

ENERGY OF THE INTERACTION OF A CHARGE WITH THE SEPARATION BOUNDARIES OF A MULTILAYER SPHERICAL QUANTUM DOT

V.I. BOICHUK, R.YU. KUBAY, I.S. SHEVCHUK

UDC 621.315.59
©2007

Ivan Franko Drohobych State Pedagogical University
(24, I. Franko Str., Drohobych 82100, Ukraine; e-mail: innashs@yahoo.com)

We present an investigation of the influence of interfaces of a multilayer spherical crystal heterostructure on the potential energy of a charged particle. The case of presence of a thin intermediate layer at the interface where dielectric permittivity is a function of the coordinates r , θ , and φ is studied. We determined a functional dependence of the charge potential energy on distance and angles by the classical Green function method. By using the derived potential of the interaction of a charge with the interface, the Schrödinger equation is solved for surface states of an electron and a hole located in the matrix of the β -HgS/CdS heterosystem. It is shown that such states should make a considerable contribution to the interband absorption coefficient.

layer at the interface of two media was first set in [21]. In works [22–24] based on solving the Poisson equation, the potential energy of the charge interaction with the separation boundaries of composite nanoheterosystems with spherical and, correspondingly, cylindrical and planar interfaces was found by the Green function method. It is shown that if the interface contains a superthin layer (of several lattice parameters in thickness), where dielectric permittivity depends on the distance to the interface and changes smoothly from one value (in the QD) to another (in the matrix), then the potential energy of interaction of a charge with the interface – as a function of distance – does not have singularities as distinct from traditional approaches [25, 26].

1. Introduction

Regardless of the fact that the investigation of nanoheterosystems of quantum dots (QDs) began more than twenty years ago [1–4], such works are still of great importance [5–11]. This is related not only to the interesting physical properties of these structures but to their use in electric circuits and optoelectronics.

The systems with interacting quantum dots have recently been studied in many works [12–16]. However, no adequate model of a single quantum dot located in the matrix has been developed till now. First of all, it concerns the shape of QD surface which can be cubic [14], cylindrical [15], spherical [16], etc. In addition, an important characteristic of the model is physical conditions at the interface. They can involve the appearance of additional strains related to the elastic and structural characteristics of a QD and the surrounding material [17, 18, 20]. The difference between the polarization properties of the media that form the heterostructure is also important [19, 20].

In most cases, the latter effects are taken into account with the use of classical calculations which assume that all physical parameters (including dielectric permittivity) change stepwise at the interface. The problem of regarding the presence of the intermediate

The next stage of the QD model specification can consist in the account of the dependence of dielectric permittivity (ε) not only on distance (r) but on the direction of the radius-vector (\vec{r}). This dependence can arise from different asymmetric physical influences on a QD. In particular, it can be related to impurities in doping a QD [6] and to the interaction with other QDs of the heterosystem [14].

In the present work, the Poisson equation for a charge at the spherical interface of a layered QD embedded in the matrix is solved. It is assumed that, at the interfaces, dielectric permittivity is a function of all three coordinates r , θ , and φ . Based on the derived general expression of the potential energy in the β -HgS/CdS heterosystem, the energy and the wave function of the ground state of an electron and a hole located in the matrix close to the interface are defined.

2. Statement of the Problem. General Theory

We consider a multilayer spherical semiconductor nanoheterosystem (Fig. 1) with corresponding $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_n$ dielectric permittivities. The separation boundaries of the heterosystem are concentric spheres with radii $R_1,$

R_2, \dots, R_{n-1} . Dielectric permittivity at the interfaces of the media in the regions with thicknesses L_1, L_2, \dots, L_{n-1} depends on the coordinates r, θ , and φ (r is the distance from the center to a fixed point in space, and θ and φ are spherical angles).

