ELECTRON RESONANCE STATES IN OPENED SPHERICAL TWO-BARRIER NANOHETEROSTRUCTURES

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The energies of electron resonance quasistationary states in opened two-barrier spherical nanoheterostructures are obtained within the effective mass approximation using the *S*-matrix theory. Numerical calculations are performed for the HgS/CdS/HgS/CdS/HgS nanosystem. The *S*-matrix poles in the complex plane of energy are studied. The quasistationary state energies and electron lifetimes in these states are obtained as functions of nanosystem geometric sizes. It is shown that the electron lifetime in an excited quasistationary state quasiperiodically depends on the sizes of nanoheterosystem wells.

Introduction

During the last few years, a new branch of solid state physics – arrays of quantum dots – has got a great interest of scientists. Quantum dots (QD) are the unique objects combining the properties of bulk semiconductors and single atoms. The temperature stability of quasiparticles spectra in QD makes possible the essential improvement of modern devices: radiation detectors, light diodes, lasers, solar batteries, etc. [1 – 4]. The unique characteristics of QD give opportunity to fabricate electron devices which have a wide perspective in the development of semiconductor technique.

Recently, the spherical complicated nanoheterosystems [3 – 4] have been created by using modern technologies. The electron, hole, and exciton spectra and their interaction between each other and with phonons were studied in [5 – 7] for such nanosystems. Multishell spherical nanosystems have more complicated quasiparticles spectra than single QD. That is why their experimental utilization receives a new impetus, while the theoretical investigation and analysis of physical properties become more complicated.

So-called opened QDs [8, 9] (began to be studied not long ago) have the basically new peculiarities. In such systems, quasiparticles being in quasistationary states can tunnel through the potential barrier penetrating into the external medium which is the potential well for them. In quasistationaty resonance states, they have a finite lifetime depending both on the physical and geometric parameters of a nanosystem. In [9], it was shown that one can see in the radiation spectra of opened spherical nanosystems only those resonance quasistationary states, the lifetime of the radiation transition between which is much smaller than the electron or hole lifetime in these states. Thus, it is possible to guide the quasiparticle spectra in opened nanoheterosystems.

In this paper, we investigate the electron spectrum and lifetimes in resonance quasistationary states of an opened spherical two-barrier nanoheterosystem (HgS/CdS/HgS/CdS/HgS).

1. Electron Hamiltonian and Wave Functions in Opened Spherical Two-barrier Nanoheterostructure

The complicated spherical nanoheterosystem (Fig. 1) consisting of two HgS shells which are the potential wells *0*, *2*, two CdS shells creating the potential barriers *1*, *3*, and the external medium HgS *4* is under study.

In a spherical coordinate system with the beginning at the center of the heterostructure, an electron has the effective mass $m(r)$ and potential energy $U(r)$ which are the functions of the distance from the center because they have different values in different media:

$$m(r) = \begin{cases} m_0, & r < r_0,\ r_1 < r < r_2,\ r > r_3, \\ m_1, & r_0 \le r \le r_1,\ r_2 \le r \le r_3, \end{cases}$$

$$U(r) = \begin{cases} 0, & r < r_0,\ r_1 < r < r_2,\ r > r_3, \\ U_e, & r_0 \le r \le r_1,\ r_2 \le r \le r_3. \end{cases} \qquad (1)$$

Due to the effective mass dependence on *r*, the Schrodinger equation has the form [10]

$$\left(-\frac{\hbar^2}{2} \vec{\nabla} \frac{1}{m(r)} \vec{\nabla} + U(\vec{r}) \right) \Psi(r) = E\, \Psi(r). \qquad (2)$$

