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## THE SPECTRA AND LIFETIMES OF ELECTRONS, HOLES, AND EXCITONS IN OPEN CYLINDRICAL QUANTUM DOTS EMBEDDED INTO QUANTUM WIRES OR WELLS

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The spectra and lifetimes of an electron, a hole, and an exciton in open cylindrical quantum dots (QDs) embedded into various environments — a cylindrical quantum wire (QW) and a plane quantum well which, in their turn, are located in a massive three-dimensional medium — have been studied theoretically. The relevant calculations were carried out in the framework of the effective mass approximation and for a rectangular potential. The analytical expression for the scattering matrix ( $S$ -matrix) has been obtained. The real part of the  $S$ -matrix pole defines the energy of a quasi-stationary state, while the imaginary one defines its halfwidth and, accordingly, the lifetime of a quasiparticle in this state. Numerical calculations of the spectra and lifetimes of an electron, a hole, and an exciton were carried out for nanoheterosystems composed on the basis of semiconductors  $\beta$ -HgS and  $\beta$ -CdS.

### 1. Introduction

The progress in studying low-dimensional semiconducting systems is connected with the development of new technologies for growing nanocrystals which allow various nanoheterosystems (two-dimensional quantum wells, one-dimensional QWs, zero-dimensional QDs) and their various combinations to be fabricated [1, 2].

The overwhelming majority of the theoretical and experimental researches of nanoheterosystems dealt with the so-called “closed” systems, i.e. the systems where the environment constitutes the maximal potential barrier for quasiparticles (electrons, holes, excitons). In such systems, the quasiparticle states with the energy lower than the potential of the environment are always stationary. The energy losses of the excited quasiparticles (e.g., excitons) are possible only owing

to their interaction with one another or with other quasiparticles or fields.

“Open” nanoheterosystems are of interest because here, contrary to the “closed” ones, there always exists an opportunity for quasiparticles to penetrate through the potential barrier into the environment [3], which creates an additional channel for the energy of quasiparticles, which were excited in the quantum well, to relax. Such a feature of the “open” systems may be important for the creation of high-speed devices free from transit-time effects.

The theory of quasi-stationary states of electrons and holes in complex spherical QDs and cylindrical QWs was developed on the basis of the  $S$ -matrix method in works [4–6]. The calculations were carried on for specific nanoheterosystems taken as examples; and the dependences of the energy spectra and the lifetimes of quasiparticles on the geometrical parameters of those nanosystems and on the dynamic characteristics of quasiparticles (e.g., the longitudinal quasi-momentum in the case of a QW) were obtained.

Until now, there has been no theory of the quasi-stationary states of electrons, holes, and excitons in “open” combined nanoheterosystems altogether. Therefore, it is interesting and important to investigate the peculiarities in the behavior of quasi-stationary states, at least in relatively simple systems. Such a problem is solved using two spatial models as examples:

1) a semiconducting QW which includes a QD separated from the other part of the QW by two identical quantum antidots (QADs) with potential barriers of finite heights (Fig. 1);

