QUASISTATIONARY ELECTRON STATES RENORMALIZED DUE TO THE INTERACTION WITH PHONONS IN OPEN SPHERICAL QUANTUM DOT

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The electron quasistationary spectrum in open spherical quantum dot is obtained within the effective mass approximation and rectangular potentials using the S-matrix method. The stationary electron spectrum is obtained for the two-well closed spherical quantum dot. It is calculated such size of the outer well, when the resonance energies coincide almost exactly with the respective energies for the open system. The established whole set of wave functions for the two-well closed quantum dot is used for the calculation of electron spectrum renormalized due to the interaction with phonons in open spherical quantum dot. The numeric calculations of the renormalized ground quasistationary state is performed for HgS/CdS/HgS/CdS nanosystem at $T = 0^\circ K$. The obtained result for the renormalized resonance energy is physically correct and satisfies limit cases.

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

INTRODUCTION

The theory of electron and hole spectra and wave functions in single and multi-shell spherical quantum dots (SQD’s) is developed for the closed [1, 2] and for the open nanoheterosystems [2, 3]. As for the exciton theory or interaction of excitons, electrons and holes with phonons in closed SQD, it is at the start point of development and is established at the base of different models for the phonon subsystem. The most spread is the dielectric continuum model for the closed nanosystems [3, 6].

The theory of electron and hole spectra in open SQD have been developed in [4, 5] within the scattering S-matrix method. It describes well the properties of electron and hole quasistationary states and life times. But it is impossible to perform the transition to the representation of second quantization over the electron (hole) variables because the wave functions are normalized at $\delta$-function. Therefore, it is also impossible to develope the theory of electron and hole spectra


renormalized due to their interaction with phonons using the traditional methods of quantum field theory.

The exit from this complicated situation is proposed in the following way: instead of the open one-well and one-barrier SQD it is observed the closed two-well SQD with very big thickness of the outer well. This thickness can be easily taken such that the electron or hole energies would almost exactly coincide to the respective resonance energies in open SQD. The obtained set of wave functions for the quasiparticle in two-well closed SQD is used for the transition to the representation of second quantization over all variables for the electron-phonon Hamiltonian. The problem of electron spectrum renormalized due to the interaction with phonons in open SQD is solved using the obtained electron-phonon Hamiltonian and the Green functions method [2].

1. HAMILTONIAN, S-MATRIX, ELECTRON SPECTRUM AND WAVE FUNCTIONS IN OPEN SPHERICAL QUANTUM DOT

The electron spectrum and wave functions in open spherical quantum dot (OSQD) are under study. Radius of inner well \( r_0 \), barrier thickness \( \Delta_1 \), height of potential barrier \( U_1 \) are assumed as fixed (Fig. 1).

According to the general theory [7] and taking into account the dependence of quasiparticle effective mass on radius one has to solve the Schrödinger equation...
with the Hamiltonian
\[ H \Psi(\vec{r}) = E \Psi(\vec{r}) \]  
\[ H = -\frac{\hbar^2}{2m(r)} \nabla^2 + U(r) \]  
where in the spherical coordinate system with the beginning in the center of OSQD, the quasiparticle has the fixed effective mass and potential energy
\[ m(r) = \begin{cases} m_0, & r < r_0, \quad r_0 < r < \infty \\ m_1, & r_0 \leq r \leq r_i = r_0 + \Delta r \end{cases} \]  

Accounting the spherical symmetry, the solution of eq.(1) is to be written as
\[ \Psi_{\ell m}(\vec{r}) = R_\ell(r)Y_{\ell m}(\theta, \varphi) \quad \ell = 0, 1, 2, \ldots \quad m = 0, \pm 1, \pm 2, \ldots \]  
where \( Y_{\ell m}(\theta, \varphi) \) – the spherical function. For the radial wave functions \( R_\ell(r) \) it is obtained the system of equations
\[ \left\{ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} + K_i^2 - \frac{\ell(\ell + 1)}{r^2} \right\} R_i(r) = 0 \quad i = 0, 1, 2, 3 \]  
where
\[ K_i^2 = \frac{2m_0}{\hbar^2}(E - U_i) = \begin{cases} k_i^2, & i = 0, 2 \\ \chi_i^2, & i = 1 \end{cases} \]  