Considering the spherical symmetry, its solution is written as

$$\Psi(\vec{r}) = R_l(r)\, Y_{lm}(\theta, \varphi), \quad l = 0, 1, 2, \ldots$$

$$m = 0, \pm 1, \pm 2, \ldots, \qquad (3)$$

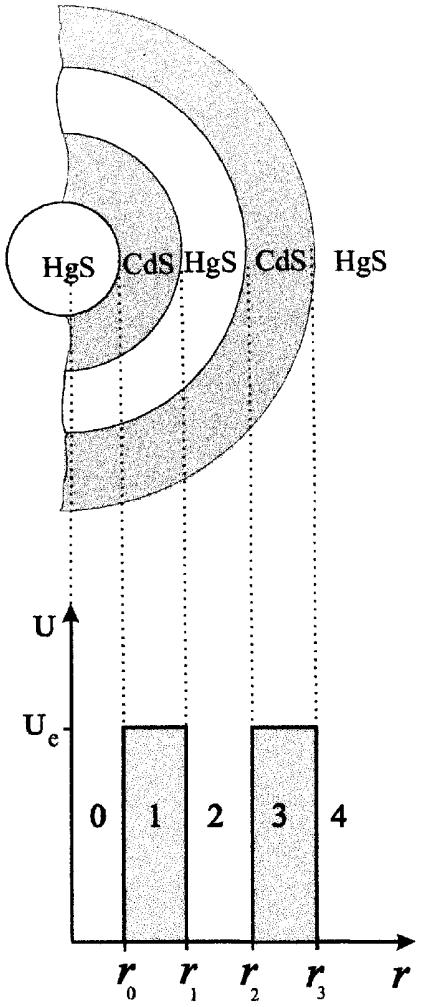

Fig. 1. Geometric scheme (*a*) and electron potential energy scheme (*b*) for the spherical nanosystem

where $R_l(r)$ is radial wave function:

$$R_l(r) = \begin{cases} R_l^{(0)}(r), & 0 \le r < r_0, \\ R_l^{(i)}(r), & r_{i-1} \le r < r_i, \quad (i = 1, 2, 3) \\ R_l^{(4)}(r), & r_3 \le r < \infty. \end{cases} \tag{4}$$

Inserting (3) in (2), we obtain the system of typical equations

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR_l^{(i)}}{dr}\right) + \left[K_i^2 - \frac{l(l+1)}{r^2}\right] R_l^{(i)}(r) = 0,$$

$(i = 1, \ldots, 4),$ (5)

where

$$K_i^2 = \frac{2m_i}{\hbar^2}(E - U_i) = \begin{cases} k^2, & i = 0, 2, 4, \\ -\chi^2, & i = 1, 3. \end{cases} \tag{6}$$

Their solutions are the linear combinations of Hankel functions of different arguments

$$R_l^{(0)}(r) = k A_l^{(0)} [h_l^-(kr) + h_l^+(kr)],$$

$$R_l^{(i)}(r) = K_i A_l^{(i)} [h_l^-(K_i r) - S_l^{(i)} h_l^+(K_i r)],$$

$(i = 1, \ldots, 3),$

$$R_l^{(4)}(r) = k A_l [h_l^-(kr) - S_l(k) h_l^+(kr)]. \tag{7}$$

The coefficient $A_l = 1/\sqrt{2\pi}$ is fixed by the normalizing condition for the radial wave function [10]:

$$\int_0^\infty R_{lk}^*(r) R_{lk'}(r) r^2 dr = \delta(k - k'). \tag{8}$$

The other unknown coefficients $A_l^{(i)}$, $S_l^{(i)}$ and scattering matrix S_l are defined by the fitting conditions for the wave functions and their derivatives as

$$R_l^{(i)}(K_i r_i) = R_l^{i+1}(K_{i+1} r_i),$$

$$\frac{1}{m_i}\frac{dR_l^{(i)}(r)}{dr}\bigg|_{r=r_i} = \frac{1}{m_{i+1}}\frac{dR_l^{(i+1)}(r)}{dr}\bigg|_{r=r_i}$$

$(i = 0, 1, \ldots, 4).$ (9)

The system of equations (9) gives an exact analytic solution for the S-matrix. In the case of spherically symmetric states ($l = 0$) which would be analysed further, $S_0 = S$ has the form

