ELECTRON ENERGY SPECTRUM IN A SPHERICAL HgS/CdS QUANTUM DOT WITH A SMOOTH BOUNDING POTENTIAL

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Within the effective mass approximation, the energy spectrum of an electron in a spherical quantum dot (QD) with the smooth behavior of the potential energy and the effective mass of a quasi-particle at the boundary between semiconductor media is calculated. It is shown that relative corrections to the electron energy caused by a spread boundary between two media are non-monotonic functions of the QD radius. These corrections increase rapidly with the QD radius, reach a maximum, and then slowly decay when the radius becomes large. The calculations reveal that the relative corrections for different energy levels of the electron in the spherical QD become closer to each other with increasing the QD radius.

1. Introduction

The calculation of the energy spectrum of quasi-particles in spherical QDs frequently uses a step-like rectangular potential or a parabolic potential, for which the exact analytical solutions of the Schrödinger equation are known. Despite the convenience of these solutions, the use of these potentials has some drawbacks.

The main drawbacks of the parabolic potential are the neglecting of a difference between the effective masses of quasi-particles inside the quantum dot and in the surrounding medium, the impossibility to obtain a continuous energy spectrum for quasi-particles with high energies, and the unboundedness of this potential at infinity. In work [1], the authors take into account the above-mentioned drawbacks of the parabolic potential and use a model potential that is parabolic within the quantum dot and constant in the surrounding medium . The energy spectrum calculation for this model is much more complicated and the calculation was performed by approximate methods. In works [2—5], the potential of the image forces and corrections to the bounding energies of an electron, caused by smooth functions of dielectric permittivity, were calculated.

The aim of this work is to calculate the energy corrections for spherically symmetric electron steady states that are caused by spreading the potential energy function and the effective mass at the interface between two media for HgS/CdS QDs.

2. Choice of a Smooth Bounding Potential

In work [2], the smooth function of dielectric permittivity at the plane boundary between two media was modelled by the equation

$$\varepsilon(z) = \frac{\varepsilon_1 + \varepsilon_2}{2}\left[1 + \frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_1 + \varepsilon_2}\tanh\left(\frac{z}{L}\right)\right]. \quad (1)$$

This shape of the diffuse spreading at the interface of the two media is confirmed by experimental data [2]. In [3—5], the following smooth functions are used at the boundary between a quantum dot and the environment

$$f(r) = \tanh\left(\frac{r - R_0}{L}\right), \quad (2)$$

$$f(r) = \frac{2}{\pi}\arctan\left(\frac{r - R_0}{L}\right). \quad (3)$$

They also use a linear approximating function

$$f(r) = \begin{cases} -1, & r < R_0 - L/2, \\ \frac{r - R_0}{L}, & R_0 - L/2 < r < R_0 + L/2, \\ 1, & r > R_0 + L/2, \end{cases} \quad (4)$$

where L is the parameter that characterizes the spread width of the interface between media.

In works [4,5], it is shown that the results of the energy spectrum calculations are less sensitive to the choice of the approximating function than to the width of the transition layer L.

In this work, in order to take into account the spread of the boundary of a HgS/CdS quantum dot, the functional dependence of the electron potential energy and its effective mass on the distance from the dot center was chosen as

$$U(r) = \frac{V}{2}\left[1 + \tanh\left(\frac{r - R_0}{L}\right)\right], \quad (5)$$

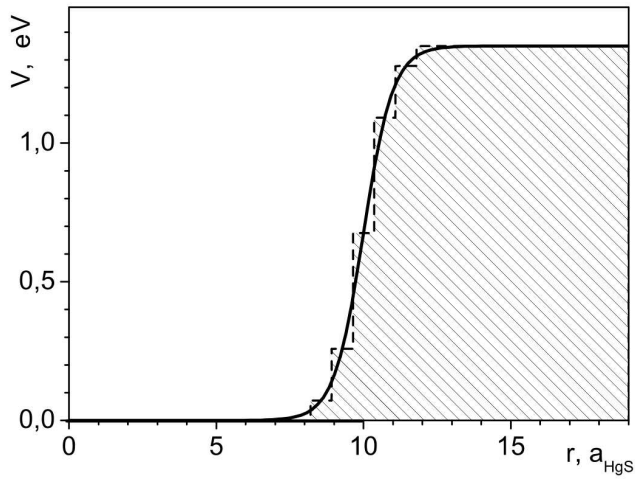

Fig. 1. Dependence $U(r)$ for the electron in a HgS/CdS QD. The solid line shows the smooth potential, and the dashed line shows the staircase-like potential