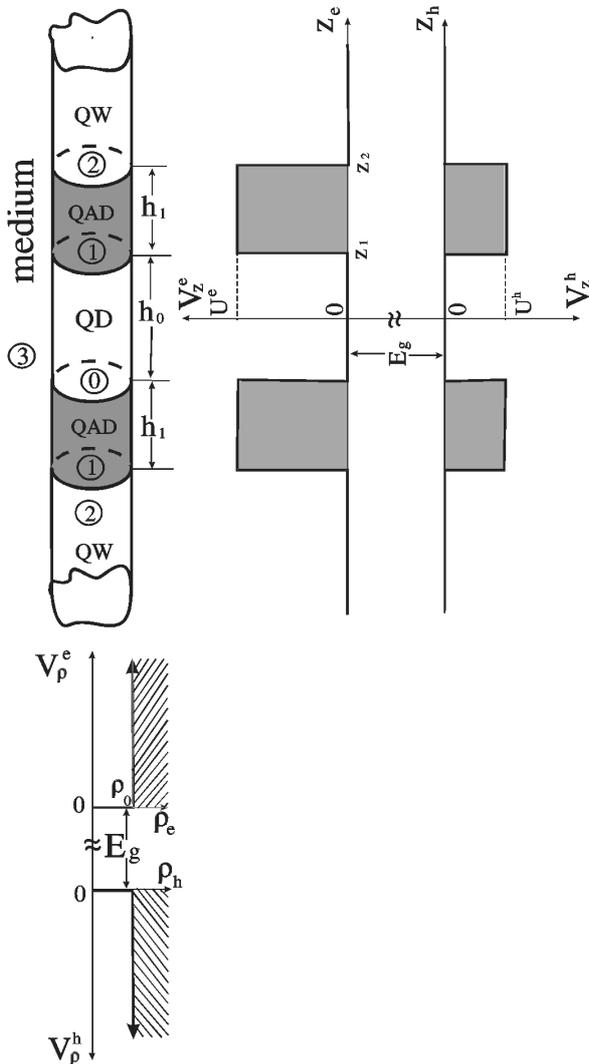


Fig. 1. Layout and the potentials  $V^{e,h}$  of cylindrical QD 0 and two cylindrical QADs 1 in QW 2 embedded into environment 3

2) a cylindrical QD and a cylindrical QAD located in a plane quantum well which, in its turn, is positioned in a massive three-dimensional environment (Fig. 2).

## 2. The Hamiltonian and the $S$ -matrix of an Electron (Hole)

### 2.1. A compound cylindrical quantum wire with an “open” quantum dot

Consider a compound semiconducting QW which contains a QD surrounded by two identical QADs. The radii of the nanowire, the QD and both the QADs are equal to  $\rho_0$ ; the heights of the QD and the QADs are  $h_0$

and  $h_1$ , respectively (Fig. 1). According to the reasons of symmetry, the origin of the cylindrical coordinate system is convenient to be chosen at the center of the QD, with the axis  $OZ$  being directed along the rotation axis of the system. It is supposed that the QW and the QD are made of materials with identical physical characteristics (effective masses, dielectric permittivities), while the material of both the QADs has different, in general, characteristics. The entire compound QW is embedded into the environment which constitutes the infinite potential barrier for any quasiparticle presenting in this system.

Owing to the finite height and width of the potential barriers of both QADs, the QW is an “open” quasi-one-dimensional system, so that quasiparticles can penetrate through the potential barriers, and their states are quasi-stationary with certain finite lifetimes.

The geometrical dimensions of the nanoheterosystem’s components are such that the approximation of effective masses is valid for an electron (hole). So, the effective masses of an electron ( $e$ ) and a hole ( $h$ ) are considered known and equal to their corresponding values in massive analogues of nanocrystals:

$$\mu^{e,h}(z) = \begin{cases} \mu_0^{e,h} & \text{in QD,} \\ \mu_1^{e,h} & \text{in QAD,} \\ \mu_0^{e,h} & \text{in QW.} \end{cases} \quad (1)$$

We also suppose that the lattice constants ( $a_0, a_1$ ) of the well (subscript 0) and barrier (subscript 1) materials are very close by value. Considering the nanosystem composed on the basis of  $\beta$ -HgS or  $\beta$ -CdS semiconductors (such a nanosystem will be studied below), we note that the lattice constants in it are such that  $(a_1 - a_0)/a_0 \leq 1\%$  (see the table). Therefore, the interfaces between subsystems are abrupt enough, which allows us to use the approximation of rectangular potential energies for an electron and a hole:

$$V^{e,h}(\rho, \varphi, z) = \begin{cases} -V_0^{e,h} & \text{in QD,} \\ -V_1^{e,h} & \text{in QAD,} \\ -V_0^{e,h} & \text{in QW.} \end{cases} \quad (2)$$

where  $V_{0,1}^{e,h}$  is the potential energy of an electron or a hole in the corresponding environment reckoned from the vacuum level. At  $\rho > \rho_0$ ,  $V^e(\rho, \varphi, z) = V^h(\rho, \varphi, z) = \infty$ .

Since the theories of the quasi-stationary spectra of an electron and a hole in the investigated system are equivalent, we present the further calculations for an electron, temporarily omitting the superscript  $e$ .