$$S(k) = e^{-2ikr_3} \{e^{2\chi(r_2 - r_3)} [m_1(-1 - ikr_3) +$$

$$+ m_0(1 + \chi r_3)] + [m_1(1 + ikr_3) + m_0(-1 + \chi r_3)] \xi_3\} /$$

$$/ \{e^{2\chi(r_2 - r_3)} [m_1(-1 + ikr_3) + m_0(1 + \chi r_3)] +$$

$$+ [m_1(1 - ikr_3) + m_0(-1 + \chi r_3)] \xi_3\}. \tag{10}$$

where

$$\xi_3 = \{-m_0 + m_1 - \chi m_0 r_2 - ikm_1 r_2 +$$

$$+ e^{2ik(r_1 - r_2)} [m_1 (-1 - ikr_2) + m_0 (1 + \chi r_2)] \xi_2\} /$$

$$/ \{- m_0 + m_1 + \chi m_0 r_2 - ikm_1 r_2 - e^{2ik(r_1 - r_2)} \times$$

$$\times [m_1 (1 + ikr_2) + m_0 (-1 + \chi r_2)] \xi_2 \}, \qquad (11)$$

$$\xi_2 = \{m_0 - m_1 + \chi m_0 r_1 + ikm_1 r_1 +$$

$$+ e^{2\chi(-r_0 + r_1)} [m_1 (1 - ikr_1) + m_0 (-1 + \chi r_1)] \xi_1 \} /$$

$$/ \{m_0 - m_1 + \chi m_0 r_1 - ikm_1 r_1 + e^{2\chi(-r_0 + r_1)} \times$$

$$\times [m_1 (1 + ikr_1) + m_0 (-1 + \chi r_1)] \xi_1 \}, \qquad (12)$$

$$\xi_1 = \frac{m_0 - m_1 + \chi m_0 r_0 + m_1 k \operatorname{ctg}(kr_0) r_0}{m_0 - m_1 - \chi m_0 r_0 + m_1 k \operatorname{ctg}(kr_0) r_0}. \qquad (13)$$

The properties of S_l at $l \neq 0$ are the same as for $l = 0$. Therefore, we shall study the electron spectrum only in spherically symmetric states.

2. Properties of *S*-matrix. Electron Spectrum in Resonance States

The S-matrix obtained in Section 1 has the properties well known from the scattering theory [11]. In the complex plane of quasimomentum, one has $k = k_1 + i k_2$. In the real axis k_1, $|S(k)| \equiv 1$, and the S-matrix poles in the imaginary plane k_2 define the stationary states of the system. So-called quasistationary states (which live during a certain time τ) of a quasiparticle in the potential field $U(r)$ correspond to the every pole of $S(K)$ in the lower semiplane $(k = k_1 - i k_2)$.

Due to the fact that the potentials of both wells in the spherical nanosystem HgS/CdS/HgS/CdS/HgS under research are equal to the potential of the external medium, there cannot be any stationary states in it. There are only resonance quasistationary states where the electron is located for a long time in the internal part of the system. Fig. 2 shows the real (Re S) and imaginary (Im S) parts of the S-matrix as functions of complex energy. Here, one can also see the location of the S-matrix pole corresponding to the lowest resonance quasistationary state. The calculations were performed for the system with material parameters: $m_0 = 0.036\, m_e$, $m_1 = 0.2\, m_e$, $a_{\mathrm{HgS}} = 5.851$ Å, $a_{\mathrm{HgS}} = 5.818$ Å, $U_e = 1.35$ eV and shell sizes: $n_0 = 15$, $\Delta_1 = 5$, $\Delta_2 = 15$, $\Delta_3 = 5$ ($\Delta_i = n_i - n_{i-1}$) (in units of lattice constant).

It is clear from Fig. 2 that the S-matrix as a function of the complex variable $\tilde{E}$ has the following characteristic behaviour: almost everywhere in the complex energy plane ($E = E_1 + i E_2$), its real and imaginary parts are smooth functions. Only in the vicinity of a pole, both have the second-order discontinuity at the point $(E_{n0}, - i \Gamma_{n0}/2)$ of the complex energy plane.

