1 \to 0$, $h_2 \to 0$ the complicated closed three-well CQD transforms into the single closed CQD inside CQW (Fig. 1a) and at $h_1 \to \infty$, $h_2 \to \infty$ — into the single open one (Fig. 1c). Obviously, the electron spectrum, herein, transforms into the quasi-stationary one with the respective resonance energies and resonance widths.

In order to obtain the electron spectrum and wave functions in the closed three-well CQD (Fig. 1b), the stationary Schrödinger equation is solved

$$\hat{H}\Psi(\mathbf{r}) = E\Psi(\mathbf{r}) \tag{1}$$

with the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2}\nabla\frac{1}{\mu(\mathbf{r})}\nabla + U(\mathbf{r}). \tag{2}$$

The electron effective masses and potentials are the following

$$\mu(\mathbf{r}) \equiv \mu(z) = \begin{cases} \mu_0, & \text{medium “0”} \\ \mu_1, & \text{medium “1”} \end{cases},$$

$$U(\mathbf{r}) \equiv U(\rho,\phi,z) = \begin{cases} \infty, & \rho > \rho_0 \\ 0, & \text{medium “0”} \\ U_0, & \text{medium “1”} \end{cases} \tag{3}$$

In the cylindrical coordinate system the variables in Eq. (1) are separated when the wave function is written as

$$\Psi_{n_z n_\rho m}(\mathbf{r}) = \frac{1}{\sqrt{\pi\rho_0^2 \left|J_{m-1}\left(X_{n_\rho m}\right) J_{m+1}\left(X_{n_\rho m}\right)\right|}} J_m\left(\frac{X_{n_\rho m}}{\rho_0}\rho\right) e^{im\varphi} F_{n_z n_\rho m}(z), \tag{4}$$

where J_m is the cylindrical Bessel function, m is the magnetic quantum number, $X_{n_\rho m}$ are zeroes of Bessel function, n_ρ is the radial quantum number determined by the number of zeroes of Bessel function at fixed m.

The solutions of Schrödinger equation for $F_{n_z n_\rho m}(z)$ function for all parts of three-well CQD are written as

$$F_{n_z n_\rho m}(z) = \begin{cases} F^{(0)}_{n_z n_\rho m} = A_0 \exp[k_1 z], & -\infty < z \le -z_4 \\ F^{(1)}_{n_z n_\rho m} = B_1 \cos(k_0 z) + B_2 \sin(k_0 z), & -z_4 \le z \le -z_3 \\ F^{(2)}_{n_z n_\rho m} = C_1 \exp[k_1 z] + C_2 \exp[-k_1 z], & -z_3 \le z \le 0 \\ F^{(3)}_{n_z n_\rho m} = D_1 \cos(k_0 z) + D_2 \sin(k_0 z), & 0 \le z \le z_0 \\ F^{(4)}_{n_z n_\rho m} = L_1 \exp[k_1 z] + L_2 \exp[-k_1 z], & z_0 \le z \le z_1 \\ F^{(5)}_{n_z n_\rho m} = M_1 \cos(k_0 z) + M_2 \sin(k_0 z), & z_1 \le z \le z_2 \\ F^{(6)}_{n_z n_\rho m} = G_1 \exp[-k_1 z], & z_2 \le z < \infty \end{cases} \tag{5}$$

where $k_0^2 = 2\mu_0 E/\hbar^2 - X^2_{n_\rho m}/\rho_0^2$, $k_1^2 = 2\mu_1(U_0 - E)/\hbar^2 + X^2_{n_\rho m}/\rho_0^2$.

