

QUASISTATIONARY AND QUASIFREE ELECTRON STATES IN OPENED QUANTUM DOTS*

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The quasistationary electron spectrum in opened spherical quantum dot is obtained within the S -matrix method and analyzed for the nanosystem HgS\CdS/HgS. It is shown that the quasiparticle spectrum becomes quasistationary when the thickness of the potential barrier CdS is more than one monoshell. For the quasibound states, the resonance energies almost do not depend on the thickness of the barrier and their life times are exponentially increasing. Analysis of the probability of electron location in quantum dot as function of energy allows to explain the paradox: why at the decreasing of the thickness, the life times defined from the S -matrix are only decreasing, while at the absence of the barrier the spectrum is stationary for all states. It is shown the existence of critical barrier thickness under which the concept of quasistationary band semi width vanishes and the states become quasifree.

Key words: quantum dot, quasistationary state, energy spectrum.

1. INTRODUCTION

The theory of electron, exciton, phonon spectra and interaction of these quasiparticles in closed nanosystems (quantum dots, wires and wells), is already developed rather well [1] and gives good correlation to experimental results. As for the theory of quasiparticles in opened nanosystems, it is only at the start point of development [2] and the theory of interaction between electrons and holes and with phonons is absent at all.

The actuality of the opened nanosystems research is caused by the presence of the additional channel of quasiparticle relaxation due to the ability of their transition through the potential barrier. This phenomenon allows to produce the super fast sensors and other nanoelectronic devices for the further utilization. Besides, while investigating the physical phenomena in opened nanosystems, there arise general theoretical questions, which were not studied in classic theory

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of quantum mechanic tunnel effect of electrons [3], or not assumed for the systems where quasiparticle effective mass was independent of spatial variables.

General theory of electron spectrum and life times in complicated opened quantum dots have been developed in ref. [4] in the framework of the S-matrix method ref. [5]. There were calculated and analyzed the resonance energies and life times of electron and hole in the opened spherical QD. The closed spherical quantum dots are already grown experimentally ref. [6]. The investigations were performed for such barrier thicknesses, where the classic quasistationary condition ($E_{n\ell} \gg \Gamma_{n\ell}$) was satisfied. Herein, it was shown that at the increasing of barrier thickness the resonance energies ($E_{n\ell}$) were almost not changing but the semi widths ($\Gamma_{n\ell}$) were increasing too. But it was not investigated the paradox: why at the decreasing of barrier thickness (Δ), the semi width ($\Gamma_{n\ell}$) increases and, consequently, the life time ($\tau_{n\ell} = \hbar/\Gamma_{n\ell}$) decreases, while at $\Delta \rightarrow 0$ (potential barrier is absent) the spectrum is to be stationary and the life times of all states are to be infinitely big?

The solution of this paradox is proposed in this paper. Here it is shown that for the very small magnitudes of barrier thicknesses the quasistationary condition is broken, *i.e.* the states are already not quasistationary. Since, the S-matrix already does not define the resonance energies and band semi widths and it is necessary to analyze the probability of electron location in QD as function of energy. Analysis shows that there is the critical value of thickness (Δ_k) delimiting quasibound ($\Delta > \Delta_k$) and quasifree ($\Delta < \Delta_k$) states. At $\Delta < \Delta_k$, the concept of quasistationary band semi width vanishes, that explains the above mentioned paradox. The energies and semi widths of the states, which are already not quasistationary and are not defined by the S-matrix poles, are now defined by maxima and semi widths of density of probability of electron location in QD as function of energy. Thus, in this paper, the quasistationary and quasifree electron states in opened nanosystem HgS/CdS/HgS are studied.

2. HAMILTONIAN, S-MATRIX, ELECTRON SPECTRUM AND WAVE FUNCTIONS IN OPENED SPHERICAL QUANTUM DOT

The electron spectrum, life times and wave functions in opened spherical quantum dot (OSQD) is under study. Radius of inner well (r_0), barrier thickness (Δ), height of potential barrier (U) are assumed as fixed (Fig. 1).