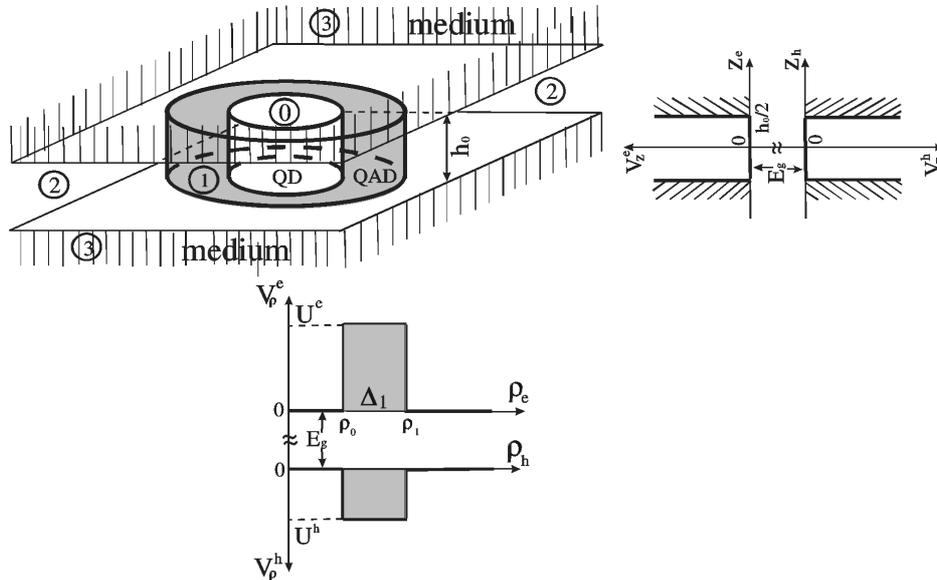


Fig. 2. Layout and the potentials  $V^{e,h}$  of cylindrical QD 0 and cylindrical QAD 1 in quantum well 2 embedded into environment 3

To study the electron quantum states, it is necessary to solve the Schrödinger equation

$$\hat{H}\psi(\vec{r}) = E\psi(\vec{r}) \quad (3)$$

with the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2} \vec{\nabla} \frac{1}{\mu(z)} \vec{\nabla} + U(\rho, \varphi, z). \quad (4)$$

According to the symmetry of the problem, it is convenient to seek the wave function  $\psi(\vec{r})$  in the form [7]

$$\begin{aligned} \Psi_{n_\rho m}(\vec{r}) &= (-\pi \rho_0^2 J_{m-1}(x_{n_\rho m}) J_{m+1}(x_{n_\rho m}))^{-1/2} \times \\ &\times J_m\left(\frac{x_{n_\rho m}}{\rho_0} \rho\right) e^{im\varphi} \varphi(z), \end{aligned} \quad (5)$$

where  $m = 0, \pm 1, \pm 2 \dots$  is the magnetic quantum number,  $J_m(x)$  is the Bessel function of an integer order,  $x_{n_\rho m}$  are the zeros of the Bessel function, and  $n_\rho$  is the radial quantum number that defines the serial number of the zero of the Bessel function at fixed  $m$ .

After having substituted solution (5) into the Schrödinger equation (3), the variables can be separated, and the equation for the  $z$ -th component of the wave function reads

$$\frac{\partial^2}{\partial z^2} \varphi(z) + \varphi(z) \left[ \frac{2\mu(z)}{\hbar^2} (E - V(\rho, \varphi, z)) - \frac{x_{n_\rho m}^2}{\rho_0^2} \right] = 0. \quad (6)$$

Since the potential energy of an electron is symmetric in the  $z$  variable, Eq. (6) is invariant with respect to the inversion transformation  $z \rightarrow -z$ . It allows  $z$  to be confined to the interval of variation from 0 to  $\infty$ . The solutions of Eq. (6) are separated into even (+) and odd (-) ones [8]:

$$\begin{aligned} \varphi^\pm(z) &= \\ &= \begin{cases} \varphi_0(z) = A^\pm (e^{ik_0 z} \pm e^{-ik_0 z}), & 0 < z \leq z_1, \\ \varphi_1(z) = B^\pm (e^{-k_1 z} + S_1^\pm e^{k_1 z}), & z_1 \leq z \leq z_2, \\ \varphi_2(z) = C^\pm (e^{-ik_0 z} + S^\pm e^{ik_0 z}), & z_2 \leq z < \infty. \end{cases} \end{aligned} \quad (7)$$

Here,  $k_0^2 = 2\mu_0/\hbar^2 E - x_{n_\rho m}^2/\rho_0^2$ ,  $k_1^2 = 2\mu_1/\hbar^2 (U - E) + x_{n_\rho m}^2/\rho_0^2$ ,  $U = V_0 - V_1$ , and  $S^\pm$  is the scattering matrix ( $S$ -matrix). The energy is reckoned “upwards” from the bottom of the potential well (environment “0”).