Within the S-matrix method [7], the solutions of eqs. (5) are taken as
\[ R_{K, \ell}(r) = R_{\ell, 1}^{(1)}(i \frac{\chi r}{K}) = i \chi A_{\ell}^{(1)} \left[ h_i (i \frac{\chi r}{K}) - S_i^{(1)} h_i^* (i \frac{\chi r}{K}) \right] \]  
\[ R_{\ell, 2}^{(2)}(kr) = k A_{\ell}^{(2)} \left[ h_i (kr) - S_i (k) h_i^* (kr) \right] \]  
where the coefficient \( A_{\ell}^{(2)} = 1/\sqrt{2\pi} \) is defined from the normalizing condition
\[ \int_0^\infty R_{\ell, i}(r) R_{\ell, j}(r) r^2 dr = \delta(k - k') \]  

The fitting conditions of the wave functions and currents of probability densities continuity determine all unknown coefficients [8] and the analytical form of \( S_{\ell} \)-matrix
\[ S_{\ell} = \begin{pmatrix} \alpha_i \frac{d}{dr_i} + \beta_i - \gamma_i \frac{d}{dr_i} & -\lambda_i \frac{d}{dr_i} & \frac{\alpha_i d}{dr_i} + \beta_i - \gamma_i \frac{d}{dr_i} - \lambda_i \frac{d}{dr_i} \\ \frac{\alpha_i d}{dr_i} - \beta_i + \gamma_i \frac{d}{dr_i} + \lambda_i \frac{d}{dr_i} & \frac{\alpha_i d}{dr_i} + \beta_i - \gamma_i \frac{d}{dr_i} - \lambda_i \frac{d}{dr_i} \end{pmatrix} h_i (kr_i) \]  

\[ \alpha_i \frac{d}{dr_i} + \beta_i - \gamma_i \frac{d}{dr_i} - \lambda_i \frac{d}{dr_i} \]
Finally, the radial wave functions \( R_{K}(r) \) are fixed by formula (7), the resonance energies and semi widths of electron quasistationary states are defined by the real and imaginary parts of \( S_{1} \)-matrix poles, eq. (9).

2. ELECTRON-PHONON HAMILTONIAN IN TWO-WELL SPHERICAL CLOSED QUANTUM DOT

The electron energy spectrum and wave functions in two-well closed SQD is obtained in order be further used for the Hamiltonian of electron-phonon interaction in open SQD. According to the developed theory [2], the electron-phonon Hamiltonian is obtained in the following way. Within the approximation of effective mass and rectangular potentials for the electron, the Schrödinger equation is solved exactly. As a result, the whole set of orthonormalized wave functions is

\[ \Psi_{p\ell m}(\vec{r}) = R_{p\ell m}(r) Y_{\ell m}(\theta, \phi), \quad (p = n, k) \] (10)

where

\[ R_{p\ell m}(r) = R_{p\ell m}^{0}(r) + R_{p\ell m}^{1}(r) \]

\[ = \left[ \frac{j_{\ell}(kr)j_{\ell}(kr_{0})}{j_{\ell}(kr_{0})} \right]_{r<r_{0}} + \left[ h_{\ell}^{+}(i\chi_{r}r_{0})/h_{\ell}^{+}(i\chi_{r}r_{0}) \right]_{r>r_{0}} \] (11)

