STATIONARY AND QUASISTATIONARY STATES OF HYDROGENIC IMPURITY IN A SPHERICAL QUANTUM ANTIDOT

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Discrete states of a hydrogenic impurity have been calculated for CdS/β-HgS spherical nanoheterostructures with various radii of a quantum antidot. The calculations are based on the exact solutions of the Poisson and Schrödinger equations and are carried out in the framework of the effective mass approximation. The dependence of discrete energy levels on the potential barrier height has been examined. The average value of electron distance in the structure concerned has been found and analyzed. The quasistationary states of the impurity have been studied, which allowed the quasistationary energy levels and the mean lifetime of an electron in those states to be determined.

1. Introduction

Localized states of charge carriers in various confined systems have been intensively studied recently. In particular, the substantial attention is given to studying quantum dots (QDs). Since the energy spectrum of current carriers in them is completely discrete, QDs possess improved optical parameters. Therefore, they are studied to be used in diode lasers, amplifiers, and biological sensors.

A lot of theoretical and experimental researches dealing with QDs have been carried out till now. The presence of impurities in QDs is also known to be able to change localized states and, hence, the properties of QDs themselves considerably. In works [1–5], the first theoretical researches of impurity states in spherical QDs have been fulfilled, and the exact solutions of the Schrödinger equation with the Coulomb interaction potential between particles have been obtained. In work [6], it was shown that the account of the exact solution of the Poisson and Schrödinger equations for a hydrogenic impurity considerably changes the spectrum in comparison with the results of works [1–5].

Recently, the attention of researchers has been drawn to the so-called quantum antidots (QADs), the internal part of which is a potential barrier for current carriers, rather than a potential well, as it occurs in QDs. If the mean free path of current carriers is longer than QAD dimensions, the discrete states are formed in such a structure in a magnetic field. In particular, in work [7], the Aharonov–Bohm effect and the Landau levels in QADs have been studied. In work [8], the quantum states of an electron in a heterosystem with a good many QADs, the energy of magnetic subbands, and the electron density of states have been determined. Discrete states can also arise in QADs, if the latter contain an impurity.

Taking all that into account, we have obtained the potential energy of interaction between the impurity ion and an electron on the basis of the exact solution of the Poisson equation for a spherical QAD with a positively charged impurity ion in its center. Using this energy, the Schrödinger equation for the discrete spectrum of the hydrogenic impurity in QAD has been solved exactly. The average distance of an electron in the nanoheterostructure has been determined. We have also studied the dependence of quasistationary states on the QAD radius. Specific calculations have been carried out for a spherical CdS/β-HgS nanoheterosystem.

2. Hydrogenic Impurity in the Middle of a Spherical QAD

Let a positively charged ion of the hydrogenic impurity be centered in the middle of a spherical nanoheterostructure with a potential barrier in the region $r \leq a$. The potential energy stemming from the

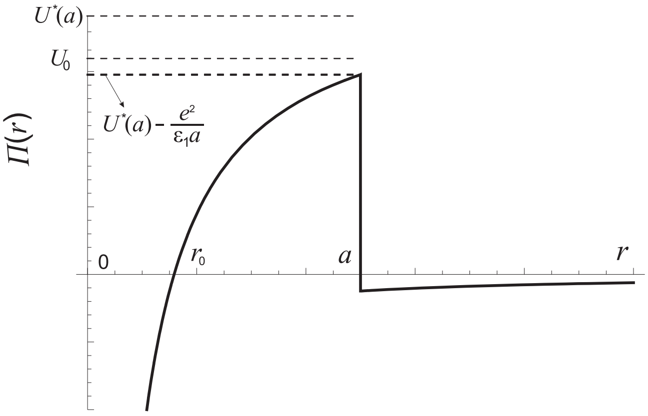

Fig. 1. Potential energy profile

band discontinuity can be given in the form

$$U(r) = \begin{cases} U_0, & r \le a, \\ 0, & r > a, \end{cases} \quad U_0 > 0. \tag{1}$$

The potential energy of interaction between an electron and the impurity ion, which is considered to be a positive point-like charge, is obtained on the basis of the solution of the Poisson equation:

$$V(r) = e^2 \begin{cases} -\dfrac{1}{\varepsilon_1 r} + \dfrac{\varepsilon_2 - \varepsilon_1}{\varepsilon_1 \varepsilon_2 a}, & r \le a, \\ -\dfrac{1}{\varepsilon_2 r}, & r > a. \end{cases} \tag{2}$$