$$m(r) = \frac{m_1 + m_2}{2}\left[1 + \frac{m_2 - m_1}{m_1 + m_2}\tanh\left(\frac{r - R_0}{L}\right)\right], \quad (6)$$

where $m_1 = 0.036m_0$ and $m_2 = 0.2m_0$ are the effective masses of the electron in the QD and in the surrounding medium, respectively, m_0 is the mass of a free electron, $V = 1.35$ eV is a relative affinity of HgS and CdS semiconductors. The energy spectrum of the quasiparticle with the effective mass (6) in the potential well (5) can be found as a solution of the Schrödinger equation

$$\left(-\frac{\hbar^2}{2}\vec{\nabla}\frac{1}{m(r)}\vec{\nabla} + U(r)\right)\psi(\vec{r}) = E\psi(\vec{r}). \quad (7)$$

It is clear that one cannot find the exact solution of Eq. (7) and it is needed to apply approximate methods. For example, the variational approach would be appropriate for the calculation of the lowest energy level, but the problem becomes too complicated for the calculation of excited levels.

In this work, we propose to solve Eq. (7) using the approximation of the smooth functions (5) and (6) by staircase-like functions which are shown in Fig. 1. The use of these functions allows us to find the exact solution of the corresponding Schrödinger equation.

The more steps the closer the approximate functions to functions (5) and (6), and the more accurate becomes the solution of Eq. (7).

3. Solution of the Schrödinger Equation

Taking into account a spherical symmetry of the problem and the staircase form of the functions $m(r)$ and $U(r)$,

$$U(r) = \sum_{i=0}^{N+1} V_i\sigma_i(r), \quad m_(r) = \sum_{i=0}^{N+1} m_i\sigma_i(r),$$

$$\sigma_i(r) = \begin{cases} 1, & r_{i-1} < r < r_i, \quad (r_{-1} \equiv 0); \\ 0, & \text{elsewhere}, \end{cases} \quad (8)$$

the radial part of the wave function can be written in the form

$$R(r) = \sum_{i=0}^{N+1} R_i\sigma_i(r). \quad (9)$$

The Schrödinger equation (7) is split into the system of $N+1$ equations for radial wave functions $R_i(r)$

$$-\frac{\hbar^2}{2m_i}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R_i(r)}{\partial r}\right) + (V_i - E)R_i(r) = 0,$$

$$i = 1, ..., N+1, \quad (10)$$

each of which corresponds to a constant potential energy V_i and a constant effective mass m_i. The solution of Eq. (10) is a linear superposition of the Bessel and Neumann functions:

$$R_i(r) = A_i j_0(k_i r) + B_i n_0(k_i r), \qquad i = 0, 1, ..., N+1, \quad (11)$$

where $k_i = \hbar^{-1}\sqrt{2m_i(E - V_i)}$. In the case $E < V_i$ the Bessel and Neumann functions are transformed to the modified spherical Bessel function $I_0(|k_i|r)$ and the Macdonald function $K_0(|k_i|r)$.

The continuity conditions for the wave function and the density flux at all points r_i lead to the system of $2(N+1)$ equations

$$\left.\begin{array}{l} R_i(r)|_{r=r_i} = R_{i+1}(r)|_{r=r_i} \\ \frac{1}{m_i}\frac{dR_i(r)}{dr}\Big|_{r=r_i} = \frac{1}{m_i}\frac{dR_{i+1}(r)}{dr}\Big|_{r=r_i} \end{array}\right\} \qquad i = 0, 1, ..., N. \quad (12)$$

Using Eq. (11) and calculating the derivatives, relations (12) yield the system of linear homogeneous equations for coefficients A_i, B_i

$$j_0(k_i r_i)A_i + n_0(k_i r_i)B_i - j_0(k_{i+1} r_i)A_{i+1} -$$

$$-n_0(k_{i+1} r_i)B_{i+1} = 0,$$

$$\frac{1}{m_i}\left[j_0'(k_i r_i)A_i + n_0'(k_i r_i)B_i\right] - \frac{1}{m_{i+1}}\Big[j_0'(k_{i+1} r_i)A_{i+1} -$$