A point charge q placed at \vec{r}_0 induces the potential $\phi(\vec{r}, \vec{r}_0)$ at a point \vec{r} of space which is a solution of the Poisson equation

$$\nabla^2 \phi(\vec{r}, \vec{r}_0) + \nabla \phi(\vec{r}, \vec{r}_0) \frac{\nabla \varepsilon(\vec{r})}{\varepsilon(\vec{r})} = -\frac{4\pi q}{\varepsilon(\vec{r})} \delta(\vec{r} - \vec{r}_0), \quad (1)$$

derived from the Maxwell equation

$$\text{div} \vec{D} = 4\pi q \delta(\vec{r} - \vec{r}_0).$$

Here,

$$\vec{D} = \varepsilon(\vec{r}) \vec{E} = -\varepsilon(\vec{r}) \nabla \phi(\vec{r}, \vec{r}_0),$$

and $\delta(\vec{r} - \vec{r}_0)$ is the Dirac delta-function. With regard for the explicit form of operators ∇^2 and ∇ in the spherical coordinate system, Eq. (1) can be rewritten as

$$\begin{aligned} & \frac{\partial^2}{\partial r^2} \phi(\vec{r}, \vec{r}_0) + \frac{2}{r} \frac{\partial}{\partial r} \phi(\vec{r}, \vec{r}_0) + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} \phi(\vec{r}, \vec{r}_0) + \\ & + \frac{1}{r^2} \frac{\cos \theta}{\sin \theta} \frac{\partial}{\partial \theta} \phi(\vec{r}, \vec{r}_0) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \phi(\vec{r}, \vec{r}_0) + \frac{1}{\varepsilon(\vec{r})} \times \\ & \times \left[\frac{\partial \varepsilon(\vec{r})}{\partial r} \frac{\partial \phi(\vec{r}, \vec{r}_0)}{\partial r} + \frac{1}{r^2} \frac{\partial \varepsilon(\vec{r})}{\partial \theta} \frac{\partial \phi(\vec{r}, \vec{r}_0)}{\partial \theta} + \right. \\ & \left. + \frac{1}{r^2 \sin^2(\theta)} \frac{\partial \varepsilon(\vec{r})}{\partial \varphi} \frac{\partial \phi(\vec{r}, \vec{r}_0)}{\partial \varphi} \right] = -\frac{4\pi q}{\varepsilon(\vec{r})} \delta(\vec{r} - \vec{r}_0). \quad (2) \end{aligned}$$

The potential energy of a charge in the self-induced polarization field is

$$U(\vec{r}) = \frac{q}{2} \phi(\vec{r}),$$

where

$$\phi(\vec{r}) = \lim_{\vec{r} \rightarrow \vec{r}_0} \left\{ \phi(\vec{r}, \vec{r}_0) - \frac{q}{\varepsilon(\vec{r})} \frac{1}{|\vec{r} - \vec{r}_0|} \right\}.$$

It is convenient to express the potential $\phi(\vec{r}, \vec{r}_0)$ through the Green function

$$\phi(\vec{r}, \vec{r}_0) = -4\pi q \cdot [\varepsilon(\vec{r}) \varepsilon(\vec{r}_0)]^{-1/2} G(\vec{r}, \vec{r}_0). \quad (3)$$

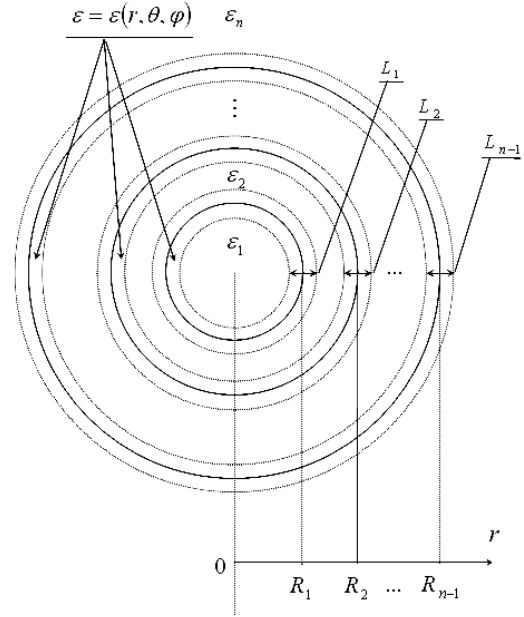


Fig. 1. Multilayer spherical nanoheterosystem model

By substituting (3) into Eq. (2), we get

$$\nabla^2 G(\vec{r}, \vec{r}_0) - V(\vec{r}) G(\vec{r}, \vec{r}_0) = \delta(\vec{r} - \vec{r}_0), \quad (4)$$

where

$$\begin{aligned} V(\vec{r}) \equiv V(r, \theta, \varphi) &= V_1(r, \theta, \varphi) + \\ &+ V_2(r, \theta, \varphi) + V_3(r, \theta, \varphi), \quad (5) \end{aligned}$$