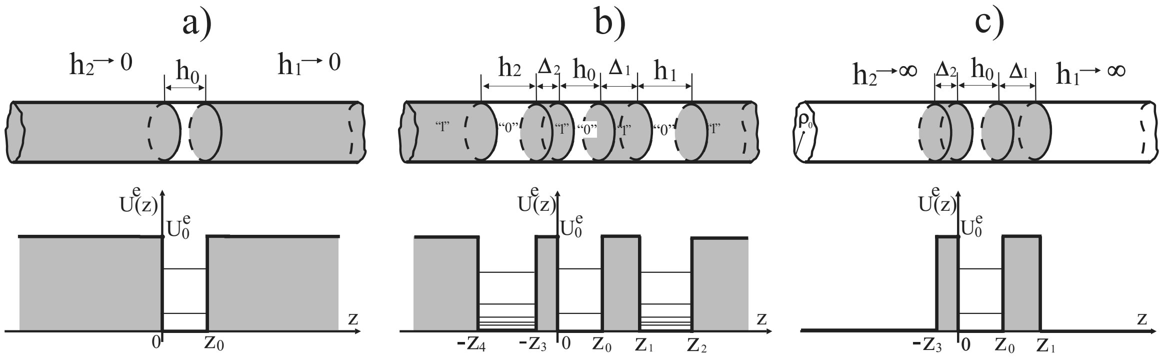

Fig. 1. Geometrical and potential energy schemes of single closed (a), three-well closed (b) and single open CQD in CQW (c).

Using the conditions of wave function and its density of current continuity at all nano-systems media interfaces ($z = -z_4$, $z = -z_3$, $z = 0$, $z = z_0$, $z = z_1$, $z = z_2$) and the normalizing condition

$$\int_{-\infty}^{+\infty} \left|F_{n_z n_\rho m}(z)\right|^2 dz = 1 \tag{6}$$

there have been obtained an analytical expressions for all the coefficients A_0, B_i, C_i, D_i, L_i, M_i, G_1, $(i = 1, 2)$ (since the electron wave functions are already fixed) and dispersion equation for the electron energy spectrum ($E_{n_z n_\rho m}$). The latter is not presented due its sophisticated form. The axial quantum number (n_z) numbers the solutions of dispersion equation at the fixed quantum numbers n_ρ, m. As a result, the electron energy spectrum ($E^e_{n_z n_\rho m}$) and wave function ($\Psi^e_{n_z n_\rho m}(\mathbf{r})$) in three-well closed CQD in CQW are completely defined.

In order to analyze in details the process of transformation of stationary spectrum in three-well closed CQD into the quasi-stationary spectrum in single open CQD, according to the theory one has to investigate the behavior of probability of electron residence inside the inner CQD at $h_1 \to \infty$, $h_2 \to \infty$

$$W^e_{n_z n_\rho m} = \int_{-z_3}^{z_1} \left|F_{n_z n_\rho m}(z)\right|^2 dz. \tag{7}$$

All numeric calculations were performed for the β-HgS/β-CdS nano-system with the well known material parameters, ref. [4]. Geometrical parameters of the three-well closed CQD were the following: quantum wire radius: $\rho_0 = 8a_{\mathrm{HgS}}$, barrier thickness: $\Delta = \Delta_1 = \Delta_2 = 2a_{\mathrm{CdS}}$, height of inner CQD: $h_0 = 15a_{\mathrm{HgS}}$. The sizes of equal ($h = h_1 = h_2$) outer wells of CQD varied from zero to physical infinity.