Summing up expressions (1) and (2), we obtain the total potential energy of an electron in the QAD as

$$\Pi(r) = \begin{cases} \dfrac{-e^2}{\varepsilon_1 r} + U^*(a), & r \le a, \\ \dfrac{-e^2}{\varepsilon_2 r}, & r > a, \end{cases} \tag{3}$$

where the effective potential barrier

$$U^*(a) = \frac{e^2(\varepsilon_2 - \varepsilon_1)}{\varepsilon_1 \varepsilon_2 a} + U_0 \tag{4}$$

is introduced. According to expression (4), the effective potential barrier depends on the heterosystem dimensions and the dielectric permittivities. In Fig. 1, the potential energy of an electron in a QAD with an impurity is shown schematically. The distance r_0 is determined from the condition $\Pi(r_0) = 0$.

The operator of total system energy is written down in the effective mass approximation as

$$\mathbf{H} = -\frac{\hbar^2}{2} \nabla \frac{1}{m^*(r)} \nabla + \Pi(r), \tag{5}$$

where

$$m^*(r) = \begin{cases} m_1^*, & r \le a, \\ m_2^*, & r > a \end{cases} \tag{6}$$

is the effective electron mass in the corresponding crystal. For potential (3), it is evident that, at $E < 0$, the spectrum is discrete; in the case $E > U^*(a) - e^2/\varepsilon_1 a$, the energy spectrum becomes completely continuous; and if $0 < E < U^*(a) - e^2/\varepsilon_1 a$, there exist quasistationary states.

3. Impurity Discrete Spectrum

The Schrödinger equation with Hamiltonian (5) for a discrete spectrum can be solved exactly. Taking the spherical symmetry of the problem into account, the wave function can be tried as a product of the radial and angular components:

$$\psi(r, \theta, \varphi) = R(r) Y_l^m(\theta, \varphi), \tag{7}$$

where $Y_l^m(\theta, \varphi)$ are the spherical functions. In this case, the radial Schrödinger equation for two regions of the coordinate r variation can be written down. If $r \le a$, the radial Schrödinger equation looks like

$$\left\{ -\frac{\hbar^2}{2m_1^*} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) - \frac{e^2}{\varepsilon_1 r} + U^*(a) + \right.$$

$$\left. + \frac{\hbar^2 l(l+1)}{2m_1^* r^2} - E \right\} R_1(r) = 0. \tag{8}$$

By introducing the dimensionless quantities

$$\xi = \alpha_{1a} r, \quad \alpha_{1a}^2 = -8m_1^* \left(E - U^*(a)\right)/\hbar^2,$$

$$\lambda_1 = 2m_1^* e^2 / \left(\varepsilon_1 \hbar^2 \alpha_{1a}\right), \quad R_1(\xi) = \xi^{-1} \rho_1(\xi),$$

we obtain, after simple transformations,

$$\frac{\partial^2 \rho_1(\xi)}{\partial \xi^2} + \left[-\frac{1}{4} + \frac{\lambda_1}{\xi} - \frac{l(l+1)}{\xi^2} \right] \rho_1(\xi) = 0. \tag{9}$$

This is the Whittaker equation which has two linearly independent solutions. One of them is unphysical, because it does not obey the condition to be finite at the coordinate origin. Therefore, the solution of Eq. (9) in the interval $r \le a$ is the function

$$\rho_1(\xi) = C_1 e^{-\xi/2} \xi^{l+1} \mathrm{M}(l + 1 - \lambda_1, 2l + 2, \xi), \tag{10}$$

where $M(a,b,x)$ is the hypergeometric function of the 1-st kind [9].

If $r > a$, we introduce dimensionless quantities

$$(\xi = \alpha_2 r)\,, \qquad \alpha_2^2 = -8m_2^* E/\hbar^2,$$

$$\lambda_2 = 2m_2^* e^2/\left(\varepsilon_2 \hbar^2 \alpha_2\right), \quad R_2(\xi) = \xi^{-1}\rho_2(\xi)\,,$$

and obtain another Whittaker equation, very similar to Eq. (9). The solution of this new equation, which satisfies the conditions of wave function finiteness in the given area, is the function [9]

$$\rho_2(\xi) = C_2 \frac{e^{-\xi/2}\xi^{-l}}{\Gamma(\,-l-\lambda_2)} \int_0^\infty dt\, e^{-\xi t}\, t^{-l-\lambda_2-1}(1+t)^{-l+\lambda_2-1}, \tag{11}$$

where $\Gamma(x)$ is the Euler gamma function [9].

