EVOLUTION OF THE ELECTRON SPECTRUM OF SPHERICALLY SYMMETRIC STATES UNDER THE TRANSITION FROM A CLOSED DOUBLE-WELL DOT TO A SIMPLE OPEN SPHERICAL QUANTUM ONE

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The theory of the electron spectrum of spherically symmetric states in a double-well spherical quantum dot (SQD) is proposed and used to study the evolution of the spectrum, provided that the dimensions Δ_2 of the external well vary from zero to infinity. The spectrum is shown to coincide, at $\Delta_2 \to 0$, with the stationary spectrum of a closed single-well SQD and to pass, at $\Delta_2 \to \infty$, to the quasistationary spectrum of an open SQD with the decay of quantum states. A mechanism responsible for the decay of quasistationary states in an open SQD is proposed for the first time. It has been found that the redistribution of the probabilities for a quasiparticle to occupy energy levels in the vicinity of the resonance energy levels is the reason for the electron to exist in an open SQD for a finite time interval. The "memory" of closed double- and open single-well nanosystems with respect to the locations of resonance levels on the energy scale is originated from the anti-crossing ("bottle-neck") effect. The way how the mathematical tool of the theory of excitons and electron-phonon interactions in open SQDs can be built on the basis of the proposed theory is demonstrated.

1. Introduction

The theory of electron and hole wave functions and spectra in simple and multilayered SQDs has been built for both closed [1–3] and open nanoheterosystems [3–5]. As for the theory of excitons or the theory of interaction of electrons, holes, and excitons with phonons in SQDs, it is only at the development stage and includes various models of the phonon subsystem in a closed system [3,6, 7]; mostly, it is the model of dielectric continuum. The theory of quasiparticles, which interact with quantum fields (phonons, photons) in closed nanosystems, is not faced with basic difficulties, because the mathematical tools of classical quantum mechanics (for excitons) [8,9] and the methods of secondary quantization with the application of Green's functions [5] work well in this case.

At the same time, if one turns to the theory of quasiparticles and their interaction with quantized fields in open nanoheterosystems, the situation looks considerably worse because of the basic problems which do arise here and concern the applicability of the mathematical methods developed for systems of quasiparticles with stationary states. The quasiparticle states in open systems are quasistationary, and it is the key point why we have neither the theory of excitons nor the theory of interaction of electrons, holes, and excitons with phonons in such nanoheterosystems now.

The theory of electron and hole spectra in open SQDs has been developed in works [4, 5] on the basis of the general S-matrix theory [10]. It well describes the properties of quasistationary energy states in these systems and the lifetimes of electrons and holes which do not interact with one another. However, as soon as the necessity of constructing the theory which would take into account the interaction between these quasiparticles (excitons) or between these quasiparticles and quantized fields (phonons, photons) arises, one meets the basic difficulties. In this case, there are no difficulties with the quantization of phonon or electromagnetic fields in nanoheterosystems, because the mathematical methods for the quantization of a field of oscillations [3] or a phonon field [11] do not depend on whether the nanosystem is closed or open.

The situation for electrons, holes, and excitons is different. According to the general theory [10], the wave functions of the quasiparticle quasistationary states in open systems are not included into the complete set of orthonormalized functions. This circumstance makes the transformation of the Hamiltonian to the particle number representation with respect to the variables of those quasiparticles impossible. Therefore, a straightforward use of the electron, hole, and exciton wave functions, which were found for open systems in the framework of the S-matrix method, does not enable one to develop a theory, where the spectra of those quasiparticles are renormalized by their interaction with phonons or photons, by using the conventional methods of the quantum field theory [3].

The way out of this complicated situation could be discovered in considering a closed double-well SQD with a very large thickness Δ_2 of the external well rather than a simple open one (with a single well and a single barrier). However, the basic question arises in this case: Which must the thickness of the external well in a closed SQD be in order that the electron energy spectrum and the relevant wave functions can be considered close (and with which accuracy?) to their counterparts in the corresponding open system? The classical literature [10] gives no answer to this question, because it analyzes thoroughly only the transformation of a quasistationary electron spectrum into a stationary one owing to the layer-barrier thickening in a simple open single-well nanosystem. But we are interested in the inverse problem: How does the stationary spectrum of an electron in a closed double-well nanosystem gradually evolve to the quasistationary one, when the dimensions of the external layer-sphere increase? In the framework of such an approach, one more important question arises, which has not been answered until now as far as we know: Why do the quasistationary states, in which the electron has a finite lifetime, exist in a simple open nanosystem, whereas the spectrum in a closed double-well nanosystem is stationary irrelatively to the width of the external well and, at first sight, cannot be transformed into a quasistationary one as $\Delta_2 \to \infty$? However, as will be shown below, the reason for such an opportunity, naturally, does exist: this is a resonance approaching ("anti-crossing") of the electron energy levels in a nanosystem with two wells, when the external well becomes expanded to infinity.