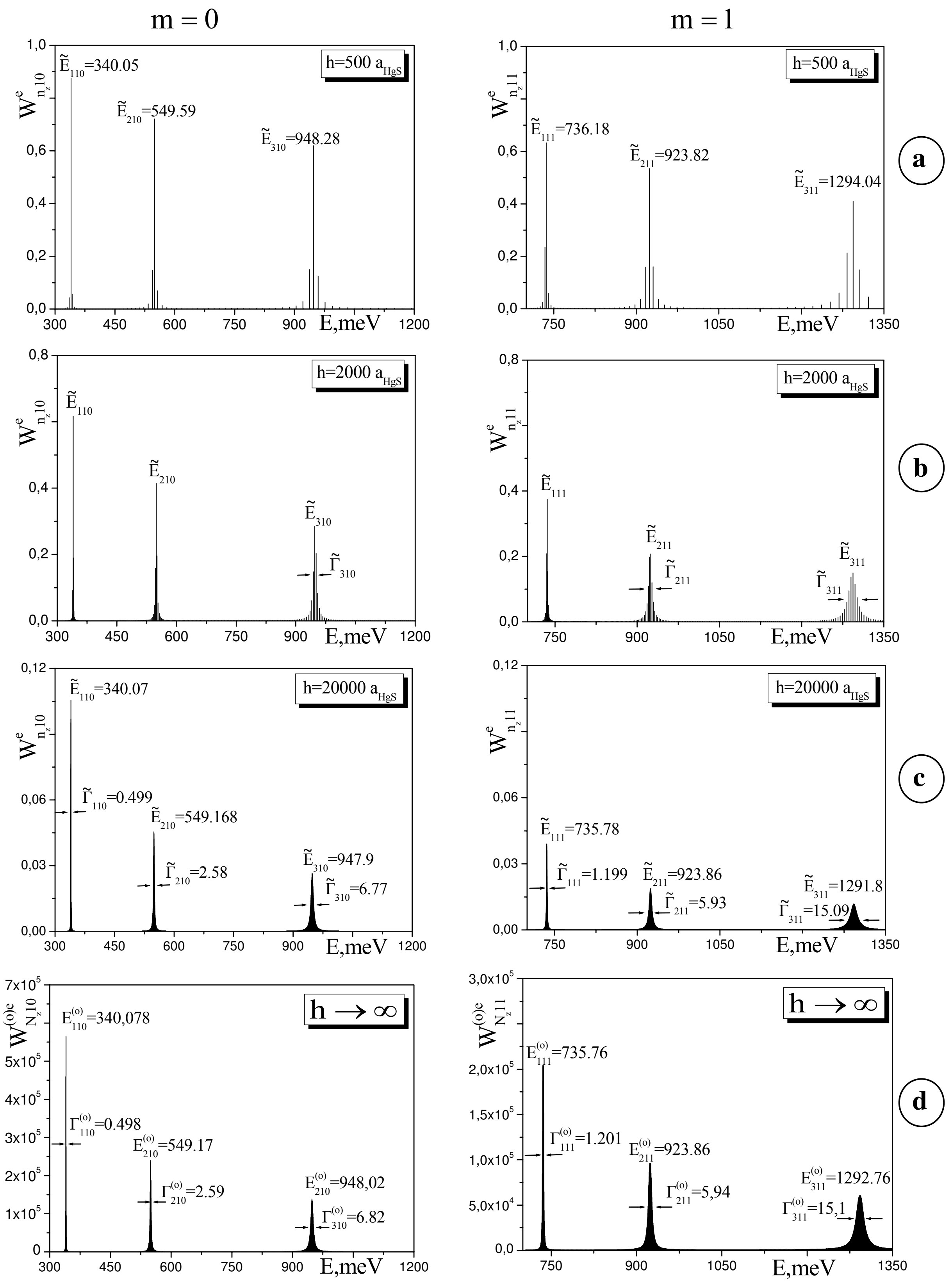

Fig. 2. Evolution of probability $W^e_{n_z 1m}(E)$ of electron residence in three inner parts of three-well closed CQD (a)–(c) at different h and $W^{(o)e}_{N_z 1m}(E)$ dependence in single open CQD inside of CQW (d) at $\rho_0 = 8a_{\mathrm{HgS}}$, $\Delta = 2a_{\mathrm{CdS}}$, $h_0 = 15a_{\mathrm{HgS}}$.

Before the analysis of the dependences of electron residence in three inner parts of the nano-system ($W^e_{n_z n_\rho m}$) at h varying, it is convenient to introduce the concept of pra-resonance energy ($\tilde{E}^e_{N_z n_\rho m}$) corresponding to the N_z-th value of the energy at which $W^e_{n_z n_\rho m}$ is maximal and pra-resonance widths of N_z-th discrete states band ($\tilde{\Gamma}^e_{N_z n_\rho m}$) — the interval of energies in the vicinity of pra-resonance one ($\tilde{E}^e_{N_z n_\rho m}$). At the boundaries of this interval the probability of electron residence in three inner parts of three-well closed CQD are two times smaller than the maximal probability ($W^e_{n_z n_\rho m}$) in the state with the pra-resonance energy ($\tilde{E}^e_{N_z n_\rho m}$).