$$V_1(r, \theta, \varphi) = \frac{1}{2r^2 \sqrt{\varepsilon}} \frac{\partial \varepsilon}{\partial r} \left[\frac{r^2}{\sqrt{\varepsilon}} \frac{\partial \varepsilon}{\partial r} \right],$$

$$V_2(r, \theta, \varphi) = \frac{1}{2r^2 \sin \theta \sqrt{\varepsilon}} \frac{\partial \varepsilon}{\partial \theta} \left[\frac{\sin \theta}{\sqrt{\varepsilon}} \frac{\partial \varepsilon}{\partial \theta} \right],$$

$$V_3(r, \theta, \varphi) = \frac{1}{2r^2 \sin^2 \theta \sqrt{\varepsilon}} \frac{\partial \varepsilon}{\partial \varphi} \left[\frac{1}{\sqrt{\varepsilon}} \frac{\partial \varepsilon}{\partial \varphi} \right].$$

The solution of Eq. (4) is derived by successive approximations with regard for a small value $V(\vec{r})$ which is discussed below. Then the Green function can be represented as a fast convergent series

$$\begin{aligned} G(\vec{r}, \vec{r}_0) &= G^{(0)}(\vec{r}, \vec{r}_0) + \\ &+ G^{(1)}(\vec{r}, \vec{r}_0) + G^{(2)}(\vec{r}, \vec{r}_0) + \dots \equiv \\ &\equiv G^{(0)}(\vec{r}, \vec{r}_0) + \Delta G(\vec{r}, \vec{r}_0). \quad (6) \end{aligned}$$

In the zero-order approximation

$$\nabla^2 G^{(0)}(\vec{r}, \vec{r}_0) = \delta(\vec{r} - \vec{r}_0).$$

To within a constant factor, $G^{(0)}(\vec{r}, \vec{r}_0)$ is a point charge potential, hence

$$G^{(0)}(\vec{r}, \vec{r}_0) = -\frac{1}{4\pi|\vec{r} - \vec{r}_0|}. \tag{7}$$

If we take formulas (3), (6), and (7) into account, the potential $\phi(\vec{r})$ is

$$\phi(\vec{r}) = -\frac{4\pi q}{\varepsilon(x_0)} \Delta G(\vec{r}_0, \vec{r}_0),$$

where

$$\Delta G(\vec{r}_0, \vec{r}_0) = G^{(1)}(\vec{r}_0, \vec{r}_0) +$$

$$+ G^{(2)}(\vec{r}_0, \vec{r}_0) + \dots + G^{(n)}(\vec{r}_0, \vec{r}_0) + \dots$$

Thus, $\phi(\vec{r})$ is determined by the corrections to the Green function of higher orders than the zero-order terms.

The next stage of work is to find these corrections. It is proved that any correction to the Green function can be determined from the recurrence equation

$$\nabla^2 G^{(n)}(\vec{r}, \vec{r}_0) = V(\vec{r}) G^{(n-1)}(\vec{r}, \vec{r}_0),$$

where

$$G^{(n)}(\vec{r}, \vec{r}_0) = \int d\vec{r}_1 d\vec{r}_2 \dots d\vec{r}_n G^{(0)}(\vec{r}, \vec{r}_1) V(\vec{r}_1) \times$$

$$\times G^{(0)}(\vec{r}_1, \vec{r}_2) V(\vec{r}_2) \dots G^{(0)}(\vec{r}_{n-1}, \vec{r}_n) V(\vec{r}_n) \times$$

$$\times G^{(0)}(\vec{r}_n, \vec{r}_0), \quad n \geq 1.$$

Then, with regard for (7), it looks as

$$G^{(n)}(\vec{r}_0, \vec{r}_0) = \left(-\frac{1}{4\pi}\right)^n \int d\vec{r}_1 d\vec{r}_2 \dots d\vec{r}_n \times$$

$$\times \frac{V(\vec{r}_1) \cdot V(\vec{r}_2) \cdot \dots \cdot V(\vec{r}_n)}{|\vec{r}_0 - \vec{r}_1| \cdot |\vec{r}_1 - \vec{r}_2| \cdot \dots \cdot |\vec{r}_{n-1} - \vec{r}_n| \cdot |\vec{r}_n - \vec{r}_0|}.$$