These and other questions were answered while studying the evolution of the spectrum and the probability density for an electron to be located in a closed double-well SQD with one potential barrier, which was the main content of this work. As a result, we obtained the spectrum and the wave functions of the electron in a closed double-well SQD, which turned out close to their counterparts in a simple open nanosystem. We also revealed, for the first time, the physical origin of the electron lifetime finiteness in the quasistationary state: the electron lifetime turned out to be the time interval, within which the probability of finding the electron in the SQD becomes redistributed over all the states in the energy interval 2Γ in the neighborhood of the resonance energy E, so that the probabilities for the electron to occupy the states with the energies $E \pm \Gamma$ become half as high as the probability to occupy the state with the resonance energy E.

2. Nanosystem Hamiltonian. Spectrum and Wave Functions

Consider the spectrum and the wave functions of the electron in a closed SQD with two potential wells and one barrier (Fig. 1,*b*). The geometrical parameters (the radius of the internal well r_0, the thickness of the layer-barrier Δ_1, and the thickness of the external well Δ_2) are indicated in Fig. 1,*b*. It is evident that, if $\Delta_2 \to 0$, the three-layer nanosystem coincides with a simple closed SQD (Fig. 1,*a*), and, if $\Delta_2 \to \infty$, it transforms into a simple open double-layer SQD (Fig. 1,*c*). Figures 1,*a*—*c* also exhibit schematically the potential energies of the electron in corresponding nanoheterosystems.

In order to analyze the evolution features of the electron spectrum and the electron wave functions in relation to the variation of the external well thickness Δ_2, we shall obtain them in the framework of the general theory [3] by solving the stationary Schrödinger equation

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

In the spherical coordinate system with the point of origin located at the SQD center, the electron is characterized by the effective mass $m(r)$ and the potential energy $U(r)$:

$$m(r) = \begin{cases} m_0, & r < r_0, \qquad r_1 < r < r_2, \\ m_1, & r_0 \le r \le r_1, \quad r_2 \le r < \infty, \end{cases} \tag{2}$$

$$U(r) = \begin{cases} 0, & r < r_0, \qquad r_1 < r < r_2, \\ U, & r_0 \le r \le r_1, \quad r_2 \le r < \infty. \end{cases} \tag{3}$$

Taking the spherical symmetry of the problem into account, the solution of Eq. (1) is tried in the form

$$\Psi_{\ell \mathrm{m}}(\vec{r}) = R_\ell(r) Y_{\ell m}(\theta, \varphi), \quad \ell = 0, 1, 2, ...,$$

$$m = 0, \pm 1, \pm 2, ..., \tag{4}$$

where $Y_{\ell m}(\theta, \varphi)$ are the spherical functions [3, 8, 9], the radial function $R_\ell(r)$ looks like

$$R_\ell(r) = R_\ell^0(r)\theta(r - r_0) +$$

$$+\sum_{i=1}^{2} R_\ell^i(r)[\theta(r_i - r) - \theta(r - r_{i-1})] + R_\ell^i(r)\theta(r - r_i), \tag{5}$$

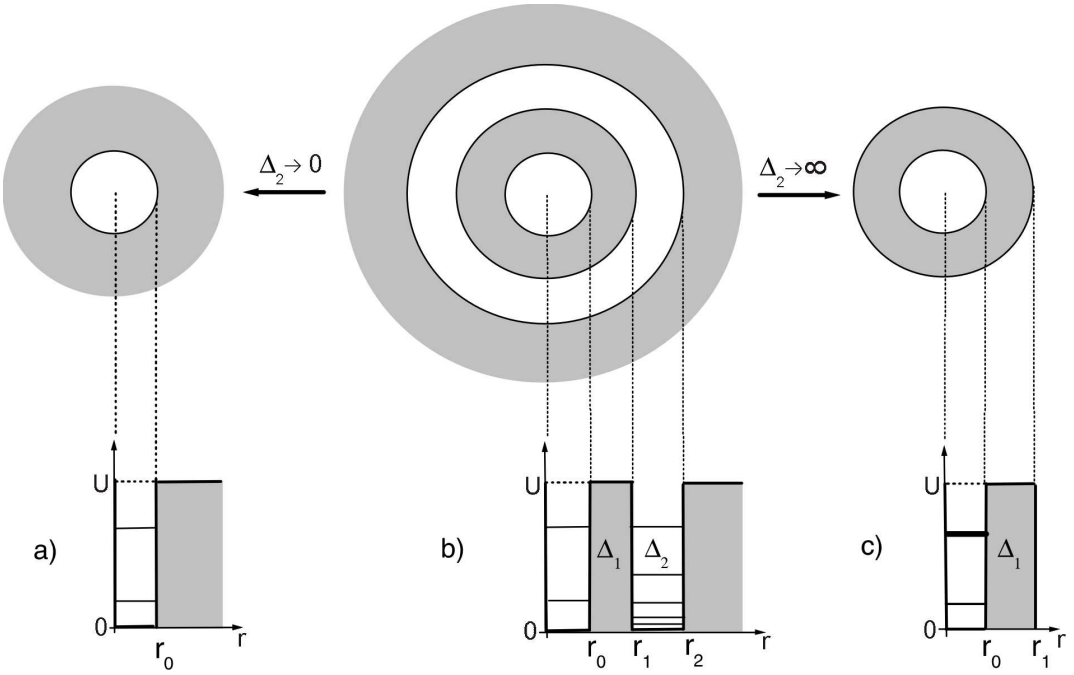

Fig. 1. Geometrical schemes of a simple closed (a), a closed double-well (b), and a simple open (c) spherical quantum dot (SQD), and the corresponding energy diagrams