Further, using the continuity conditions for the wave function and the probability density current at all the medium interfaces

$$\begin{cases} \varphi_0(z)|_{z=z_1} = \varphi_1(z)|_{z=z_1}, \\ \varphi_1(z)|_{z=z_2} = \varphi_2(z)|_{z=z_2}, \\ \frac{1}{\mu_0} \varphi_0'(z)|_{z=z_1} = \frac{1}{\mu_1} \varphi_1'(z)|_{z=z_1}, \\ \frac{1}{\mu_1} \varphi_1'(z)|_{z=z_2} = \frac{1}{\mu_0} \varphi_2'(z)|_{z=z_2} \end{cases} \quad (8)$$

and the normalization condition for the wave function

$$\int_0^\infty \varphi_{k_0}^{*\pm}(z) \varphi_{k_0'}^\pm(z) dz = \delta(k_0 - k_0'), \quad (9)$$

we obtain the analytical expressions for all the coefficients  $A^\pm$ ,  $B^\pm$ , and  $C^\pm$ . We omit the cumbersome analytical expressions for these coefficients and will not consider the features of the wave

functions of quasi-stationary states of an electron and a hole. Instead, we confine ourselves to the analysis and calculation of the  $S$ -matrix which looks like

$$S^\pm = \frac{S_1^\pm(\mu_0 k_1 + i\mu_1 k_0) \exp[(k_1 - ik_0)z_2] - (\mu_0 k_1 - i\mu_1 k_0) \exp[-(k_1 + ik_0)z_2]}{(\mu_0 k_1 + i\mu_1 k_0) \exp[-(k_1 - ik_0)z_2] - S_1(\mu_0 k_1 - i\mu_1 k_0) \exp[(k_1 + ik_0)z_2]}, \quad (10)$$

where

$$S_1^\pm = \frac{\exp(-2k_1 z_1) \left[ k_1 \mu_0 \begin{Bmatrix} \cos(k_0 z_1) \\ \sin(k_0 z_1) \end{Bmatrix} \mp k_0 \mu_1 \begin{Bmatrix} \sin(k_0 z_1) \\ \cos(k_0 z_1) \end{Bmatrix} \right]}{k_1 \mu_0 \begin{Bmatrix} \cos(k_0 z_1) \\ \sin(k_0 z_1) \end{Bmatrix} \pm k_0 \mu_1 \begin{Bmatrix} \sin(k_0 z_1) \\ \cos(k_0 z_1) \end{Bmatrix}}. \quad (11)$$

According to the general theory [3], the real parts of the  $S$ -matrix poles in the complex plane of energies

$$\tilde{E}_{n_z n_\rho m} = E_{n_z n_\rho m} - i\Gamma_{n_z n_\rho m}/2 \quad (12)$$

define the energies of the quasi-stationary states ( $E_{n_z n_\rho m}$ ), while the relevant imaginary parts their halfwidths ( $\Gamma_{n_z n_\rho m}$ ). The quantum number  $n_z$  numbers the poles of the  $S$ -matrix, provided the quantum numbers  $n_\rho$  and  $m$  are fixed. The level halfwidth is connected to the electron (hole) lifetime in the state  $|n_z n_\rho m\rangle$  by the relationship

$$\tau_p = \frac{\hbar}{\Gamma_p} \quad (p = n_z n_\rho m). \quad (13)$$

Thus, formulae (10)–(13) determine the energy spectrum and the lifetimes of an electron and a hole in the quasi-stationary states which are formed in a quasi-one-dimensional “open” cylindrical QD embedded into a cylindrical QW.

## 2.2. A plane quantum well with a quasi-plane cylindrical quantum dot

Consider a compound semiconducting quantum well which contains a cylindrical QD surrounded by a cylindrical QAD. The radii of the QD and QAD are, respectively,  $\rho_0$  and  $\rho_1$ , and the heights of the dot and antidot are equal to  $h_0$  both (Fig. 2). The origin of the cylindrical coordinate system is selected at the center of the QD, with the axis  $OZ$  being directed along the rotation axis of the system.