A general expression of the self-induced potential with regard for the Green function corrections is given by

$$U(\vec{r}_0) = -\frac{2\pi q^2}{\varepsilon(\vec{r}_0)} \left(\frac{1}{(4\pi)^2} \int d\vec{r} \frac{V(\vec{r})}{(\vec{r}_0 - \vec{r})^2} -$$

$$-\frac{1}{(4\pi)^3} \int d\vec{r}_1 d\vec{r}_2 \frac{V(\vec{r}_1) V(\vec{r}_2)}{|\vec{r}_0 - \vec{r}_1| |\vec{r}_1 - \vec{r}_2| |\vec{r}_2 - \vec{r}_0|} + \dots +$$

$$+ \left(-\frac{1}{4\pi}\right)^n \int d\vec{r}_1 d\vec{r}_2 \dots d\vec{r}_n \times$$

$$\times \frac{V(\vec{r}_1) \cdot V(\vec{r}_2) \cdot \dots \cdot V(\vec{r}_n)}{|\vec{r}_0 - \vec{r}_1| \cdot |\vec{r}_1 - \vec{r}_2| \cdot \dots \cdot |\vec{r}_{n-1} - \vec{r}_n| \cdot |\vec{r}_n - \vec{r}_0|} + \dots \Big). \tag{8}$$

These results are rather general. In order to specify them, we need to regard the explicit form of functions $V(\vec{r})$. For this purpose, it is necessary to specify the function $\varepsilon(\vec{r})$. Here, we assume that it is a continuous smooth function of spherical coordinates,

$$\varepsilon(\vec{r}) \equiv \varepsilon(r, \theta, \varphi) = \frac{1}{2} [1 - S(r, \theta, \varphi)] \sum_{i=1}^n \varepsilon_i,$$

where

$$S(r, \theta, \varphi) = \gamma_1 f\left(\frac{r - R_1}{L_1}\right) f\left(\cos \theta + \frac{R_1}{L_1}\right) \times$$

$$\times f\left(\sin \varphi + \frac{R_1}{L_1}\right) + \sum_{i=1}^{n-2} \left[\gamma_{i+1} f\left(\frac{r - R_i}{L_i}\right) \times$$

$$\times f\left(\cos \theta + \frac{R_i}{L_i}\right) f\left(\sin \varphi + \frac{R_i}{L_i}\right) f\left(\frac{r - R_{i+1}}{L_{i+1}}\right) \times$$

$$\times f\left(\cos \theta + \frac{R_{i+1}}{L_{i+1}}\right) f\left(\sin \varphi + \frac{R_{i+1}}{L_{i+1}}\right) \Big] -$$

$$- \gamma_n f\left(\frac{r - R_{n-1}}{L_{n-1}}\right) f\left(\cos \theta + \frac{R_{n-1}}{L_{n-1}}\right) f\left(\sin \varphi + \frac{R_{n-1}}{L_{n-1}}\right),$$

$$\gamma_i = \frac{\varepsilon_i}{\sum_{i=1}^n \varepsilon_i}, \tag{9}$$

ε_i is the dielectric permittivity of the i -th medium, and n is the number of layers of a single quantum dot. In $S(r, \theta, \varphi)$, the presence of many surfaces that make a layered spherical structure is taken into account.

Moreover, it contains some unknown function $f(x)$ which should satisfy the conditions

$$f\left(|x| \geq \frac{1}{2}\right) = \pm 1, \quad f'\left(|x| \geq \frac{1}{2}\right) = 0.$$

Imposing these conditions makes it possible for the dielectric permittivity $\varepsilon(r, \theta, \varphi)$ to become a continuous function.

As seen from formula (9), the parameters γ_i ($i = \overline{1, n}$) are small. The presence of γ_i in the function $S(r, \theta, \varphi)$ and, therefore, in the function $\varepsilon(r, \theta, \varphi)$, as well as in $V_1(r, \theta, \varphi)$, $V_2(r, \theta, \varphi)$, and $V_3(r, \theta, \varphi)$, allows us to expand them into power series in γ_i :