and $\theta(r_i - r)$ is the Heaviside function. The functions $R^i_\ell(r)$ obey the system of equations

$$\left\{\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + K_i^2 - \frac{\ell(\ell+1)}{r^2}\right\} R^i_\ell(r) = 0, \quad i = 0,1,2,3, \tag{6}$$

whence they are obtained as the linear combinations of Bessel functions

$$R^i_\ell(K_i r) = A^i_\ell J_\ell(K_i r) + B^i_\ell N_\ell(K_i r). \tag{7}$$

Here,

$$J_\ell(K_i r) = \begin{cases} j_\ell(k_i r), \\ h^+_\ell(i\chi_i r), \end{cases}$$

$$N_\ell(K_i r) = \begin{cases} n_\ell(k_i r), & U_i \geq E, \\ h^-_\ell(i\chi_i r), & U_i \leq E, \end{cases} \tag{8}$$

$$K_i^2 = \frac{2m_i}{\hbar}(E - U_i) = \begin{cases} k_i^2, i = 0,2, \\ -\chi_i^2, i = 1. \end{cases} \tag{9}$$

Taking the boundary conditions that the wave functions and their density flows are continuous at all the system's boundaries —

$$\left.\begin{array}{l} R^i_\ell(r)|_{r=r_i} = R^{i+1}_\ell(r)|_{r=r_i} \\ \frac{1}{m_i}\frac{dR^i_\ell(r)}{dr}\Big|_{r=r_i} = \frac{1}{m_{i+1}}\frac{dR^{i+1}_\ell(r)}{dr}\Big|_{r=r_i} \end{array}\right\}, \quad i = 0,1,2,3, \tag{10}$$

— and the condition of normalization

$$\int_0^\infty |R_\ell(r)|^2 r^2 dr = 1 \tag{11}$$

into account, the coefficients A^i_ℓ and B^i_ℓ and, therefore, the complete set of electron wave functions and the electron energy spectrum $E_{n\ell}$ can be determined unambiguously. Since the corresponding analytical expressions are cumbersome, they are not presented in the explicit form, and the relevant results will be analyzed numerically in the next section.

Nevertheless, we would like to exhibit here the dispersion equation and the wave functions of the electron in a closed single-well system in their explicit forms, because, in the next section, the evolution of the electron spectrum of spherically symmetric states with $\ell = 0$, which accompanies the variation of the external well width Δ_2 in a three-layer SQD from the case of a

closed single-well nanosystem (with $\Delta_2 = 0$) to that of an open one (with $\Delta_2 \to \infty$), will be analyzed in detail. These expressions follow from the theory expounded above, if one puts $\Delta_2 \to 0$, and, in the energy range $E \le U$, which is of interest to us, look like

$$\frac{j_1(kr_0)}{j_0(kr_0)} = i\frac{\chi m_0}{km_1}\frac{h_1^+(i\chi r_0)}{h_0^+(i\chi r_0)}, \tag{12}$$

$$R_{n0}(r) =$$

$$= \left\{ j_0(k_n r)/j_0(k_n r)\,\big|_{r\le r_0} + h_0^+(i\chi_n r)/h_0^+(i\chi_n r)\big|_{r\ge r_0} \right\} /$$

$$\left\{ \frac{r_0^3}{2}\left[1 + \left|\frac{j_1(k_n r_0)}{j_0(k_n r_0)}\right|^2\right] + \right.$$

$$\left. + \left|h_0^+(i\chi_n r_0)\right|^{-2} \int\limits_0^\infty r^2 \left|h_0^+(i\chi_n r)\right|^2 dr \right\}, \tag{13}$$

where the subscript $n = 1, 2, 3\ldots$ enumerates the energy states E_{n0}, which are determined by the solutions of the dispersion equation (12). Naturally, these expressions coincide with those obtained earlier for the case $\ell = 0$ in works [1–3].

The spectrum and the wave functions of the electron in a simple open nanosystem cannot be obtained, in principle, making the limiting analytical transition $\Delta_2 \to \infty$ in the corresponding expressions for a closed double-well system. For the systems of such a type, according to the general theory, the S-matrix method [3, 10] is used to solve the Schrödinger equation (1). In terms of the subsystem components, which correspond to Fig. 1, *c*, the wave functions of the spherically symmetric states ($\ell = 0$) look like

$$R_{n0}(r) =$$

$$= \begin{cases} R_0^{(0)}(r) = k\mathrm{A}_0^{(0)}\left[h_0^-(kr) + h_0^+(kr)\right] \\ R_0^{(1)}(r) = i\chi\mathrm{A}_0^{(1)}\left[h_0^-(i\chi r) - S_0^{(1)}h_0^+(i\chi r)\right] \\ R_0^{(2)}(r) = k\mathrm{A}_0^{(2)}\left[h_0^-(kr) - S_0(k)h_0^+(kr)\right] \end{cases}. \tag{14}$$