Fig. 2 presents the results for the probability $W^e_{n_z 1m}$ ($m = 0, 1$) of electron residence in three inner parts of the three-well closed CQD calculated at different h magnitudes. From Fig. 2a it is clear that when the outer CQDs height is rather small ($h = 500a_{\mathrm{HgS}}$), the probability of electron residence at all three pra-resonance levels ($\tilde{E}^e_{N_z 1m}$) are more than two times bigger than the probability of its location at both (or one) neighbour levels. Thus, the concept of these QSSs width still does not appear.

When the outer CQDs have the size: $h = 2000a_{\mathrm{HgS}}$ (Fig. 2b), the lower QSSs with pra-resonance energies ($\tilde{E}^e_{110}$, $\tilde{E}^e_{210}$, $\tilde{E}^e_{111}$) still have not widths but for the upper QSSs with the resonance energies ($\tilde{E}^e_{310}$, $\tilde{E}^e_{211}$, $\tilde{E}^e_{311}$) there are the conditions for the appearence of the discrete bands widths ($\tilde{\Gamma}^e_{310}$, $\tilde{\Gamma}^e_{211}$, $\tilde{\Gamma}^e_{311}$). When the height of outer CQDs is: $h = 20000a_{\mathrm{HgS}}$ (Fig. 2c) already all quasi-discrete bands are characterized by pra-resonance energies ($\tilde{E}^e_{N_z n_\rho m}$) and widths ($\tilde{\Gamma}^e_{N_z n_\rho m}$).

Comparing Fig. 2c with Fig. 2d one can also see that the pra-resonance energies ($\tilde{E}^e_{N_z n_\rho m}$) and the respective widths ($\tilde{\Gamma}^e_{N_z n_\rho m}$) in the three-well CQD inside of CQW are almost coinciding with the resonance energies ($E^{(o)e}_{N_z n_\rho m}$) and widths ($\Gamma^{(o)e}_{N_z n_\rho m}$) in the single open CQD in CQW obtained within the S-matrix method [4]. We must note that the probabilities are naturally differently normalized.

III. QUASI-STATIONARY ELECTRON STATES IN QAD WITH DONOR IMPURITY

The electron energy spectrum in ZnS/CdS semiconductor QAD with donor impurity, placed into the center of a nano-system is studied. The Coulomb potential of the impurity together with the rectangular potential of QAD create two potential wells for the electron: deep — near the center of spherical nano-system and shallow — near its boundary (Fig. 3). The depth of shallow well and barrier width between the potential wells depend on QAD radius. Evidently, the stationary spectrum of electron localized out of the QAD is observed for the negative energies and for the positive ones — the series of QSSs of electron localized in the deep potential well, characterized by the finite life times due to the ability of quasi-particle tunneling through the potential barrier.

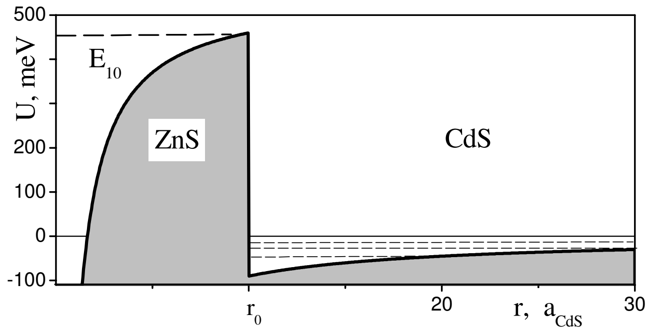

Fig. 3. Potential energy scheme and electron energy spectrum in ZnS/CdS QAD.