$$\begin{aligned} V_1(r, \theta, \varphi) &= -\frac{1}{2r^2} \frac{\partial}{\partial r} \left[r^2 \frac{\partial}{\partial r} [S(r, \theta, \varphi)] \right] - \\ &\quad - \frac{S(r, \theta, \varphi)}{2r^2} \frac{\partial}{\partial r} \left[r^2 \frac{\partial}{\partial r} [S(r, \theta, \varphi)] \right] - \\ &\quad - \frac{1}{4} \left[\frac{\partial}{\partial r} [S(r, \theta, \varphi)] \right]^2 - \dots, \\ V_2(r, \theta, \varphi) &= -\frac{1}{2r^2 \sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \frac{\partial}{\partial \theta} [S(r, \theta, \varphi)] \right] - \\ &\quad - \frac{S(r, \theta, \varphi)}{2r^2 \sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \frac{\partial}{\partial \theta} [S(r, \theta, \varphi)] \right] - \\ &\quad - \frac{1}{4r^2} \left[\frac{\partial}{\partial \theta} [S(r, \theta, \varphi)] \right]^2 - \dots, \\ V_3(r, \theta, \varphi) &= -\frac{1}{2r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} [S(r, \theta, \varphi)] - \\ &\quad - \frac{S(r, \theta, \varphi)}{2r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} [S(r, \theta, \varphi)] - \\ &\quad - \frac{1}{4r^2 \sin^2 \theta} \left[\frac{\partial}{\partial \varphi} [S(r, \theta, \varphi)] \right]^2 - \dots. \end{aligned}$$

However, the calculation of the potential which does not depend on the angles θ and φ shows that the maximum contribution to the potential energy $U(r_0)$ (about 98%) is given by the term that contains γ_i raised to the first power [1]. Thus, in the expressions $V_1(r, \theta, \varphi)$,

$V_2(r, \theta, \varphi)$, and $V_3(r, \theta, \varphi)$, one can take the first term and neglect the rest. Then, according to (5), we get

$$V(r, \theta, \varphi) \approx -\frac{1}{2} \nabla^2 S(r, \theta, \varphi).$$

In addition, this restriction leaves only the first term in formula (8) since all the rest are proportional to γ_i^m , where $m \geq 2$, $i = \overline{1, n}$. By taking the above-mentioned reasoning into account, we can write

$$\begin{aligned} U(\vec{r}_0) &\equiv U(r_0, \theta_0, \varphi_0) = \\ &= \frac{q^2}{16\pi\varepsilon(r_0, \theta_0, \varphi_0)} \int_0^{2\pi} d\varphi \int_0^\pi d\theta \sin \theta \times \\ &\quad \times \int_0^\infty dr r^2 \frac{\nabla^2 S(r, \theta, \varphi)}{r^2 + r_0^2 - 2rr_0 \cos \theta}. \end{aligned} \quad (10)$$

Expression (10) defines a final form of the potential energy of interaction of a charged particle with interfaces of the multilayer spherical nanoheterosystem. In such a system, it takes into account the presence of the interfaces which are thin layers with dielectric permittivities dependent on the spherical coordinates r , θ , and φ .

3. The β -HgS/CdS Nanoheterosystem

The structures that consist of two, three, and even four layers are studied experimentally. In every case, it is easy to obtain analytical expressions for $U(r_0, \theta_0, \varphi_0)$, in particular, for the β -HgS/CdS system ($\varepsilon_1 = 11.3$, $\varepsilon_2 = 5.2$) for which

$$\varepsilon(r_0, \theta_0, \varphi_0) = \frac{\varepsilon_1 + \varepsilon_2}{2} [1 - S(r_0, \theta_0, \varphi_0)],$$

where

$$\begin{aligned} S(r_0, \theta_0, \varphi_0) &= \gamma f\left(\frac{r_0 - R}{L}\right) \times \\ &\quad \times f\left(\cos(\theta_0) + \frac{R}{L}\right) f\left(\sin(\varphi_0) + \frac{R}{L}\right), \end{aligned}$$

$$\gamma = \frac{\varepsilon_1 - \varepsilon_2}{\varepsilon_1 + \varepsilon_2}.$$

A detailed determination of $U(r_0, \theta_0, \varphi_0)$ is possible after the specification of the function $f = f(x)$. For the

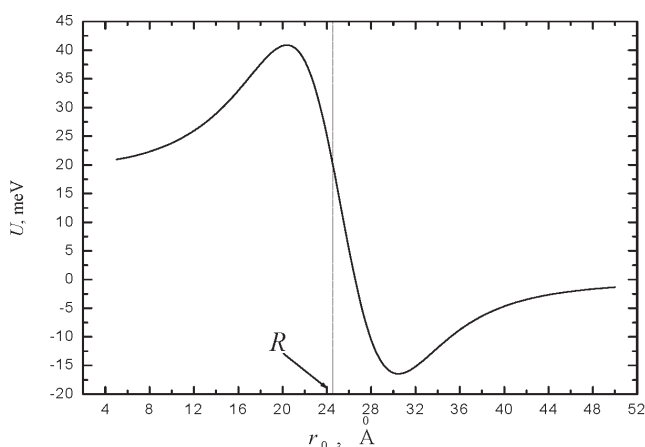


Fig. 2. Dependence of the potential energy of interaction of a charged particle with the interface on the distance to the nanocrystal center