The coefficient $A_0^{(2)} = 1/\sqrt{2\pi}$ is determined by the normalization condition [10]

$$\int\limits_0^\infty R_{0k}^*(r)R_{0k'}(r)r^2dr = \delta(k - k'), \tag{15}$$

while the other unknown coefficients A_0^0, A_0^1, and S_0^1 and the S_0-matrix are determined unequivocally from the boundary conditions

$$R_0^{(i)}(\mathrm{K}_i r_i) = R_0^{(i+1)}(\mathrm{K}_{i+1} r_i,)$$

$$\frac{1}{m_i}\frac{dR_0^{(i)}(\mathrm{K}_i r)}{dr}\bigg|_{r=r_i} = \frac{1}{m_{i+1}}\frac{dR_0^{(i+1)}(\mathrm{K}_{i+1} r)}{dr}\bigg|_{r=r_{i+1}} . \tag{16}$$

In such a way, we find the system of orthonormalized functions $R_0(r)$; they correspond to the quasistationary states, which are determined by the poles of the S_0-matrix. The remaining part of the work deals with the analysis of the probability density only. Therefore, the cumbersome analytical expressions for $R_0(r)$ will not be written down explicitly. Instead, we propose the explicit expression of the S_0-matrix for the spherically symmetric states:

$$S_0(k) = e^{-2ikr_1} \times$$

$$\times \left\{ e^{2\chi(r_0 - r_1)}\left[m_0(\chi r_1 + 1) - m_1(ikr_1 + 1)\right] + \right.$$

$$\left. + \left[m_0(\chi r_1 - 1) + m_1(ikr_1 + 1)\right]\xi \right\} /$$

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

$$\left. + \left[m_0(\chi r_1 - 1) - m_1(ikr_1 - 1)\right]\xi \right\}, \tag{17}$$

where

$$\xi = \left\{ m_0 - m_1 + \chi m_0 r_0 + ikm_1 r_0 - e^{-2ikr_0} \times \right.$$

$$\left. \times \left[m_0(\chi r_0 + 1) - m_1(ikr_0 + 1)\right] \right\} /$$

$$/ \left\{ m_0 - m_1 - \chi m_0 r_0 + ikm_1 r_0 + e^{-2ikr_0} \times \right.$$

$$\left. \times \left[m_0(\chi r_0 - 1) + m_1(ikr_0 + 1)\right] \right\}. \tag{18}$$

It will be used to determine the energy spectrum E_{n0} and the decay parameters Γ_{n0} as the real and imaginary parts, respectively, of the S-matrix poles.

It is the poles of the S_0-matrix (17) and the radial wave functions $R_{n0}(r)$ (14) that comprise the energy spectrum and the wave functions of electron in the closed double-well system in the limiting case $\Delta_2 \to \infty$, which will be demonstrated in detail in the next section.

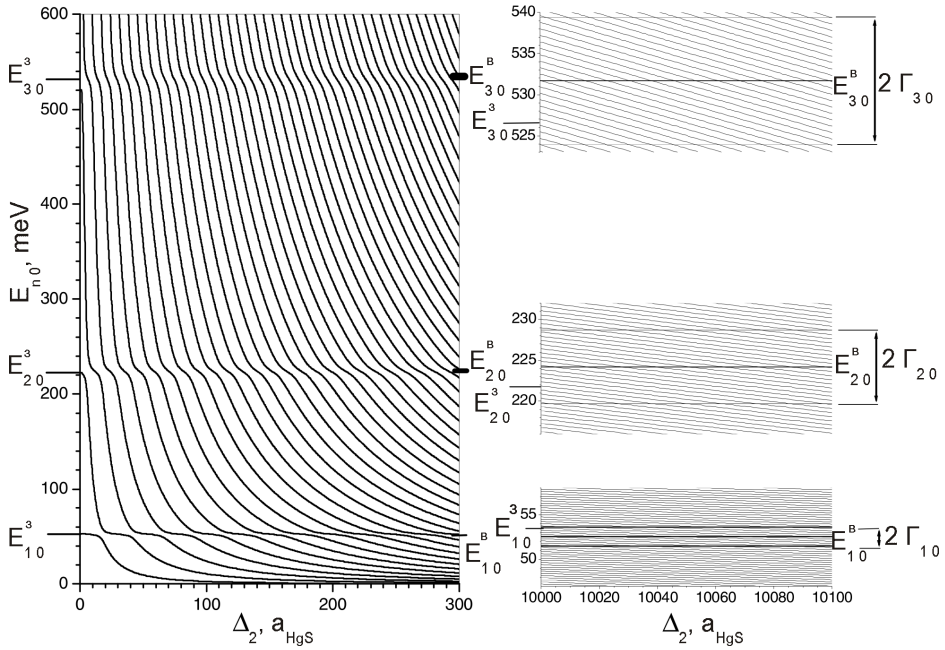

Fig. 2. Dependence of the electron spectrum on the thickness Δ_2 of the external SQD well

3. Properties of the Electron Spectrum in a Closed Double-well SQD. The physical origins of the quasistationary states in an open SQD

The calculations of the electron spectrum were carried out, according to the expounded theory, for a closed double-well SQD (HgS/CdS/HgS/CdS) with the following parameters which are in good agreement with the rectangular potential model (a small difference between the lattice constants of contacting layers): $m_{\rm HgS} = 0.036$, $m_{\rm CdS} = 0.2$, $U = 1350$ meV, $a_{\rm HgS} = 5.851$ Å, and $a_{\rm CdS} = 5.818$ Å.