The study of energy spectrum in this nano-system in the framework of scattering matrix method meets the problem of finding the S-matrix poles in the complex energy plane. Therefore, the investigation of QSSs of electron interacting with donor impurity placed into the center of QAD is performed according to the method developed in the previous Section.

The closed semiconductor spherical nano-system — QAD with r_0 radius is embedded into the spherical shell with radius r_1 being impenetrable for the electron. The limit case of r_1 increasing transforms the closed nano-system into the open one. Thus, the electron energy spectrum in QAD with donor impurity can be obtained as limit transition at $r_1 \to \infty$ of energy spectrum for the closed nano-system.

Solving again the Schrödinger Eq. (1) in spherical coordinate system with the amiltonian

$$\hat{H} = -\frac{\hbar^2}{2}\nabla\frac{1}{\mu(r)}\nabla - \frac{e^2}{\varepsilon r} + V(r), \tag{8}$$

where

$$\mu(r) = \begin{cases} \mu_0, & r < r_0 \\ \mu_1, & r \geq r_0 \end{cases}, \qquad V(r) = \begin{cases} V_0, & r < r_0 \\ 0, & r \geq r_0 \end{cases} \tag{9}$$

and introducing the values

$$\xi_0 = \frac{\sqrt{8\mu_0(E_{n\ell} - V_0)}}{\hbar}, \qquad \xi_1 = \frac{\sqrt{8\mu_1 E_{n\ell}}}{\hbar}, \tag{10}$$

$$\eta_{0,1} = \frac{2\mu_{0,1}e^2}{\varepsilon\xi_{0,1}\hbar^2} \tag{11}$$

the radial wave function can be written as

$$R_{n\ell}(r) = \begin{cases} \dfrac{\chi_0(\xi_0 r)}{r}, & r < r_0 \\ \dfrac{\chi_1(\xi_1 r)}{r}, & r > r_0 \end{cases}. \tag{12}$$

Finally, two differential equations are obtained

$$\frac{1}{\xi_0^2}\frac{\partial^2 \chi_0(\xi_0 r)}{\partial r^2}+\left(-\frac{1}{4}-\frac{\eta_0}{\xi_0 r}+\frac{1/4-(\ell+1/2)^2}{\xi_0^2 r^2}\right)\chi_0(\xi_0 r)=0, \qquad r<r_0, \tag{13}$$

$$\frac{1}{\xi_1^2}\frac{\partial^2 \chi_1(\xi_1 r)}{\partial r^2}+\left(-\frac{1}{4}-\frac{\eta_1}{\xi_1 r}+\frac{1/4-(\ell+1/2)^2}{\xi_1^2 r^2}\right)\chi_1(\xi_1 r)=0, \qquad r>r_0. \tag{14}$$

Their general solution can be written within the Whittaker functions [6, 7]

$$\chi_0(\xi_0\, r)=A_0 M(\eta_0,\, \ell+1/2,\, \xi_0\, r), \qquad \chi_1(\xi_1\, r)=A_1\, W(\eta_1,\, \ell+1/2,\, \xi_1\, r). \tag{15}$$

The Whittaker functions are expressed through the hyper geometrical functions of the first and second kind $F(\alpha,\gamma,z)$, $G(\alpha,\gamma,z)$. Finally, the radial wave function is written as

$$R_{n\ell}(r)=\begin{cases} A_0\exp\left[-\xi_0\, r/2\right] r^\ell\, F(\ell+1+\eta_0,\ 2\ell+2,\ \xi_0 r), & r<r_0,\\ A_1\exp\left[-\xi_1\, r/2\right] r^\ell\, G(\ell+1+\eta_1,\ 2\ell+2,\ \xi_1 r), & r>r_0. \end{cases} \tag{16}$$