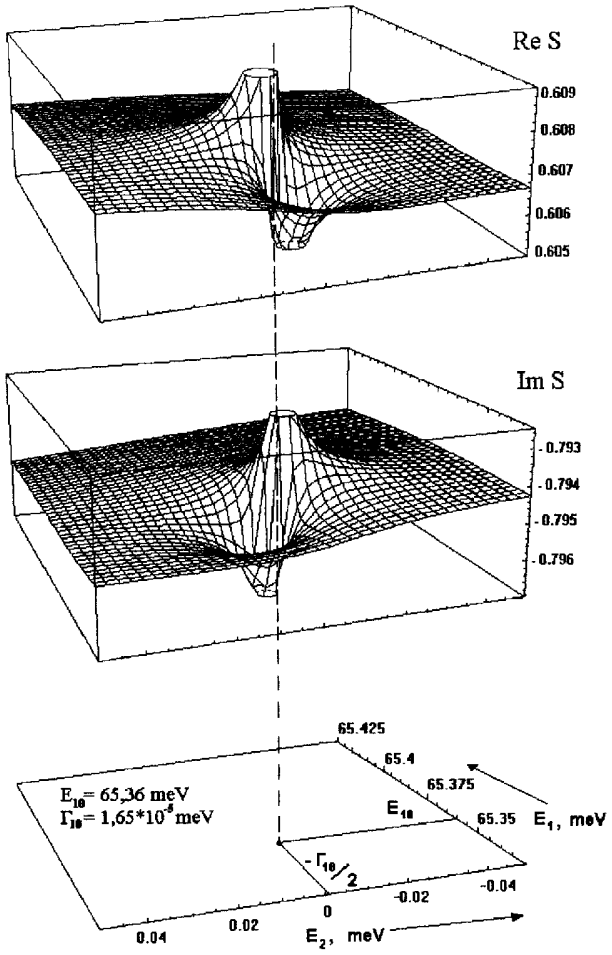

Fig. 2. Dependences of the real and imagionary parts of the scattering matrix S on $\tilde{E}$ and location of the pole in the complex plane for state $|100\rangle$ at $n_0 = 15$, $\Delta_1 = 5$, $\Delta_2 = 15$, $\Delta_3 = 5$ in units of lattice constant

Numerical results for the S-matrix and location of its pole in the complex energy plane make it possible to investigate the electron resonance quasistationary states energies E and lifetimes τ dependences on geometric sizes of the nanosystem.

Fig. 3 shows the electron resonance energies E_{n0} and lifetimes τ_{n0} in spherically symmetric quasistationary states of the opened two-barrier nanoheterostructure HgS/CdS/HgS/CdS/HgS as functions of core radius r_0 at fixed sizes of the system shells. One can see from the figure that these dependences are nonmonotonous. The reason is obvious because if the heights of both internal potential barriers

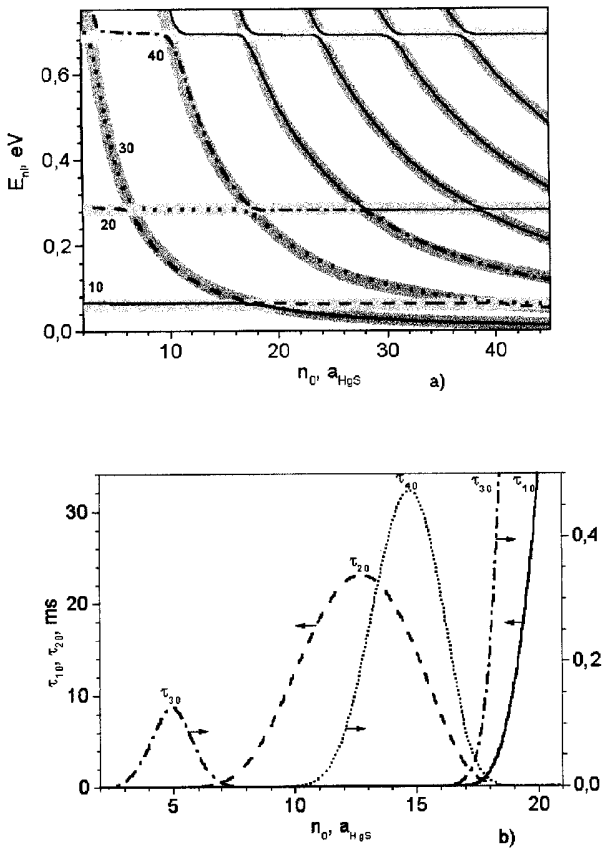

Fig. 3. Dependences of electron resonance energies E_{n0} and lifetimes τ_{n0} on n_0 at $\Delta_1 = 5$, $\Delta_2 = 15$, $\Delta_3 = 5$