Let us analyze now the evolution of the electron spectrum in the symmetric states with $\ell = 0$ in relation to the variation of the external well width Δ_2, provided that the SQD radius $r_0 = 20a_{\rm HgS}$ and the thickness of the internal barrier $\Delta_1 = a_{\rm CdS}$ remain constant. The thickness of the external barrier-medium is assumed infinite.

The dependence of the spectrum E_{n0} on the thickness of the external well Δ_2 is shown in Fig. 2. From the figure, one can see that the spectrum obtained at $\Delta_2 = 0$ coincides with the spectrum in a closed single-well SQD, as it has to be: $E^{\rm cl}_{10} = 53.38$ meV, $E^{\rm cl}_{20} = 223.99$ meV, and $E^{\rm cl}_{30} = 526.85$ meV. Figure 2 also illustrates that the energies of all the three levels gradually decrease as the value of Δ_2 grows, until they approach, from below, the region of the first "bottle-neck", which is formed owing to the first levels created by the internal and external wells coming closer. We recall that the mechanisms of the anti-crossing ("bottle neck") emergence were discussed a lot of times [1, 5]. They are associated with the repulsion between the levels of both potential wells owing to their interaction which appears because the height of the potential barrier is finite.

We are interested in the process of formation of quasistationary states. The latter, as follows from the calculations of the S_0-matrix (and can be seen from Fig. 2), possess the following energy characteristics: the resonance energies $E^{\rm op}_{10} = 52.55$ meV, $E^{\rm op}_{20} = 224.18$ meV, and $E^{\rm op}_{30} = 531.67$ meV; and the halfwidths $\Gamma_{10} = 1.065$ meV, $\Gamma_{20} = 4.49$ meV, and $\Gamma_{30} = 7.722$ meV.

Now, Fig. 2 makes evident that all the anti-crossings are located in the vicinities of the relevant resonance energies. Therefore, in order to elucidate the origin and the mechanism of formation of the quasistationary states as $\Delta_2 \to \infty$, we must study the anti-crossing properties in detail. Figure 2 shows that they are as follows.

In the energy interval around an arbitrary quasistationary state energy, the "bottle necks" decrease and the lines of both levels that form them gradually change their slopes from vertical to horizontal ones as the value of Δ_2 increases (Fig. 2,*a*). In so doing, the spectrum density grows more quickly than the "bottle

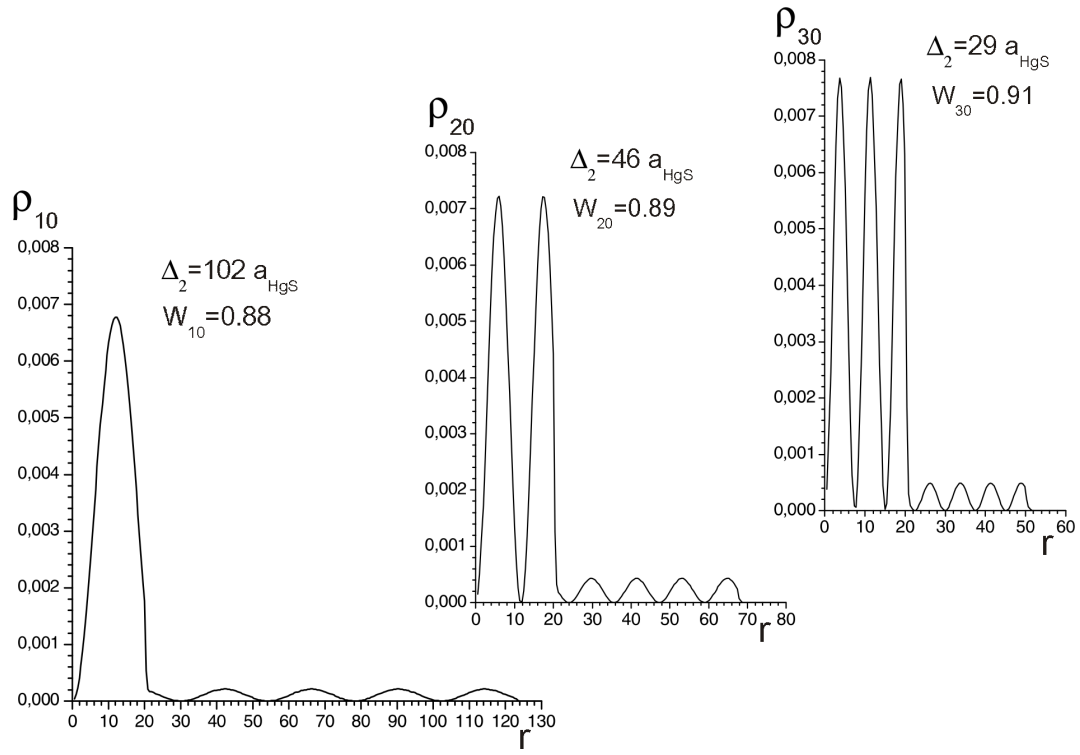

Fig. 3. Probability density distributions $\rho_{n0}(r)$ of the electron in a double-well SQD in various ($n = 1, 2, 3$) states which are transformed to quasistationary ones if $\Delta_2 \to \infty$