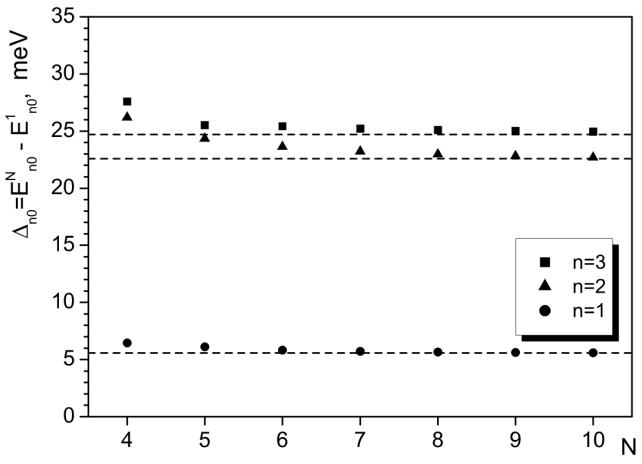

Fig. 2. Dependences of the absolute corrections to the energy levels E_{10}, E_{20}, E_{30} in a HgS/CdS QD of radius $r_0 = 15a_{\mathrm{HgS}}$ on N

$$-n_0'(k_{i+1}r_i)B_{i+1}\Big] = 0, \quad i = 0, 1, ..., N. \tag{13}$$

where

$$j_0'(k_i r_i) = \left.\frac{dj_0(k_i r)}{dr}\right|_{r=r_i} = -k_i j_i(k_i r_i), \tag{14}$$

$$n_0'(k_i r_i) = \left.\frac{dn_0(k_i r)}{dr}\right|_{r=r_i} = -k_i n_i(k_i r_i). \tag{15}$$

Two coefficients are determined from the finiteness of the wave functions at $r \to 0$ and $r \to \infty$:

$$B_0 = 0, \qquad B_{N+1} = 0. \tag{16}$$

The other $2(N+1)$ unknown coefficients are determined by system (17) and the normalization condition

$$\int_0^\infty |R(r)|^2 r^2 dr = 1. \tag{17}$$

The system of linear homogeneous equations for coefficients A_i and B_i has non-trivial solutions if the determinant built from the Bessel functions of the first and second kinds, and their derivatives are equal to zero. From this condition, we obtain a dispersion equation for the electron energy spectrum in a quantum dot with smooth boundary.

4. Results of Numerical Calculations

In order to obtain the optimal number of steps N in the approximate functions $V(r)$ and $m(r)$, we performed the calculations of the electron energies in spherically symmetric states for various values of N. Fig. 2 shows the results of calculations of corrections to the electron energies in spherically symmetric states

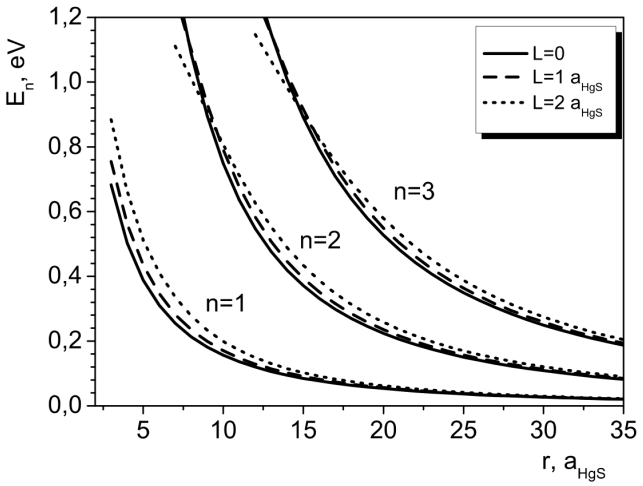

Fig. 3. Dependences of the electron energy spectrum on the HgS/CdS QD radius for various parameters of the boundary spreading

$$\Delta_{n0} = E^N_{n0} - E^1_{n0}, \tag{18}$$

where E^N_{n0} are the steady-state energies of the electron in the model potential with N steps, and E^1_{n0} are the steady-state energies of the electron in a rectangular potential (1 step).

Fig. 2 shows that the absolute values of corrections reach saturation with increase in N. For higher excited states, the saturation is observed at a higher number of steps. Taking into account that the increase in N complicates the numerical calculations significantly, we choose N ensuring that the errors of the absolute values of corrections will not exceed 5% even for excited states.