heterostructure under consideration, this function is unknown. But the analysis shows that the final results do not qualitatively depend on a specific form of this function provided that it is smooth. Here, we assume that

$$f(x) = \tan H(x).$$

Then Eq. (10) for the structure under consideration can be written as

$$U(r_0, \theta_0, \varphi_0) =$$

$$= \frac{q^2 \gamma}{8\pi \varepsilon(r_0, \theta_0, \varphi_0)} \int_0^{2\pi} d\varphi \int_0^\pi d\theta \sin(\theta) \times \\ \times \int_0^\infty dr \frac{P(r, \theta, \varphi) + Q(r, \theta, \varphi) + R(r, \theta, \varphi)}{r^2 + r_0^2 - 2rr_0 \cos \theta_0},$$

where

$$P(r, \theta, \varphi) = \frac{r}{L} \sec H^2 \left(\frac{r-R}{L} \right) \left[1 - \frac{r}{L} \tanh \left(\frac{r-R}{L} \right) \right] \times \\ \times \tan H \left(\cos(\theta) + \frac{R}{L} \right) \tanh \left(\sin(\varphi) + \frac{R}{L} \right),$$

$$Q(r, \theta, \varphi) = -\tanh \left(\frac{r-R}{L} \right) \sec H^2 \left(\cos(\theta) + \frac{R}{L} \right) \times$$

$$\times \left[\cos(\theta) + \sin^2(\theta) \tanh \left(\cos(\theta) + \frac{R}{L} \right) \right] \times$$

$$\times \tan H \left(\sin(\varphi) + \frac{R}{L} \right),$$

$$R(r, \theta, \varphi) = -\tanh \left(\frac{r-R}{L} \right) \operatorname{cosec}^2(\theta) \times$$

$$\times \tanh \left(\cos(\theta) + \frac{R}{L} \right) \sec H^2 \left(\sin(\varphi) + \frac{R}{L} \right) \times$$

$$\times \left[\frac{\sin(\varphi)}{2} + \cos^2(\varphi) \tanh \left(\sin(\varphi) + \frac{R}{L} \right) \right].$$

In Fig. 2, an explicit form of the potential energy of interaction of a charged particle with the interface is shown for the studied crystal at $R = 5a$, $L = a$, $\theta = \pi/4$, $\varphi = \pi/2$, where $a = 4.851 \text{ \AA}$ is the lattice parameter of β -HgS. It is seen from the plot that the curve is continuous and it changes nonmonotonically in the region of the intermediate layer. This means that, in contrast to the classical case where dielectric permittivity of the heterosystem changes abruptly, $U(r_0, \theta_0, \varphi_0)$ is not a discontinuous function. Moreover, it is also limited in the whole interval, where the coordinate varies.

The coordinate dependence of the potential energy of a charge interacting with the interface makes it possible to find the total energy of a particle.

Let the particle be in the matrix (CdS). As is known, its dielectric permittivity is less than that of a QD (β -HgS). Then, as seen from Fig. 2, the interaction potential in the region $r_0 > R$ is negative, and a particle is attracted to the separation boundary. In this case, the bound states of an electron or a hole can arise at the interface. In order to find the energies and the wave functions of these states, it is necessary to solve the Schrödinger equation

$$\hat{H}\psi(\vec{r}_0) = E\psi(\vec{r}_0), \tag{11}$$

where

$$\hat{H} = \hat{H}_k + \hat{H}_p, \quad \hat{H}_k = -\frac{\hbar^2}{2m_{e,h}^{\text{CdS}}} \nabla_{\vec{r}_0}^2, \quad \hat{H}_p = U(\vec{r}_0),$$

and $m_{e,h}^{\text{CdS}}$ is the effective mass of a charged particle ($m_e^{\text{CdS}} = 0.2m_0, m_h^{\text{CdS}} = 0.7m_0$). Since it is difficult to solve Eq. (11) exactly, we use the variational method. For the sake of simplicity, we consider the case where $U(\vec{r}_0) \equiv U(r_0)$ [27]. That is why $\psi(\vec{r}_0) \equiv \psi(r_0)$ for the ground state. A trial wave function of this state is chosen as