necks" become narrower. Therefore, as one can see from Fig. 1,*b*, in the case where the values of Δ_2 are large, more and more energy levels, which correspond to the stationary states in the closed double-well SQD, fall into the energy intervals around the energies $E_{n0}^{\rm op}$ of the open SQD which contain the quasistationary states characterized by the halfwidths Γ_{n0}. Since the distinction between the anti-crossing lines and the other lines of the spectrum becomes eliminated at large Δ_2-values (and even more so at $\Delta_2 \to \infty$), it may appear that the "memory" of the system, which contains the information on the existence of the isolated states, the energies of which, at small Δ_2-values, corresponded to linear sections in the dependences $E_{n0}(\Delta_2)$ and which were coupled to such stationary SQD states, in which the electron is mainly localized in the internal well, also becomes erased. Certainly, such a "memory" does exist in the system, but the complete body of information is contained not so much in the energy spectrum as in the wave functions of the corresponding states. Nevertheless, in order to elucidate the origin of why the quasistationary states with the halfwidths Γ_{n0} and the corresponding lifetimes $\tau_{n0} = \hbar/\Gamma_{n0}$ do arise in an open system, it will be sufficient to analyze the density of the electron probability distribution in the nanosystem $\rho_{n0}(r) = r^2|R_{n0}(r)|^2$ rather than the wave functions themselves.

The examples of such dependences $\rho_{n0}(r)$ in the states with the energies close to the energies of stationary states in a closed SQD with two wells are depicted in Fig. 3. The results obtained testify that if the dimensions of the internal well ($r_0 = 20a_{\rm HgS}$) and the barrier ($\Delta_1 = a_{\rm CdS}$) are taken fixed and the size of the external well is selected according to the condition that the dependences $\rho_{n0}(r)$ should possess the same numbers of maxima within its limits (here, this number equals 4), the electron probability distribution will have the same number of maxima (1, 2, or 3) within the first well as that for the corresponding simple closed SQD with the principal quantum number $n = 1, 2, 3$ has. The probabilities for the electron to be located in the internal well or in the barrier are close to each other in this case ($W_{10} = 0.88$, $W_{20} = 0.89$, and $W_{30} = 0.91$).

The evolution of the probabilities $W_{n0} = \int\limits_0^{r_1+\Delta_1} \rho_{n0}(r)\, dr$ for the electron to be located either in the internal well or in the barrier with the variation of

the external well thickness is shown in Fig. 4. This figure illustrates the redistribution process of the probability for the electron to occupy the states with various energies in the closed double-well SQD. Simultaneously, it reveals obviously the gradual emergence of discrete quasistationary bands, which accompanies the growth of Δ_2, and their transformation into continuous quasistationary bands which are peaked at the resonance energies E^v_{n0} and have the halfwidths Γ_{n0} (the lifetime $\tau_{n0} = \hbar/\Gamma_{n0}$).

Let us analyze the evolution of the probabilities W_{n0} for the electron to occupy various states in two internal SQD layers as the parameter Δ_2 changes. But first let us introduce the concept of the quasistationary state bandwidth $2\tilde{\Gamma}_{n0}$. We define it as the energy interval, which is located about the resonance energy $\tilde{E}_{n0}$ and whose edge values $\tilde{E}_{n0} \pm \tilde{\Gamma}_{n0}$ correspond to the states, in which the probability W_{n0} for the electron to be located in two internal SQD layers is half as much as the probability $\tilde{W}_{n0}$ for the electron to occupy the state with the resonance energy $\tilde{E}_{n0}$. As is seen from Fig. 4,*a*, if the external well is narrow enough ($\Delta_2 = 200a_{\rm HgS}$), the probabilities $\tilde{W}_{10}$ and $\tilde{W}_{20}$ are more than twice as large as the corresponding probabilities W_{n0} for those levels which are located aside. The probability $\tilde{W}_{30}$ exceeds the probability W_{n0} for the neighbor, towards the higher energies, state by a factor of more than two, and that for the neighbor, towards the lower energies, state by a factor of less than two. This circumstance, i.e. the large probability values for two neighbor states, is caused by the fact that just these states form the anti-crossing at $\Delta_2 = 200a_{\rm HgS}$. Therefore, no sufficient conditions come true yet at $\Delta_2 = 200a_{\rm HgS}$ for the quasistationary band to appear.

From Fig. 4,*b*, one can see that, provided the external well is rather thick ($\Delta_2 = 1000a_{\rm HgS}$), there are no components contributing to the discrete band around the lowest quasistationary state $\tilde{E}_{10}$, but near the second, $\tilde{E}_{20}$, and third, $\tilde{E}_{30}$, resonance quasistationary states, there are already states which satisfy the condition for the halfwidths $\tilde{\Gamma}_{20}$ and $\tilde{\Gamma}_{30}$ of the corresponding bands to emerge. At the thickness $\Delta_2 = 10000a_{\rm HgS}$ (Fig. 4,*c*), all the three quasistationary discrete bands have their halfwidths. While comparing Figs. 4,*c* and *d*, one can see that the positions of the resonance energy levels in the closed double-well (Fig. 4,*c*) and open single-well (Fig. 4,*d*) SQDs, as well as the widths of the discrete bands, are practically identical, although their normalizations are different, of course.