– the radial wave functions of discrete spectrum stationary states, with the energies \( (E_{\ell \ell}) \) defined by the dispersion equations

\[ \frac{\ell}{k_{0}r_{0}} \frac{j_{\ell+1}(kr_{0})}{j_{\ell}(kr_{0})} = i \chi_{r} \frac{m_{0}}{m_{1}} \left[ \frac{\ell}{\ell+1} \frac{h_{\ell+1}^{+}(i\chi_{r}r_{0})}{h_{\ell}^{+}(i\chi_{r}r_{0})} \right], \quad (\ell = 0,1,2,...) \] (12)

where

\[ k_{0} = \hbar^{-1} \sqrt{2m_{0}(U-|E|)}, \quad \chi_{r} = \hbar^{-1} \sqrt{2m_{1} |E|}, \] (13)

\( j_{\ell}, h_{\ell}^{+}, h_{\ell}^{-} \) – Bessel and Hankel spherical functions.

Performing the transition to the representation of occupation numbers over the whole set of wave functions (10) we obtain the Hamiltonian of electron subsystem

\[ H_{e} = \sum_{p\ell m} E_{p\ell m} a_{p\ell m}^{+} a_{p\ell m}. \] (14)

The phonon spectra and polarization of heterosystem potential field are defined in the framework of dielectric continuum model, where it is assumed that the QD (0) and the outer medium (1) are characterized by the fixed magnitudes of
dielectric constants: \( \varepsilon_{00} \), \( \varepsilon_{0\infty} \), \( \varepsilon_{10} \), \( \varepsilon_{1\infty} \) and optical phonon energies: \( \Omega_{L0} \), \( \Omega_{L1} \). In the framework of this model, the Hamiltonian of confined phonons in the representation of occupation numbers has the form

\[
H_L = \sum_{l=0}^{1} \sum_{s_l,\ell,m} \Omega_{L_l} \left( b_{s_l,\ell,m}^+ b_{s_l,\ell,m} + \frac{1}{2} \right).
\] (15)

We must note, that according to the dielectric continuum model, there are also the interface phonons in the system under research but their interaction with electron are not observed in this paper.

The Hamiltonian of electron-confined-phonons interaction in the representation of second quantization over the all variables of the system is found using the polarization potential field and whole set of orthonormalized wave functions of stationary states (10)

\[
H_{v-L} = \sum_{l=0}^{1} \sum_{p_l} \sum_{m_l} \Phi_{p_l,m_l}^{j_{s_l} m_l} (s_l,\ell,m) a_{p_l,m_l}^+ a_{p_l,m_l} \left( b_{s_l,\ell,m}^+ b_{s_l,\ell,-m} + \frac{1}{2} \right)
\] (16)

containing binding functions

\[
\Phi_{p_l,m_l}^{j_{s_l} m_l} (s_l,\ell,m) = \left( Y_{v,L} \right)_{p_l,m_l}^{j_{s_l} m_l} \left( F_{v,L} \right)_{p_l,\ell}^{j_{s_l} m_l}, \ (i=0,1)
\] (17)

where \( \left( Y_{v,L} \right)_{p_l,m_l}^{j_{s_l} m_l} \) and \( \left( F_{v,L} \right)_{p_l,\ell}^{j_{s_l} m_l} \) are produced by spherical and radial functions, respectively

\[
\left( Y_{v,L} \right)_{p_l,m_l}^{j_{s_l} m_l} = \int_0^\infty d\theta d\phi Y_{j_{s_l} m_l}^* (\theta,\phi) Y_{p_l,m_l} (\theta,\phi),
\] (18)

\[
\left( F_{v,L} \right)_{p_l,\ell}^{j_{s_l} m_l} = \frac{4\pi \Omega_{L v} e^2}{\ell_0^2} \left( \frac{1}{\varepsilon_{0\infty}} - \frac{1}{\varepsilon_{00}} \right) \left( k_{n_l} r_0 j_{i-1} \left( k_{n_l} r_0 \right) \right)^{-1} \times
\]