According to the general theory [5] and taking into account the dependence of quasiparticle effective mass on radius one has to solve the Schrödinger equation

$$H \Psi(\vec{r}) = E \Psi(\vec{r}) \quad (1)$$

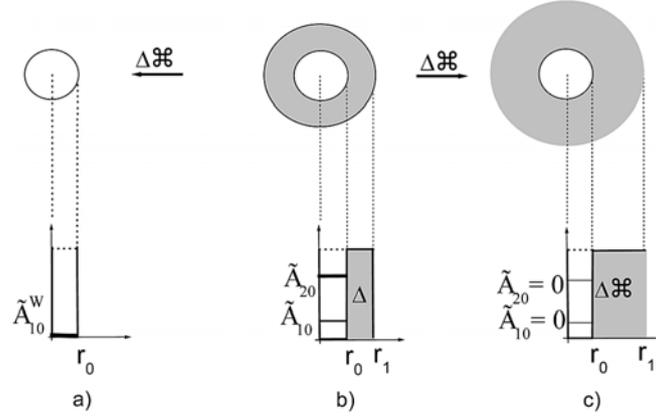


Fig. 1 – Geometrical schemes of nanosystems, potential energies, and several energy levels.

with the Hamiltonian

$$H = -\frac{\hbar^2}{2} \vec{\nabla} \frac{1}{m(r)} \vec{\nabla} + U(r) \quad (2)$$

where in the spherical coordinate system with the beginning in the center of OSQD, the quasiparticle has the fixed effective mass and potential energy

$$m(r) = \begin{cases} m_0, & r < r_0, \quad r_1 < r < \infty \\ m_1, & r_0 \leq r \leq r_1 = r_0 + \Delta, \end{cases} \quad (3)$$

$$U(r) = \begin{cases} U_{0,2} = 0, & r < r_0, \quad r_1 < r < \infty \\ U_1, & r_0 \leq r \leq r_1. \end{cases} \quad (4)$$

Accounting the spherical symmetry, the solution of eq. (1) is to be written as

$$\Psi_{\ell m}(\vec{r}) = R_{\ell}(r) Y_{\ell m}(\theta, \varphi) \quad \ell = 0, 1, 2, \dots \quad m = 0, \pm 1, \pm 2, \dots \quad (5)$$

where $Y_{\ell m}(\theta, \varphi)$ – the spherical function. For the radial wave functions ($R_{\ell}(r)$) it is obtained the system of equations

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

where

$$K_i^2 = \frac{2m_i}{\hbar} (E - U_i) = \begin{cases} k_i^2, & i = 0, 2 \\ -\chi_i^2, & i = 1. \end{cases} \quad (7)$$

Within the S-matrix method [5], the solutions of eqs. (6) are to be taken as

$$R_{K\ell}(r) = \begin{cases} R_\ell^{(0)}(kr) = kA_\ell^{(0)} [h_\ell^-(kr) + h_\ell^+(kr)] \\ R_\ell^{(1)}(i\chi r) = i\chi A_\ell^{(1)} [h_\ell^-(i\chi r) - S_\ell^{(1)} h_\ell^+(i\chi r)] \\ R_\ell^{(2)}(kr) = kA_\ell^{(2)} [h_\ell^-(kr) - S_\ell(k) h_\ell^+(kr)] \end{cases} \quad (8)$$

where coefficient $A_\ell^{(2)} = 1/\sqrt{2\pi}$ is defined from the normalizing condition

$$\int_0^\infty R_{k\ell}^*(r) R_{k'\ell}(r) r^2 dr = \delta(k - k'), \quad (9)$$

which accounts the unequal to zero probability of quasiparticle transition from the internal space of OSQD to the infinity. The fitting conditions of the wave functions and currents of probability densities continuity

$$\begin{cases} R_\ell^{(0)}(kr_0) = R_\ell^{(1)}(i\chi r_0), \\ R_\ell^{(1)}(i\chi r_1) = R_\ell^{(2)}(kr_2), \\ \left. \frac{1}{m_0} \frac{dR_\ell^{(0)}(kr)}{dr} \right|_{r=r_0} = \left. \frac{1}{m_1} \frac{dR_\ell^{(1)}(i\chi r)}{dr} \right|_{r=r_0}, \\ \left. \frac{1}{m_1} \frac{dR_\ell^{(1)}(i\chi r)}{dr} \right|_{r=r_1} = \left. \frac{1}{m_0} \frac{dR_\ell^{(2)}(kr)}{dr} \right|_{r=r_1} \end{cases}, \quad (10)$$