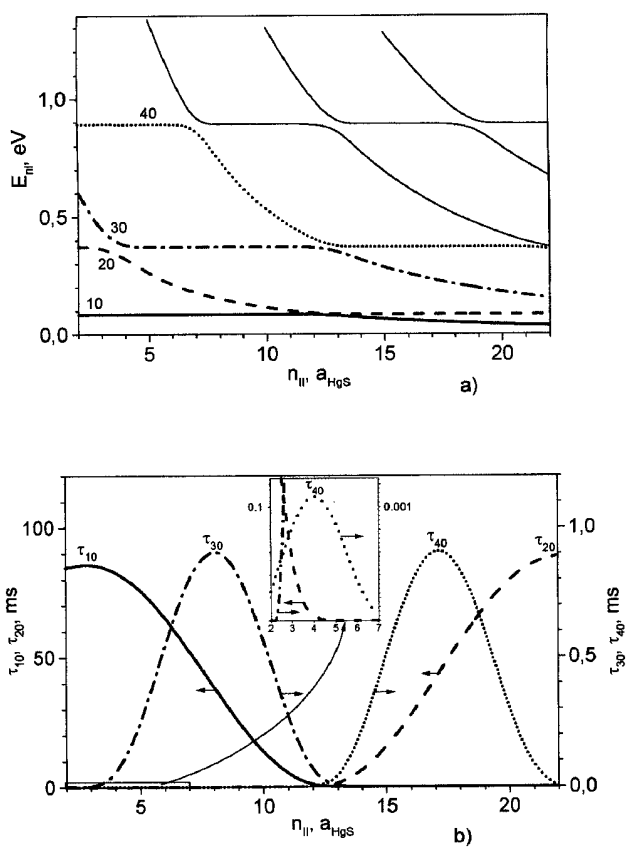

Fig. 4. Dependences of electron resonance energies E_{n0} and lifetimes τ_{n0} on Δ_2 at $n_0 = 15$, $\Delta_1 = 5$, $\Delta_3 = 5$

would be infinite, the electron states would be stationary and the spectrum at $l = 0$ would be located in the region of energies reflected in Fig. 3 by respective grey bands. Herein, it is clear that electron levels $|n\,00\rangle_2$ located in the second well (medium *2*) must not be changed when n_0 (the number of monoshells in well *0*) is varied because a change in the internal well size brings to a change in the external well curvature and does not influence its width. Thus, the energy levels must be located on the boundaries of horizontal grey bands. If an electron would be located in the internal well (zeroth medium), then its energy levels must be shifted into region of lower energies confined by the decreasing bands when the well size increases. Since, an electron in the spherical nanosystem with two isolated infinite potential quantum wells in spherically symmetric states would be characterized by the spectrum with two crossed groups of energy levels at the fixed thickness of the second well (Δ_2) and variable size of the first well (n_0).

The real nanosystem HgS/CdS/HgS/CdS/HgS contains potential barriers of finite height, which means that the electron moves in the field of finite potential in the space between the wells. Herein, the presence of the second barrier (Δ_3) brings to the fact that the states are now resonant and quasistationary because the quasiparticle can perform an infinite movement; the presence of the first barrier causes the effect of repulsing levels since the symmetry of both groups of states (due to both wells) is the same.

It is obvious that the resonance energy levels borned by the quantum well *0* (see Fig. 1) are shifted to the bottom when its sizes increase, and the levels borned by the quantum well *2* almost do not depend on n_0. Such behaviour of quantum system energy levels causes the existence of the regions of repulsing levels and characteristic cascade dependence of the level on n_0. Herein, the regions, where E_{no} are close to the horisontal, belong to the states where the electron is located generally, in the potential well *2*, and those where E_{n0} are decreasing belong to the

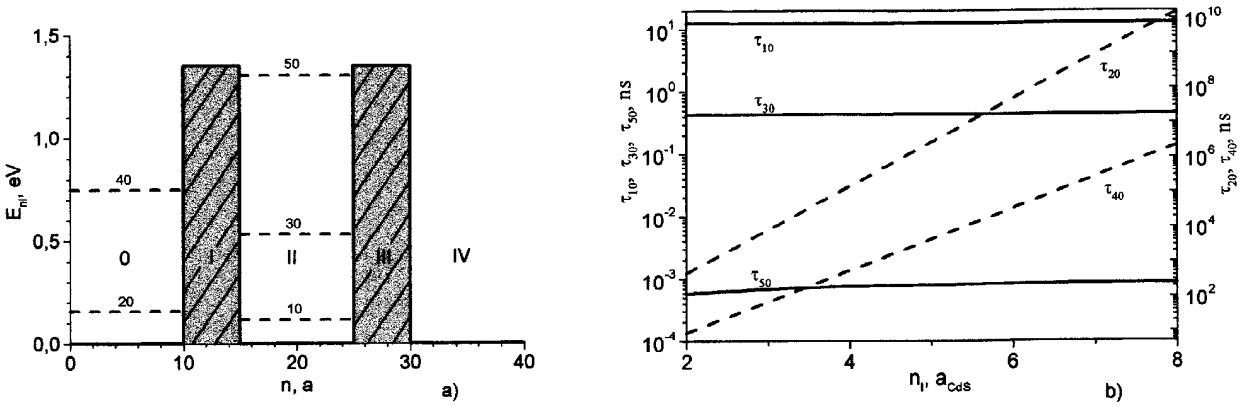

Fig. 5. Scheme of electron potential energy location of resonance levels (*a*) and electron lifetimes dependences on barrier thickness Δ_1 at $n_0 = 15$, $\Delta_2 = 15$, $\Delta_3 = 5$ (*b*)

states where the electron is located generally, in core *0*.