\[
\times \int_0^{\infty} d\rho r^2 j_r (k_{s_l} r) R^{v0}_{p_l,\ell} (r) R^{v0}_{p_l,\ell} (r),
\] (19)

\[
\left( F_{v,L} \right)_{p_l,\ell}^{j_{s_l} m_l} = \lim_{\ell_0 \to \infty} \frac{4\pi \Omega_{L v} e^2}{\ell_0^2} \left( \frac{1}{\varepsilon_{0\infty}} - \frac{1}{\varepsilon_{00}} \right) \left( k_{s_l} r_l \right)^{-1} \times
\]

\[
\times \int_0^{\infty} d\rho R^{v0}_{p_l,\ell} (r) R^{v0}_{p_l,\ell} (r) r^2 \left[ n_l (k_{s_l r_l} j_r (k_{s_l} r) - j_r (k_{s_l} r) n_l (k_{s_l}, r)) \right] dr.
\] (20)

Herein, \( k_{i0} \) and \( k_s \) coefficients are obtained from the equations
where \( s_0 \) and \( s_1 \) denote the nodes of the respective equations.

Finally, the Hamiltonian of electron-confined-phonon system in spherical QD is defined as

\[
H = H_e + H_L + H_{e-L},
\]

making possible the use of Green functions method [2] for the obtaining of electron spectrum renormalized due to interaction with phonons.

The renormalization of ground resonance electron level \( E_{00}^{(0)} \) due to confined phonons of OSQD \( \phi_a \) are found as limit magnitude of \( N \)-th renormalized level \( \lim_{\Delta_z \to \infty} E_{N0}^{(c)}(\Delta_z) \) of the respective closed \( (c) \) nanosystem at physical infinitely big thickness of outer shell-well. As far, as electron spectrum in closed SQD is essentially multi-level one, since in order to calculate its renormalization due to the interaction with phonons, it is convenient to use the Green functions method [9]. According to it, at rather low temperature (\( T \approx 0^\circ K \)) the renormalized electron energy levels for the states \( |\mu\rangle = |n, \ell, m\rangle \) of closed SQD are defined by the poles of electron Green function Fourier image

\[
G_{\mu}^{(c)}(\omega) = \frac{1}{\omega - E_{\mu}^{(c)} - M_{\mu}^{(c)}(\omega)},
\]

where \( E_{\mu}^{(c)} \) – electron energies in the states \( |\mu\rangle = |n, \ell, m\rangle \) (without interaction with phonons). The diagonal mass operator \( M_{\mu}^{(c)} = M_{\mu\mu}^{(c)} \) in the case of weak electron-phonon binding (realized in the system under research due to the small difference \( (\epsilon_{00} - \epsilon_{m}) \)) in one-phonon approximation is written as

\[
M_{\mu\mu}^{(c)}(\omega) = \sum_{l=0}^{\ell} \sum_{l=0}^{\ell} \sum_{m=-\ell}^{\ell} \left| Y_{l m} \right|^2 (2\ell+1) \sum_{n_{00}} \sum_{n_{0\ell}} \sum_{n_{\ell\ell}} \sum_{n{m}} \left( E_{l}^{(d)} \right)_{\mu}^{n_{00} + n_{0\ell} + n_{\ell\ell} + n_{m} - \Omega_{0} - \Omega_{L}}.
\]

In this expression the electron in state \( |n, \ell, m\rangle \) interacts with with four modes \( (i = 0, 1, 2, 3) \) of confined phonons through all electron states in heterosystem.

From the structure of mass operator one can see that electron-phonon interaction takes off the degeneration of electron levels over the magnetic quantum number \( m \) at \( \ell \neq 0 \). The weak electron-phonon binding and, thus, the weak frequency dependence of \( M_{\mu}^{(c)}(\omega) \) brings to the fact that the energy of renormalized level can be written as
\[ \tilde{E}_{q}^{(c)} = E_{q}^{(c)} + \Delta E_{q}^{(c)} + \Delta E_{q}^{(i)} \]  
(25)

where the total shift of energy level \( \Delta E_{q}^{(c)} \) consists of partial shifts \( \sum_{i=1}^{4} \Delta E_{q_{i}}^{(c)} \).