Owing to the finite height and width of the potential barrier of the QAD, the quantum well is a

quasi-plane “open” system, so that quasiparticles can penetrate through the potential barriers, and their states are quasi-stationary and possess certain finite lifetimes.

It is adopted that all the components of the nanosystem obey the same geometrical and physical conditions, as in the previous case. Therefore, the effective masses and the potential energies of an electron and a hole can be assigned in the form

$$\mu^{e,h}(\rho) = \begin{cases} \mu_0^{e,h} & \text{in QD,} \\ \mu_1^{e,h} & \text{in QAD,} \\ \mu_0^{e,h} & \text{in quantum well,} \end{cases} \quad (14)$$

$$V^{e,h}(\rho, \varphi, z) = \begin{cases} -V_0^{e,h} & \text{in QD,} \\ -V_1^{e,h} & \text{in QAD,} \\ -V_0^{e,h} & \text{in quantum well.} \end{cases} \quad (15)$$

where  $V_{0,1}^{e,h}$  is the potential energy of an electron or a hole in a corresponding environment reckoned from the vacuum level. At  $|z| > h_0/2$ ,  $V^e(\rho, \varphi, z) = V^h(\rho, \varphi, z) = \infty$ . According to the symmetry of the problem, it is convenient to seek for a solution of Eq. (3) in the form

$$\psi_{n_z}(\vec{r}) = R(\rho) e^{im\varphi} \sqrt{\frac{2}{h_0}} \begin{cases} \cos \frac{\pi n_z z}{h_0}, & n_z = 1, 3, \dots, \\ \sin \frac{\pi n_z z}{h_0}, & n_z = 2, 4, \dots, \end{cases} \quad (16)$$

where  $n_z$  is the axial quantum number.

The substitution of function (16) into the Schrödinger equation (3) gives the equation for the radial wave function  $R(\rho)$ :

$$\left[ \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} - \frac{m^2}{\rho^2} + \frac{2\mu(\rho)}{\hbar^2} (E - V(\rho, \varphi, z)) - \frac{\pi^2 n_z^2}{h_0^2} \right] \times R(\rho) = 0, \quad (17)$$

the solutions of which are the linear combinations of the Hankel functions:

$$R_{n_z m}(\rho) = \begin{cases} R_{n_z m}^{(0)}(\rho) = A_m^{(0)} [H_m^-(k_0 \rho) + H_m^+(k_0 \rho)], & \rho < \rho_0 \\ R_{n_z m}^{(1)}(\rho) = A_m^{(1)} [H_m^-(k_1 \rho) + S_{n_z m}^1(E) H_m^+(k_1 \rho)], & \rho_0 \leq \rho \leq \rho_1 \\ R_{n_z m}^{(2)}(\rho) = A_m^{(2)} [H_m^-(k_0 \rho) + S_{n_z m}(E) H_m^+(k_0 \rho)], & \rho > \rho_1. \end{cases} \quad (18)$$

Here,  $k_0^2 = 2\mu_0/(\hbar^2 E) - \pi^2 n_z^2/h_0^2$ ,  $k_1^2 = 2\mu_1/[\hbar^2 (U - E)] + \pi^2 n_z^2/h_0^2$ ,  $U = V_0 - V_1$ , and  $S_{n_z m}$

is the scattering matrix ( $S$ -matrix). The energy is reckoned “upwards” from the bottom of the potential well (environment “0”).

Further, using the continuity conditions of the wave function and the probability density current at all the medium interfaces

$$\begin{cases} R_{n_z m}^{(0)}(\rho) \Big|_{\rho=\rho_0} = R_{n_z m}^{(1)}(\rho) \Big|_{\rho=\rho_0}, \\ R_{n_z m}^{(1)}(\rho) \Big|_{\rho=\rho_1} = R_{n_z m}^{(2)}(\rho) \Big|_{\rho=\rho_1}, \\ \frac{1}{\mu_0} R_{n_z m}^{\prime(0)}(\rho) \Big|_{\rho=\rho_0} = \frac{1}{\mu_1} R_{n_z m}^{\prime(1)}(\rho) \Big|_{\rho=\rho_0}, \\ \frac{1}{\mu_1} R_{n_z m}^{\prime(1)}(\rho) \Big|_{\rho=\rho_1} = \frac{1}{\mu_0} R_{n_z m}^{\prime(2)}(\rho) \Big|_{\rho=\rho_1} \end{cases} \quad (19)$$