$$\psi(r_0) \equiv \psi(r_0, \alpha) = A \exp\left(-\alpha(r_0 - R)^2\right),$$

where α is a variational parameter. The factor A is found from the normalizing condition

$$\int d\tau |\psi(r_0, \alpha)|^2 = 1.$$

Therefore,

$$A = \frac{1}{\sqrt{F_0}},$$

where

$$F_0 = \int_0^\infty dr_0 r_0^2 \exp\left(-2\alpha(r_0 - R)^2\right).$$

The necessary functional used in this method is represented by the formula

$$\begin{aligned} \int d\tau \psi(r_0, \alpha) \hat{H} \psi(r_0, \alpha) &= \int_0^\infty dr_0 r_0^2 \psi(r_0, \alpha) \hat{H} \psi(r_0, \alpha) = \\ &= \int_0^\infty dr_0 r_0^2 \psi(r_0, \alpha) \left(\hat{H}_k + \hat{H}_p \right) \psi(r_0, \alpha) = \\ &= \int_0^\infty dr_0 r_0^2 \psi(r_0, \alpha) \hat{H}_k \psi(r_0, \alpha) + \\ &+ \int_0^\infty dr_0 r_0^2 \psi(r_0, \alpha) \hat{H}_p \psi(r_0, \alpha). \end{aligned}$$

Thus, the term which describes the kinetic energy of a particle is defined as

$$E_k = -\frac{\hbar^2}{2m_{e,h}^{\text{CdS}}} A^2 F_1,$$

where

$$F_1 = \int_0^\infty dr_0 \exp\left(-2\alpha(r_0 - R)^2\right) \times$$

$$\times \left[(2\alpha r_0 (r_0 - R))^2 - 4\alpha r_0 (r_0 - R) - 2\alpha r_0^2 \right],$$

and the potential energy of interaction of a charge with the interface is determined by the expression

$$E_p = A^2 F_2,$$

where

$$F_2 = \int_0^\infty dr_0 r_0^2 \exp\left(-2\alpha(r_0 - R)^2\right) U(r_0).$$

The total energy of a particle is found by minimizing the sum of both terms

$$E_0 = \min \langle \psi(r_0, \alpha) | \hat{H} | \psi(r_0, \alpha) \rangle = \min (E_k + E_p).$$

The specific calculations performed for the β -HgS/CdS heterosystem show that, for an electron in the matrix, there is a bound state with an energy of -2.45 meV. The mean distance between a charged particle and the interface determined by the expression

$$\langle r \rangle = \int_0^\infty dr r^3 \psi_0^2(r)$$

is 809 \AA for an electron in this state.

The analogous calculations were also carried out for a hole. The energy of the bound state in this case is -3.52 meV, and the mean distance makes 264 \AA .

An explicit form of the ground-state wave functions of an electron and a hole makes it possible to determine the overlapping integral that enters the formula of the interband transition probability and defines the coefficient of absorption of electromagnetic waves. The calculation of the overlapping integral

$$I = \int_0^\infty dr r^2 \psi_e(r) \psi_h(r)$$

showed that $I = 0.44$ for the states under consideration, that is, it is quite large.

Thus, we have solved the Poisson equation for a spherical quantum dot by taking intermediate layers at the separation boundaries into account. Based on the found potential of interaction of a charge with the interface, the Schrödinger equation for surface states of an electron and a hole located in the matrix was solved for the β -HgS/CdS heterosystem. It has been shown that such states should make a considerable contribution to the coefficient of interband absorption.