determine all unknown coefficients (ref. [7]) and analytical form of S_ℓ -matrix

$$S_\ell = \frac{\left(\alpha_\ell \frac{d}{dr_1} + \beta_\ell - \gamma_\ell \frac{d}{dr_1} - \lambda_\ell \right) h_\ell^-(kr_1)}{\left(\alpha_\ell \frac{d}{dr_1} - \beta_\ell + \gamma_\ell \frac{d}{dr_1} + \lambda_\ell \right) h_\ell^+(kr_1)}. \quad (11)$$

Finally, the radial wave functions ($R_{K\ell}(r)$) are fixed by formula (8), the resonance energies and semi widths of electron quasistationary states are defined by the real and imaginary part of S_ℓ -matrix (11) poles. The life time in the respective quasistationary state according to ref. [5] are given by the relationship

$$\tau_{n\ell} = \hbar / \Gamma_{n\ell}. \quad (12)$$

Finally, it is to be noted that at the condition $m_0 = m_1 = m$, $\chi \Delta \gg 1$ for $\ell = 0$ from the S -matrix there are obtained the following expressions for the resonance energies (\bar{E}_{n0}) and quasistationary states band semi widths ($\bar{\Gamma}_{n0}$)

$$\bar{E}_{n0} = \frac{\hbar^2 k_n^2}{2m}; \quad \bar{\Gamma}_{n0} = 16 \bar{E}_{n0} e^{-2\chi_n \Delta} \frac{\chi_n^3 k_n}{(\chi_n^2 + k_n^2)^2 (1 + \chi_n r_0)} \quad (13)$$

where k_n and χ_n are determined by the equation

$$k_n \operatorname{ctg} k_n r_0 + \chi_n = 0. \quad (14)$$

Formulas (13), (14) are in analogy to the results of ref. [4] obtained for the energy spectrum of quasiparticle with effective mass m in OSQD.

3. EVOLUTION OF ELECTRON SPECTRAL PARAMETERS IN OSQD AS FUNCTIONS OF WELL RADIUS AND BARRIER THICKNESS

Using the obtained information for the electron S_{nl} -matrix and wave functions in HgS/CdS/HgS OSQD we have performed the computer calculations and detail analysis of spectral parameters evolution not only for the quasistationary (quasibound) but also for the quasifree states. Physical parameters were taken the following: $m_{\text{HgS}} = 0.036$; $m_{\text{CdS}} = 0.2$; $U_e = 1350$ meV.

In Fig. 2 the dependences of energy (E_{nl}) and semi width (Γ_{nl}) on the thickness of the barrier (Δ) at different QD radii (r_0) are shown. Fig. 2 proves that the increasing of r_0 causes the shift not only of resonance energies but also of all bands of quasistationary states into the region of smaller energies. At the fixed Δ their semi widths become smaller due to the increasing of barrier height above the respective level. At any fixed r_0 the increasing of Δ brings to the thinning of bands and at $\Delta \rightarrow \infty$ they are transformed into the energy levels of stationary spectrum in closed spherical QD (Fig. 1c).

From Fig. 2 it is obvious that the quasistationary condition of electron states is satisfied rather well for the thicknesses of one lattice constant of CdS crystal and more. When $\Delta \geq a_{\text{CdS}}$, the resonance energies almost do not depend on Δ and life times are exponential functions with linear power over Δ (as in approximated formula (13)).

Comparison of exact resonance energies E_{nl} , band semi widths Γ_{nl} , averaged \bar{E}_{nl} , $\bar{\Gamma}_{nl}$ and approximated E_{nl}^* , Γ_{nl}^* (calculated within averaged effective mass $\bar{m} = \frac{1}{2}(m_{\text{HgS}} + m_{\text{CdS}})$ and approximated $m^* = m_{\text{HgS}}$) for the symmetric states ($\ell = 0$) shows (Fig. 2) that, qualitatively, all dependences on Δ and r_0 are similar while quantitatively $\bar{E}_{n0} < E_{n0} < E_{n0}^*$, $\bar{\Gamma}_{n0} < \Gamma_{n0} < \Gamma_{n0}^*$. The difference between the corresponding magnitudes is caused not so by approximated formula (13) but by the manner of averaging, where \bar{m} is much bigger than some