and the normalization condition for the wave function

$$\int_0^\infty R_{n_z m k_0}^*(\rho) R_{n_z m k_0'}(\rho) \rho d\rho = \delta(k_0 - k_0'), \quad (20)$$

we obtain the analytical expressions for all the coefficients  $A_m^{(0)}$ ,  $A_m^{(1)}$ ,  $A_m^{(2)}$ , and  $S_{n_z m}^1$  and the  $S$ -matrix. In particular,

$$S_{n_z n_\rho m} = \frac{\mu_0 k_1 \left[ \frac{H_m^-(k_1 \rho_1) + S_{n_z n_\rho m}^1 H_m^+(k_1 \rho_1)}{H_m^-(k_1 \rho_1) + S_{n_z n_\rho m}^1 H_m^+(k_1 \rho_1)} H_m^-(k_0 \rho_1) - H_m^-(k_0 \rho_1) \right]}{k_0 \mu_1 \left[ H_m^+(k_0 \rho_1) - \frac{\mu_0 k_1}{\mu_1 k_0} \frac{H_m^-(k_1 \rho_1) + S_{n_z n_\rho m}^1 H_m^+(k_1 \rho_1)}{H_m^-(k_1 \rho_1) + S_{n_z n_\rho m}^1 H_m^+(k_1 \rho_1)} H_m^+(k_0 \rho_1) \right]}, \quad (21)$$

where

$$S_{n_z n_\rho m}^1 = \frac{\mu_1 k_0 \left[ \frac{J_m'(k_0 \rho_0)}{J_m(k_0 \rho_0)} H_m^-(k_1 \rho_0) - H_m^-(k_1 \rho_0) \right]}{H_m^+(k_1 \rho_0) - \frac{\mu_1 k_0}{\mu_0 k_1} \frac{J_m'(k_0 \rho_0)}{J_m(k_0 \rho_0)} H_m^+(k_1 \rho_0)}. \quad (22)$$

We note that the energies of quasi-stationary states and their lifetimes are characterized, similarly to the previously analyzed nanosystem, by three quantum numbers ( $n_z$ ,  $n_\rho$ , and  $m$ ). The quantum number  $n_\rho$  numbers the poles of the  $S$ -matrix, provided the quantum numbers  $n_z$  and  $m$  are fixed.

Thus, formulae (12), (13), (21), and (22) determine the energy spectrum and the lifetimes of an electron and a hole in quasi-stationary states formed in a plane quantum well with an “open” cylindrical QD.

### 3. Analysis and Discussion of Results

The specific calculations of the quasi-stationary state energies and quasiparticle lifetimes were carried on for two types of the systems made up on the basis of  $\beta$ -HgS and  $\beta$ -CdS semiconductors and described above. The parameters of these semiconductors are quoted in the Table.

In Fig. 3, the dependences of the quasi-stationary state energies of an electron and a hole  $E_{n_z n_\rho m}^{e,h(I,II)}$  on the barrier thickness in a QW ( $I$ ) and a quantum well ( $II$ ) at the fixed height and radius of the QD are shown. From the figure, one can see that the energy values in the

Crystal	$\mu^e(\mu_0)$	$\mu^h(\mu_0)$	$V^e$ (eV)	$V^h$ (eV)	$a$ (Å)	$\varepsilon$	$E_g$
CdS	0.2	0.7	3.8	6.3	5.818	5.5	2.5
HgS	0.036	0.044	5.15	5.65	5.851	11.36	0.5