1. A.I. Ekimov and A.A. Onushchenko, Pis'ma Zh. Eksp. Teor. Fiz. **34**, 363 (1981).
2. A.I. Ekimov and A.A. Onushchenko, Pis'ma Zh. Eksp. Teor. Fiz. **40**, 337 (1984).
3. A.I. Ekimov and A.A. Onushchenko, Fiz. Tekhn. Polupr. **16**, 1215 (1982).
4. Al.L. Efros and A.L. Efros, Fiz. Tekhn. Polupr. **16**, 1209 (1982).
5. N.V. Kryzhanovskaya, A.H. Hladyshev, S.A. Blokhin *et al.*, Fiz. Tekhn. Polupr. **38**, 867 (2004).
6. N.V. Kryzhanovskaya, A.H. Hladyshev, S.A. Blokhin *et al.*, Fiz. Tekhn. Polupr. **39**, 1230 (2005).
7. E.P. Pokatilov, V.A. Fonoberov, V.M. Fomin, and J.T. Devrees, Phys. Rev. B **64**, 24532 (2001).
8. I.M. Kupchak, D.V. Korbutyak, Yu.V. Kryuchenko, A.V. Sachenko, I.O. Sokolovsky, and O.M. Sreset, Fiz. Tekhn. Polupr. **40**, 98 (2006).
9. V.A. Kumbachinsky, V.A. Rogozin, V.G. Kytin *et al.*, Fiz. Tekhn. Polupr. **40**, 215 (2006).
10. Volodin V.A., Yakimov A.I., Dvurechensky A.V. *et al.*, Fiz. Tekhn. Polupr. **40**, 207 (2006).
11. G.A. Kachurin, S.G. Cherkova, V.A. Volodin, D.M. Marin, D.I. Getelbaum, and H. Becker, Fiz. Tekhn. Polupr. **40**, 75 (2006).
12. V.I. Boichuk and V.B. Holskyi, Ukr. Fiz. Zh. **46**, 342 (2001).
13. V. Boichuk, V. Holskyi, and I. Shevchuk, Shevchenko Sci. Soc. Coll. Phys. Papers **5**, 107 (2002).
14. V.I. Boichuk, I.V. Bilynskiy, and V.B. Holskyi, Ukr. Fiz. Zh. **48**, 56 (2003).
15. V.I. Boichuk and V.B. Holskyi, Nauk. Zapysky NaUKMA **23**, 50 (2004).
16. V.I. Boichuk and V.B. Holskyi, Zh. Fiz. Dosl. **8**, 122 (2004).
17. Weidong Sheng and Sean-Pierre Leburton, Phys. Rev. B. **64**, 153302 (2001).
18. A.I. Yakimov, N.P. Stepina, A.V. Dvurechenski, and A.I. Nikifirov, Phys. Rev. B **63**, 045312 (2001).
19. Weidong Sheng and Sean-Pierre Leburton, Phys. Rev. Lett. **88**, 167401 (2002).
20. F. Hatami, W.T. Masselink, L. Schrottke, J.W. Tomm, V. Talalaev, C. Kristukat, and A.R. Goni, Phys. Rev. B **67**, 085306 (2003).
21. T. Nakamura, J. Phys. Soc. Japan **52**, 973 (1983).
22. V.I. Boichuk and R.Yu. Kubay, Fiz. Tverd. Tela **43**, 226 (2001).
23. V.I. Boichuk, R.Yu. Kubay, and R.I. Pazyuk, Shevchenko Sci. Soc. Coll. Phys. Papers **5**, 119 (2002).
24. V.I. Boichuk, R.Yu. Kubay, I.S. Shevchuk, and I.P. Kogoutiuk, Shevchenko Sci. Soc. Coll. Phys. Papers **5**, 128 (2002).
25. V.I. Boichuk, R.Yu. Kubay, and I.V. Bilynskiy, J. Phys. Studies **3**, 187 (1999).
26. V.I. Boichuk, I.V. Bilynskiy, R.Yu. Kubay, Ukr. Fiz. Zh. **45**, 236 (2000).
27. V.I. Boichuk and R.Yu. Kubay, J. Phys. Studies **3**, 492 (1999).

Received 19.02.07

ЕНЕРГІЯ ВЗАЄМОДІЇ ЗАРЯДУ З МЕЖАМИ ПОДІЛУ БАГАТОШАРОВОЇ СФЕРИЧНОЇ КВАНТОВОЇ ТОЧКИ

V.I. Boichuk, R.Yu. Kubay, I.S. Shevchuk

Резюме

Досліджено вплив меж поділу багатошарової сферичної кристалічної гетероструктури на потенціальну енергію зарядженої частинки. Розглядається випадок, коли біля меж поділу існує тонкий проміжний шар, в якому діелектрична проникність є функцією координат r , θ і φ . Методом класичних функцій Гріна визначено функціональну залежність потенціальної енергії заряду від відстані та кутів. На основі знайденого потенціалу взаємодії заряду з межею поділу розв'язано рівняння Шредінгера для поверхневих станів електрона та дірки гетеросистеми β -HgS/CdS, що знаходяться у матриці. Показано, що такі стани повинні давати певний внесок у коефіцієнт міжзонного поглинання.