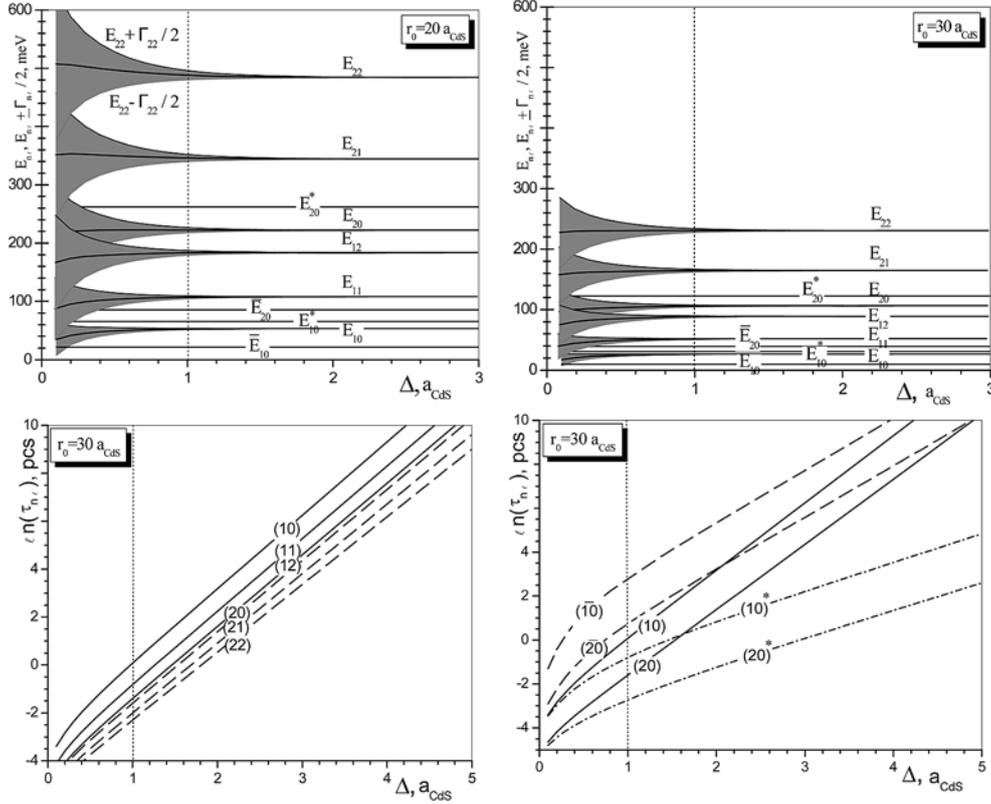


Fig. 2 – Dependences of resonance energies E_{n0} , \bar{E}_{n0} , E_{n0}^* and $\ell n\tau_{n0}$, $\ell n\bar{\tau}_{n\ell}$, $\ell n\tau_{n0}^*$ on barrier thickness Δ .

effective m^* . The condition $m^* = m_{\text{HgS}}$ defines the electron spectral characteristics $(E_{n\ell}^*, \Gamma_{n\ell}^*)$ more exact than \bar{m} . It is clear, because the probability of quasiparticle location in HgS space is much bigger than probability of its location in CdS.

Although the effective mass approximation at $\Delta \leq a_{\text{CdS}}$ practically does not give the numeric results correlating to the experimental data (ref. [5]) obtained for HgS\CdS\HgS nanosystem, nevertheless the analytical theory is formally true. Thus, it has to explain (at least qualitatively) why, at the decreasing of barrier thickness, the semi widths of all bands obtained from $S_{n\ell}$ -matrix are only increasing, while from the physical considerations it is clear that at $\Delta = 0$ (barrier is absent) the electron spectrum is to be continuous and stationary, the life times in all states are to be infinite and, since, $\Gamma_{n\ell} = 0$.