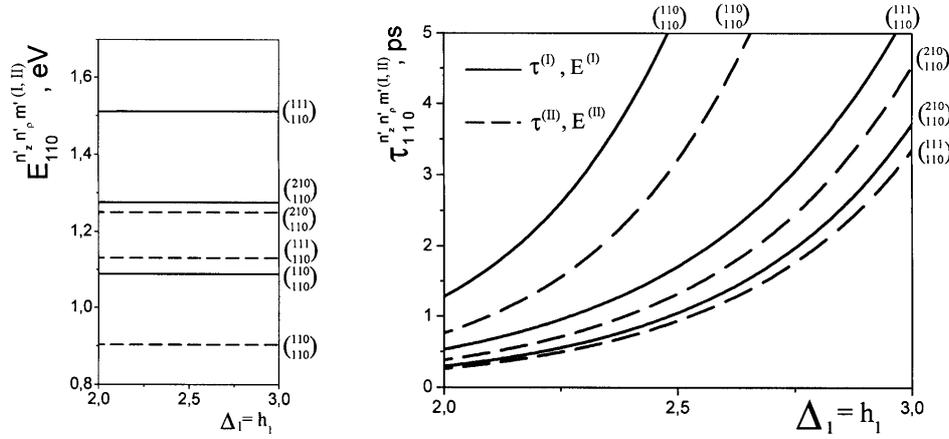


Fig. 6. Dependences of  $E_{110}^{n'_z n'_\rho m'(I,II)}$  and  $\tau_{110}^{n'_z n'_\rho m'(I,II)}$  on the barrier dimensions ( $\Delta_1 = h_1$ ) at  $h_0 = 2\rho_0 = 8a_{\text{HgS}} = \text{const}$

In Fig. 6, we show the dependences of the exciton excitation energies  $E_{110}^{n'_z n'_\rho m'(I,II)}$  and the exciton lifetimes  $\tau_{110}^{n'_z n'_\rho m'(I,II)}$  in the bottom part to the spectrum on the barrier thickness. The dependences were calculated by the formulae

$$E_{n_z n_\rho m}^{n'_z n'_\rho m'(I,II)} = E_{n_z n_\rho m}^e(I,II) + E_{n_z n_\rho m}^h(I,II) + E_g \text{HgS} \quad (23)$$

$$\frac{1}{\tau_{n_z n_\rho m}^{n'_z n'_\rho m'(I,II)}} = \frac{1}{\tau_{n_z n_\rho m}^e(I,II)} + \frac{1}{\tau_{n_z n_\rho m}^h(I,II)}, \quad (24)$$

which do not take into account the electron–hole Coulomb interaction, considering it as such that does not affect the obtained results qualitatively. From the figure, one can see that the energies of exciton states depend weakly on the barrier dimensions in both cases of a quantum wire and a quantum well, while their lifetimes grow exponentially as the barrier thickens. It turned out that, despite the barrier dimensions, both the energies and lifetimes of the ground quasi-stationary state of excitons in a QW are greater than those in a quantum well ( $E_{110}^{110(I)} > E_{110}^{110(II)}$ ,  $\tau_{110}^{110(I)} > \tau_{110}^{110(II)}$ ). However, it is not so for excited states. In particular, one can see that  $E_{110}^{210(I)} > E_{110}^{210(II)}$ , but  $\tau_{110}^{210(I)} < \tau_{110}^{210(II)}$ .

Thus, the general conclusion is that the spectral characteristics and lifetimes of the quasiparticles, although having qualitatively similar dependences on the geometrical parameters of the nanosystem, differ considerably by value, depending on the dimensionality of the space, into which the quasiparticles can escape from the same open QD.

Since the exciton states of the Breit–Wigner type turned out to be well localized in the space of a QD, they

would possess a sufficient lifetime (about picoseconds) to be observed experimentally.

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СПЕКТРИ І ЧАСИ ЖИТТЯ ЕЛЕКТРОНА, ДІРКИ ТА ЕКСИТОНА У ВІДКРИТИХ ЦИЛІНДРИЧНИХ КВАНТОВИХ ТОЧКАХ, ЩО РОЗТАШОВАНІ У КВАНТОВИХ ДРОТАХ АБО КВАНТОВИХ ЯМАХ

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Резюме

Теоретично досліджено спектри і часи життя електронів, дірок та екситонів у відкритих циліндричних квантових точках, що розташовані в різних середовищах: у циліндричному квантовому дроді і в плоскій квантовій ямі, які, в свою чергу, перебувають у масивному тривимірному середовищі. Розрахунок спектрів та часів життя виконано у наближенні ефективних мас

та прямокутного потенціалу. Розв'язується рівняння Шредінгера з використанням умов неперервності хвильової функції та потоку густини ймовірності на всіх межах поділу наногетеросистем. Отримано аналітичний вираз для матриці розсіяння ( $S$ -матриці). Дійсна частина полюсів  $S$ -матриці визначає енергію

квазістаціонарного стану, уявна — його півширину, а відповідно і час життя квазічастинки в цьому стані. Числові розрахунки спектрів та часів життя електрона, дірки і екситона виконано для наногетеросистем на основі напівпровідників  $\beta$ -HgS і  $\beta$ -CdS.