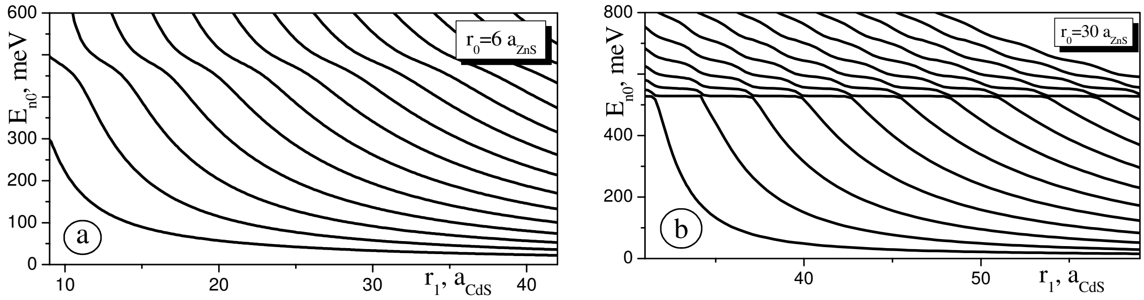

Fig. 4. Evolution of energy spectrum on radius (r_1) for the electron bound by donor impurity in nano-system: (a) $r_0 = 6a_{\mathrm{ZnS}}$; (b) $r_0 = 30a_{\mathrm{ZnS}}$.

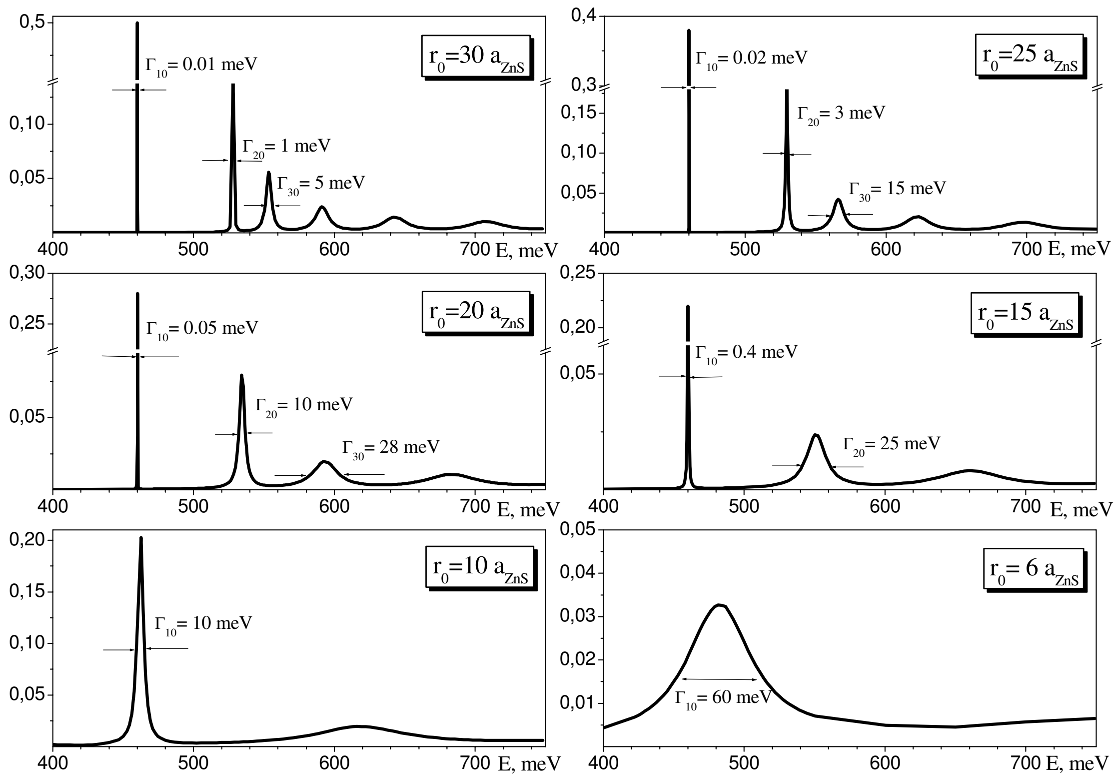

Fig. 5. Quasi-stationary energy spectrum of electron bound by donor impurity in QAD calculated at $r_0 = 30,\ 25,\ 20,\ 15,\ 10,\ 6a_{\mathrm{ZnS}}$.