Now it is easy to understand the dependence of electron lifetime in quasistationary states $\tau_{n0}(r_0)$ (Fig. 3,*b*). It is clear from the Fig. 3,*a* that, in the region $n_0 \leq 18$, the lowest resonance level belongs to a quasistationary state where the electron is located in the quantum well *2*, from which its easy to tunnel through the last potential barrier *3* into the external medium; consequently, the electron lifetime in this state is small (Fig. 3,*b*).

The other situation is in the region $n_0 > 18$ where the core sizes are such that the electron with the smallest energy is generally located in the quantum well *0* from which it is harder to penetrate (through the two barriers) into the external medium; since, the lifetime in this state increases. A monotonous and rapid increase in the lifetime τ_{10} in the region $n_0 > 18$ is also caused by the smaller magnitude of the energy level; thus, the height of the potential barrier, through which the electron has to tunnel into the external medium, becomes higher.

The dependence $\tau_{20}(n_0)$ has the other character than τ_{10}. From Fig. 3,*b*, one can see that the τ_{20} curve has one maximum in the vicinity $n_0 \approx 13$. Analysing E_{20} as a function of n_0, it becomes clear that, at small n_0 magnitudes, the electron is generally located in the second well *2*, where its lifetime is small. When n_0 increases, the energy decays, corresponding to the electron moving into the first well, from which it is harder to penetrate into the external medium; thus, its lifetime in this state becomes bigger reaching the maximum at $n_0 \approx 13$. A further increase in n_0 makes the resonance energy closer to the lowest electron level in the second well. Thus, it again moves into the second well *2*, from which it is easier to tunnel into the external medium, and the lifetime in this state becomes smaller.

Analysing E_{30} by analogy, it is clear that τ_{30} as a function of n_0 must have two maxima that is seen in Fig. 3,*b*.

The general conclusion is the following. The electron lifetimes in resonance states corresponding to the regions of decreasing energies are big and are small in the states where the resonance energies weakly depend on n. The number of maxima on the τ_{n0} curve is defined by the number of decreasing energy regions which is caused by the width of the external well: the bigger the latter, the bigger is the number of maxima in every τ_{n0} curve. The effective sizes of the barriers (through which a quasiparticle has to tunnel) become bigger and the magnitudes of maxima also increase (Fig. 3,*b*) because the decreasing energy regions are located lower for a fixed state when n_0 increases.

Fig. 4 shows the results of calculation of the resonance energy E_{n0} and electron lifetime τ_{n0} as functions of the second well thickness Δ_2 when all other sizes of the nanosystem are fixed. It is clear from Fig. 4,*a* that the horisontal regions of the $E_{n0}(\Delta_2)$ dependences correspond to the states where an electron is located in the HgS core. Electron lifetime in these states is several orders bigger than that in states where it is generally located in the potential well *2* (decreasing energy regions).

In Fig. 5,*b*, the electron lifetime τ_{n0} dependences on the thickness of the first barrier Δ_1 are presented for fixed geometric sizes of other nanosystem parts. The energy levels almost do not depend on the barrier thickness and are formally depicted in the energy scheme (Fig. 5,*a*) in those wells, where the electron in the respective state is mostly located. Fig. 5 proves

that the electron lifetimes in states $|100\rangle$, $|300\rangle$, $|500\rangle$ do not depend on barrier *1* thickness Δ_1. In states $|200\rangle$ and $|400\rangle$, the lifetimes are increasing exponentially because of the 'power" of the barrier through which the electron in well *0* tunnels into the external medium.

From the obtained results, one can make the general conclusion. In the opened HgS/CdS/HgS/CdS/HgS nanosystem under research, there are short- and long-lived quasistationary resonance states. The location of the respective levels on the energy scale strongly depends on the sizes of potential wells and weakly depends on barriers' sizes. Only in the long-lived states, the electron lifetimes strongly (exponentially) depend on the thickness of the potential barrier *1*. The lifetimes in all states exponentially depend on the thickness of the external barrier *3*. In the radiation spectra of opened spherical nanosystems, there are reflected only those resonance states, the radiation lifetime between which is much smaller than the electron lifetime in this state.