Figure 4 illustrates well the process of formation of the quasistationary state bands with their key

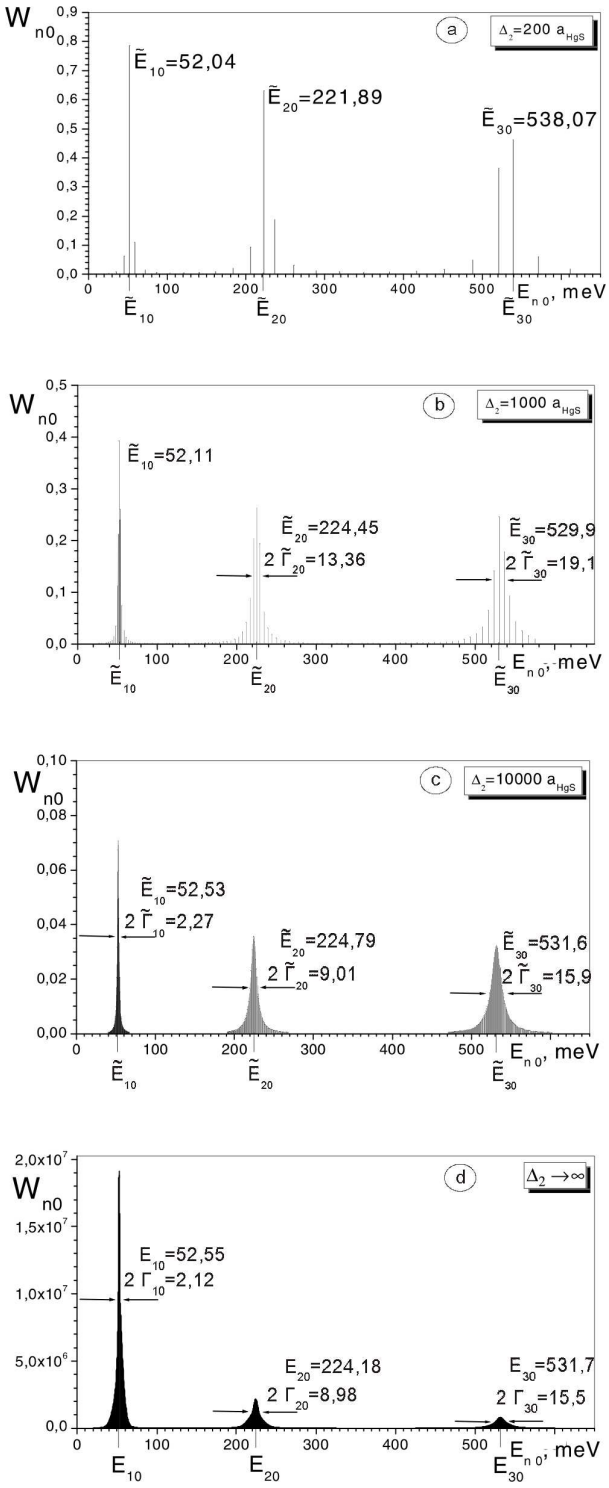

Fig. 4. Evolution of the probabilities $\tilde{W}_{n0}$ for the electron to be located in two internal layers of a closed SQD and to possess the energy in the vicinity of the resonance ones (*a*–*c*), and the energy dependence of the probabilities W_{n0} in a simple open SQD (*d*)

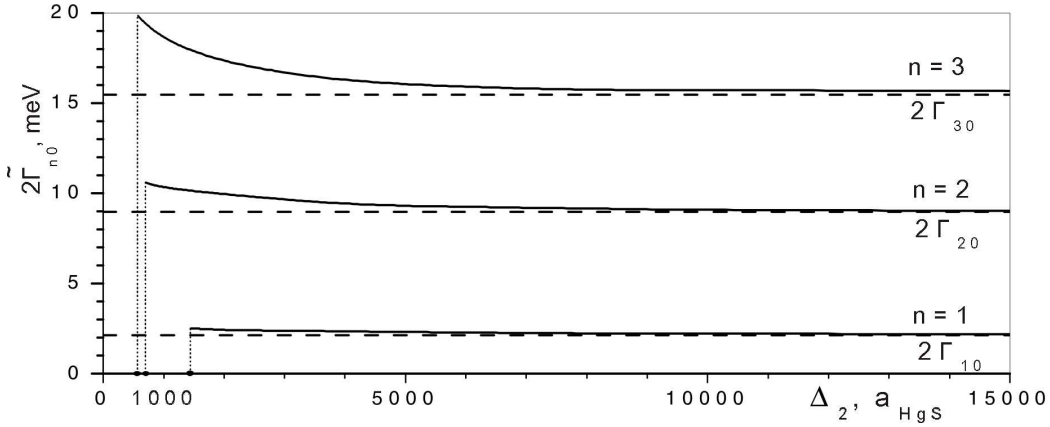

Fig. 5. Dependences of the discrete peak width $2\tilde{\Gamma}$ of the quasistationary states on the thickness Δ_2 of the external well

characteristics — the resonance energies $E_{n0}^{\rm op}$ and the halfwidths Γ_{n0} — when the dimensions of the external well of a closed SQD increase. From Fig. 4, one can see how the probability for the electron to be located in both internal SQD layers becomes redistributed between various states as the quantity Δ_2 grows. At small Δ_2-values (Fig. 4,*a*), the probabilities are large for the resonance states and relatively small for the others. As Δ_2 increases (Fig. 4,*b*), the probabilities decrease in the resonance states but relatively increase in the neighbor ones. Since the growth of Δ_2 stimulates the narrower intervals between the energy levels, very large values of Δ_2 (Fig. 4,*c*) bring about the appearance of the Lorentzian-like peaks with the halfwidths $\tilde{\Gamma}_{n0}$ which are located around the resonance energies and, at $\Delta_2 \to \infty$, transform into the quasistationary bands with the halfwidths Γ_{n0} (Fig. 4,*d*).