Using the conditions of wave function and density of current continuity at the media interface at $r = r_0$ [7] together with the condition $\chi_1(r_1) = 0$, the dispersion equation for the defining of discrete energy spectrum of electron in closed nano-system is obtained. At the base of the latter at $r_1 \to \infty$, likewise in the previous Section, the quasi-stationary spectrum of electron in QAD with donor impurity is studied.

The increasing of the potential well width ($\Delta r = r_1 - r_0$) brings to the decreasing of the distance between the discrete energy levels of a closed nano-system. Among the great number of levels there are the ones, corresponding to the states of electron bound by the impurity in the core of a nano-system. They can be defined by the probability of electron residence in the core of nano-system

$$W^e_{n\ell} = \int_0^{r_0} |R_{n\ell}(r)|^2 \, r^2 dr. \tag{17}$$

When $r_1 \to \infty$, at the background of the continuous spectrum, the quasi-stationary spectrum of the electron bound by donor impurity in QAD appears.

The numeric calculation of electron energy spectrum was performed for ZnS/CdS QAD at $\ell = 0$. Fig. 4 shows the dependence of electron spectrum in a nano-system with the donor impurity on r_1 radius. It is clear that when the radius increases the width of the outer potential well increases too. Consequently, the size quantization becomes smaller and energy levels, corresponding to the states of electron localized in the outer well, shift into the region of lower energies and become closer to each other. The anti-crossing effect is observed for the states of the electron localized in the nano-system core. The increasing of the core radius (r_0) causes that of the number of states of electron localized by the impurity in the inner potential well. It is reflected in the behavior of $E_{n\ell}(r_1)$ (Fig. 4b). When $r_1 \to \infty$, these stationary states are transformed into the quasi-stationary with the energy coinciding to the energy of the respective stationary states where the electron with bigger probability is in the core of a nano-system. The finite life time is determined by the semi-width of the respective levels.

Fig. 5 presents the energy spectrum of the electron bound by the impurity in QAD with different radii (r_0) calculated at $r_1 > 5000a_{\mathrm{CdS}}$. It is clear that at the increasing of the QAD radius the QSSs energies shift into the region of lower energies. Herein, the widths of the levels become smaller. It is to be noted that even higher of the potential barrier: $-\dfrac{e^2}{\varepsilon r_0} + V_0$, there are the resonance states of electron characterized by the finite width.

IV. CONCLUSIONS

In the paper the theory of origin and evolution of electron discrete bands of probability distribution over the energy in the closed three-well CQD in CQW depending on the sizes of outer wells was developed.

It is established that the spectral parameters of electron in single open two-barrier CQD in CQW can always and with good exactness be approximated by the respective spectral parameters in three-well closed CQD in CQW.

The approved method allows obtaining QSSs of the electron bound by donor impurity in QAD (without using the S-matrix method) and studying their dependences on geometric parameters of a nano-system.

It is shown that at the increasing of the QAD radius the energies of quasi-stationary states of the electron bound by donor impurity are shifting into the low-energy range of spectrum. Herein, their semi-widths are decreasing.

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СТАЦІОНАРНИЙ І КВАЗІСТАЦІОНАРНИЙ СПЕКТРИ ЕЛЕКТРОНА У КВАНТОВОМУ ДРОТІ ТА КВАНТОВІЙ АНТИТОЧЦІ З ДОМІШКОЮ

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У роботі досліджено квазістаціонарні стани електрона у відкритій напівпровідниковій циліндричній квантовій точці, що розташована у квантовому дроті та сферичній квантовій антиточці з донорною домішкою. Задачі розв'язано за допомогою функції розподілу ймовірності знаходження електрона у відповідних закритих наносистемах. Обґрунтований на прикладі першої наносистеми метод дав змогу дослідити квазістаціонарний спектр електрона, зв'язаного донорною домішкою у квантовій антиточці без використання методу S-матриці.