3. ELECTRON SPECTRUM RENORMALIZED DUE TO CONFINED-PHONONS, CONSIDERING DISCRETE STATES

Analytical and computer calculations are performed for closed nanosystem HgS/CdS/HgS/CdS transforming into open nanosystem HgS/CdS/HgS when the thickness of the outer well tends to infinity. Physical parameters of the systems are presented in Table 1.

<table>
<thead>
<tr>
<th>Physical parameters</th>
<th>m_a \ (m_e)</th>
<th>a \ (\AA)</th>
<th>E^* \ (eV)</th>
<th>V \ (eV)</th>
<th>\Omega \ (meV)</th>
<th>\varepsilon \ (meV)</th>
<th>\varepsilon_0</th>
</tr>
</thead>
<tbody>
<tr>
<td>CdS</td>
<td>0.2</td>
<td>5.818</td>
<td>2.5</td>
<td>3.65</td>
<td>57.2</td>
<td>5.5</td>
<td>9.1</td>
</tr>
<tr>
<td>HgS</td>
<td>0.036</td>
<td>5.851</td>
<td>0.5</td>
<td>5.0</td>
<td>27.8</td>
<td>11.36</td>
<td>18.2</td>
</tr>
</tbody>
</table>

In the framework of Green functions method it is performed the calculation of the renormalized electron energies located near the resonance quasistationary states. The results of computer calculations are shown in Figs. 2, 3. From these figures one can see that at the increasing of the outer potential well width (\( \Delta_2 \)), the magnitudes of the partial shifts of electron energy levels are decreasing, tending to the respective magnitudes for the open spherical quantum dot HgS/CdS/HgS in limit case. Such behavior of the curves can be explained in the following way.

The influence of the confined phonons of the core at the electron spectrum is bigger, the bigger is the probability of quasiparticle residence in it. At the increasing of the outer potential well width (HgS) it is observed the tendency of quasiparticle „penetration” from the core into the outer well HgS. It causes the decreasing of interaction between electron and confined phonons of the core (Figs. 2, 3). The essential weakening of this interaction contributes to the redistribution of the probability of electron residence in the big region of the space at the increasing of \( \Delta_2 \) magnitude.

This result gives the opportunity to study the electron- and hole-phonon interaction in open quantum dots, using for the theoretical calculations of the wave functions and energy spectra of quasiparticles obtained for the respective closed systems for the limit case of infinitely deep outer potential well.
Fig. 2 – Dependence of the partial energy shift ($\Delta E$) due to the interaction between electron in ground state and confined phonons of the core HgS on the width of the outer potential well $\Delta_1$.

Fig. 3 – Dependences of the partial energy shift ($\Delta E$) due to the interaction between electron in ground state and confined phonons of the core HgS on the width of the barrier CdS ($\Delta_1$).

CONCLUSIONS

The electron energy spectrum and wave functions are obtained for the two-well closed SQD. It is shown how does this stationary spectrum transits into the quasistationary one for the open SQD when the outer well thickness tends to infinity. The spectra of confined polarizational phonons and energy of electron
photon interaction in closed two-well SQD are obtained in the framework of dielectric continuum model.

Within the Green functions method (at T = 0°K) it is performed the calculation of those electron energy levels renormalized due to phonons, which at rather big thickness of outer well coincide to the resonance energy of ground quasistationary electron state renormalized due phonons in OSQD.

It is shown that at the increasing thickness of the OSQD barrier, the magnitude of the resonance energy shift due to phonons tends to saturation or to the respective magnitude for the single closed system, as it must be from the physical considerations.

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