For $L = 1a_{\mathrm{HgS}}$ (where a_{HgS} is the lattice period of HgS), this condition is fulfilled for $N = 7$. With increase in L, the absolute corrections increase, which also helps to satisfy the imposed conditions. Thus all following calculations were carried out for the model functions of the potential and the effective mass for $N = 7$.

Fig. 3 shows the electron spectrum dependence on the quantum dot size for various parameters of the boundary spreading. It can be seen that the spread of the boundary does not change qualitatively the dependence of the energy spectrum on the QD size. In order to present the quantitative influence of the smooth boundary on

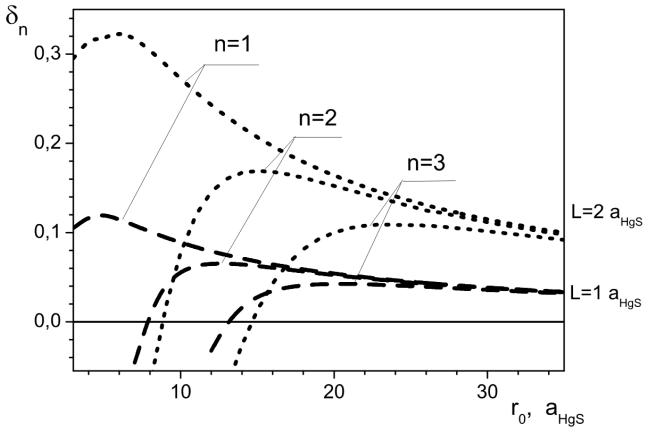

Fig. 4. Dependences of the relative corrections to energy levels for $n = 1, 2, 3$ on the size of a HgS/CdS QD for various spread parameters L

three lowest energy levels, we show the results of calculations of the relative corrections to the spherically symmetric states for various parameters L in Fig. 4.

$$\delta_{n0} = \frac{\Delta_{n0}}{E^1_{n0}} = \frac{E^N_{n0} - E^1_{n0}}{E^1_{n0}}, \tag{19}$$

Figs. 3 and 4 show that although the absolute values of corrections to the basic energy level are the smallest, the relative correction is the biggest. With increase in the spreading parameter twice as much, the relative correction also increases twice as much. The interesting and unexpected feature is that, with increase in the size of a quantum dot, the relative corrections for all energy levels first increase and then decrease and become closer to each other. This behavior of corrections is quite understandable. As the size of a quantum dot increases, the energy levels gradually draw into it. The every new level that appears in the dot is placed near the top of the spread potential well, where the well is wider than the rectangular well. In this case, a correction may be even negative, because the energy level in the spread potential well may be located lower than that in the corresponding rectangular well. This can be seen in Fig. 2 for every energy level. The increase in the quantum dot size leads to a decrease in the energy of steady states. The absolute corrections also decrease. As a result, the relative corrections for large quantum dots become hardly sensitive to the change in the quantum dot radius. Fig. 4 shows that the decrease in the potential barrier height leads to a decrease of relative corrections, a decrease in the speed of their approaching to each other, and a decrease of their sensitivity to the quantum dot size.

5. Conclusions

The spread of the boundary between the spherical quantum dot and the surrounding medium leads to the shift of the energy levels to higher energies. Only the levels that are located near the top of the potential well can be pulled down more to the well. For the big enough quantum dots, the values of relative corrections for different energy levels are the same.

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ЕНЕРГЕТИЧНИЙ СПЕКТР ЕЛЕКТРОНА У СФЕРИЧНІЙ КВАНТОВІЙ ТОЧЦІ HgS/CdS З ПЛАВНИМ ОБМЕЖУЮЧИМ ПОТЕНЦІАЛОМ

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Р е з ю м е

У рамках наближення ефективних мас розраховано енергетичний спектр електрона у сферичній квантовій точці (КТ) з плавними залежностями потенціальної енергії та ефективної маси квазічастинки на межі поділу напівпровідникових середовищ. Показано, що відносні поправки до енергій електрона, зумовлені розмитою межею поділу середовищ, є немонотонні функції радіуса КТ, зі збільшенням якого поправки швидко зростають, досягають максимуму і повільно спадають для КТ великих розмірів. У результаті розрахунків виявилось, що відносні поправки для різних енергетичних рівнів електрона у сферичній КТ з ростом її радіуса зближаються між собою.