The emergence of the halfwidths $\tilde{\Gamma}_{n0}$ of the discrete peaks of quasistationary states in a closed double-well SQD, their dependence on Δ_2, and their convergence, as $\Delta_2 \to \infty$, to the halfwidths Γ_{n0} of continuous bands of a simple open SQD (the amplitudes of Γ_{n0} are determined as the imaginary parts of the poles of the corresponding S-matrix) are illustrated well by Fig. 5. From this figure, it is evident that the formation of the discrete bands of quasistationary states proceeds from larger to smaller halfwidths as Δ_2 increases.

Thus, we are able to assume that the energy spectrum and the wave functions of a closed double-well SQD can always approximate those of a simple open SQD with a sufficient accuracy. This circumstance allows one to develop, on this basis, both the theory of excitons and the theory of phonon interaction for simple open systems.

At last, we note that, since the halfwidths Γ_{n0} of the quasistationary energy bands are coupled to the corresponding lifetimes $\tau_{n0} = \hbar/\Gamma_{n0}$, the results obtained enable the lifetime τ_{n0} to be interpreted as the time interval, during which the probability distribution for the quasiparticle to be located in the quantum dot of the open system is transformed into a peak with the halfwidth Γ_{n0} around the resonance energy E_{n0}. Since these states belong to the whole system, this means that, within this time interval, the quasiparticle formed in the SQD nucleus, where it was in a certain resonance state, penetrates through the potential barrier and moves in the free space of the open system [10].

Now, it becomes also clear why, in contrast to the dispersion equation which defines the energy spectrum of closed systems only, the S-matrix gives both the spectrum and the halfwidths of the quasistationary states. It is so, because, as one can see from the analysis presented above, the S-matrix can be expressed unambiguously in terms of the wave functions of the open system. Therefore, it contains the information concerning not only the energy of resonance states but, owing to its dependence on the probability density distribution, the halfwidth of the quasistationary state band in the open system. Whereas, such information in the closed system can be obtained only in terms of the energy distribution of the probability for the electron to be located in either of the internal SQD layers, which is possible only provided that the wave functions are known, as has been demonstrated in this work.

4. Conclusions

1. The stationary electron spectrum in a closed double-well nanosystem gradually transforms into a

quasistationary one if the thickness of the external layer-sphere tends to infinity.

2. The halfwidth of the discrete band of quasistationary electron states in a closed double-well system tends asymptotically to that of the continuous quasistationary band in the simple open system if the thickness of the external layer-sphere tends to infinity.

3. The electron wave functions in a double-well nanosystem with a large enough but finite thickness of the layer-well are included into the complete set of wave functions and can serve, with the necessary accuracy, as the basis for changing over to the particle number representation over the electron variables in open systems, if the electron interaction with phonon and photon fields are taken into account. Thus, we obtain an opportunity to construct the theory of electron-phonon or electron-photon interaction in open nanosystems.

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ЕВОЛЮЦІЯ ЕЛЕКТРОННОГО СПЕКТРА СФЕРИЧНО-СИМЕТРИЧНИХ СТАНІВ ПРИ ПЕРЕХОДІ ВІД ЗАКРИТОЇ ДВОЯМНОЇ ДО ПРОСТОЇ ВІДКРИТОЇ СФЕРИЧНОЇ КВАНТОВОЇ ТОЧКИ

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Р е з ю м е

Побудовано теорію і досліджено еволюцію спектра сферично-симетричних станів електрона двоямної сферичної квантової точки (СКТ) при зміні розмірів зовнішньої ями Δ_2 від нуля до нескінченності. Показано що при $\Delta_2 \to 0$ спектр збігається зі стаціонарним спектром одноямної закритої СКТ, а при $\Delta_2 \to \infty$ він переходить у квазістаціонарний спектр простої відкритої СКТ із затуханням квантових станів. Вперше виявлено механізм виникнення затухання квазістаціонарних станів у відкритій СКТ і встановлено, що причиною, яка зумовлює існування часу життя електрона у відкритій СКТ протягом певного часу, є перерозподіл ймовірностей перебування квазічастинки на всіх рівнях енергій в околі резонансних енергій. "Пам'ять" двоямної закритої наносистеми про положення резонансних рівнів (як і простої відкритої) у шкалі енергій зумовлена існуванням ефекту антикросингу ("пляшкового горла"). Показано, як на основі викладеної теорії може бути розвинутий математичний апарат теорії екситонів та електрон-фононної взаємодії у відкритих СКТ.