In order to explain this paradox, it is performed the calculation of probability of electron location in QD space over the radial functions of opened system in quasistationary states $|n\ell\rangle$

$$W_{n\ell}(E) = \int_0^{r_0+\Delta} |R_{n\ell}(E)|^2 r^2 dr. \quad (15)$$

Functions $W_{n0}(E)$ at fixed $r_0 = 30a_{\text{HgS}}$ for different barrier thicknesses (Δ) are shown in Fig. 3.

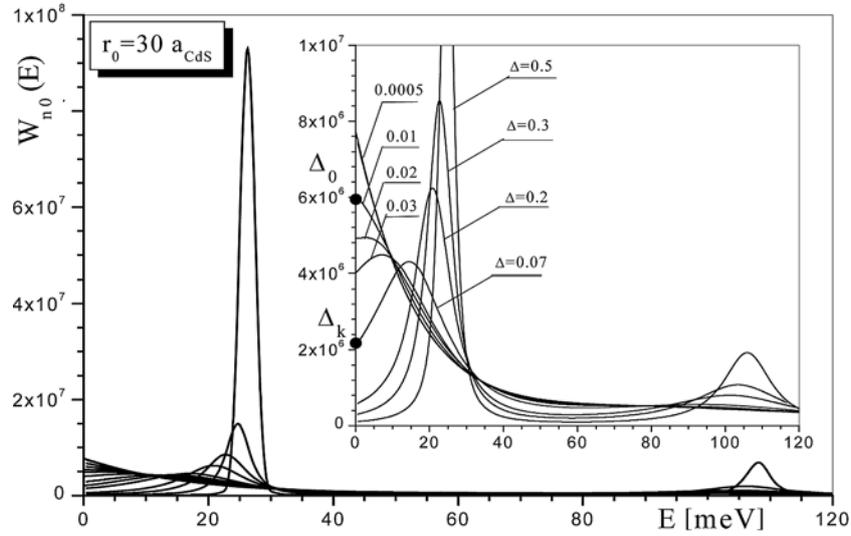


Fig. 3 – Dependence of W_{n0} on E at $r_0 = 30a_{\text{CdS}}$ for different barrier thicknesses (Δ).

From the figure it is clear that at $\Delta \geq a_{\text{CdS}}$, function $W_{10}(E)$ is like Lorentz curve with cut off low energy wing (at $E = 0$). Maxima of curves $W_{n0}(E)$ correspond to the resonance energies ($E_{n0}^w = E_{n0}$), and their semi widths ($\Gamma_{n0}^w = \Gamma_{n0}$) – to the semi width defined from the $S_{n\ell}$ -matrix poles.

From Fig. 3 one can see that at the decreasing of Δ , the low energy wing $W_{10}(E)$ is cut off more and more and at the thicknesses smaller than critical ($\Delta = \Delta_k$) it is fixed by the condition

$$W_{10}(E = 0, \Delta_k) = \frac{1}{2} W_{10}(E_{10}, \Delta_k), \quad (16)$$

the concept of Lorentz curve semi width (Γ_{n0}) vanishes. Thus, the critical thickness (Δ_k) can be assumed as minimal one at which the lowest quasistationary (quasibound) state is created. The condition (16) is more accurate than the rough condition $\Gamma_{10} \ll E_{10}$ for the quasistationary states.

From Fig. 3 inset it is quite clear that when Δ varies from Δ_k to Δ_0 , fixed by the condition

$$W_{10}(E = 0, \Delta_0) = W_{10}(E_{10}, \Delta_0), \quad (17)$$

the low energy wing of Lorentz curve is totally cut off till the maximum of W_{10} . In this region it is convenient to introduce the concept of band semi width ($\bar{\Gamma}_{n\ell}$) fixed by the condition

$$W_{10}(E = 0, \Delta) = W_{10}(2E_{10}, \Delta) \quad (18)$$

at which there arises the concept of quasi resonance energy level ($\bar{E}_{n\ell}$) corresponding to the maximum of $W_{10}(E, \Delta)$ function. When Δ varies from Δ_k to Δ_0 , the magnitudes of $\bar{\Gamma}_{n\ell}$ and $\bar{E}_{n\ell}$ are decreasing and maxima of probability of electron location in QD is of the order or smaller than maxima of probability of its location outside the QD. Therefore, it is convenient to call such states the quasifree resonance. The states arising at $\Delta < \Delta_0$ are not characterized by semi width and are not resonance.

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