Having the functions $\rho_1(\xi)$ and $\rho_2(\xi)$ in explicit form and satisfying the boundary conditions, we can determine the energy spectrum of the electron in the heterosystem.

4. Quasistationary States of Impurity

We will solve the problem of the electron penetration through a barrier making use of the "irradiation" condition. That is, we assume that the electron moves so that its coordinate r increases only (it starts to move from within the barrier). This condition demands that only incident waves should be taken into account in the outer medium (matrix) for calculations. In such a formulation of the problem, there are no stationary states. However, the "irradiation" condition chooses definite states, which will be referred to as quasistationary ones [10], from the whole spectrum. We assume that the particle penetration began long ago, so that a considerable fraction of particles are already outside the barrier. Then, the wave function, which is a solution of the non-stationary Schrödinger equation, can be presented in the form

$$\psi(\mathbf{r},t) = \psi(\mathbf{r}) \exp\left(-i\frac{\tilde{E}}{\hbar}t\right), \tag{12}$$

where the quantity $\tilde{E}$ is complex-valued, and it cannot be considered therefore as the particle energy. We assume that

$$\tilde{E} = E - \frac{i\hbar}{2}\delta, \tag{13}$$

where E is the energy of a quasistationary level. Then, the probability to find every particle within the barrier (the region $r \le a$) is determined as follows:

$$W(t) = \int_{r\le a} d\mathbf{r}\psi^*(\mathbf{r},t)\,\psi(\mathbf{r},t) = e^{-\delta t}\int_{r\le a} d\mathbf{r}\psi^*(\mathbf{r})\,\psi(\mathbf{r}), \tag{14}$$

that is,

$$W(t) = W(0)\,e^{-\delta t}. \tag{15}$$

The quantity δ is the decay constant, $\Delta E = \hbar\delta/2$ is the quasistationary level width, and $\tau = 1/\delta$ denotes the mean lifetime of a particle in the state $\psi(\mathbf{r},0) = \psi(\mathbf{r})$.

If function (12) is substituted into the non-stationary Schrödinger equation with Hamiltonian (5), it is possible to separate the coordinate variables and the time, which yields the equation

$$\mathbf{H}\psi(\mathbf{r}) = \tilde{E}\psi(\mathbf{r})\,. \tag{16}$$

The wave function, owing to the spherical symmetry, can be tried in form (7). Thus, we obtained the radial equation which is to be solved in two regions.

1. Region $r \le a$. Introducing the notations

$$\xi = \alpha_1 r; \quad \alpha_1^2 = 2m_1^*\left(\tilde{E} - U^*(a)\right)/\hbar^2,$$

$$\beta_1 = -m_1^* e^2/\left(\varepsilon_1\hbar^2\alpha_1\right), \quad R_1(\xi) = \xi^{-1}\rho_1(\xi)\,,$$

we obtain the radial equation as the Coulomb equation:

$$\frac{\partial^2\rho_1(\xi)}{\partial\xi^2} + \left[1 - \frac{2\beta_1}{\xi} - \frac{l(l+1)}{\xi^2}\right]\rho_1(\xi) = 0. \tag{17}$$

Its solution, which satisfies the condition that the wave function has to be finite, is written down in the form

$$\rho_1(\xi) = C_{11}\frac{2^l e^{-\pi\beta_1/2}\left|\Gamma(l+1+i\beta_1)\right|}{\Gamma(2l+2)} e^{-i\xi}\xi^{l+1}\times$$

$$\times \mathrm{M}(l+1-i\beta_1, 2l+2, 2i\xi)\,. \tag{18}$$

2. Region $r > a$. Introducing the dimensionless quantities

$$\xi = \alpha_2 r, \quad \alpha_2^2 = 2m_2^*\left(\tilde{E}\right)/\hbar^2,$$

$$\beta_2 = -m_2^* e^2/\left(\varepsilon_2\hbar^2\alpha_2\right), \quad R_2(\xi) = \xi^{-1}\rho_2(\xi)\,,$$

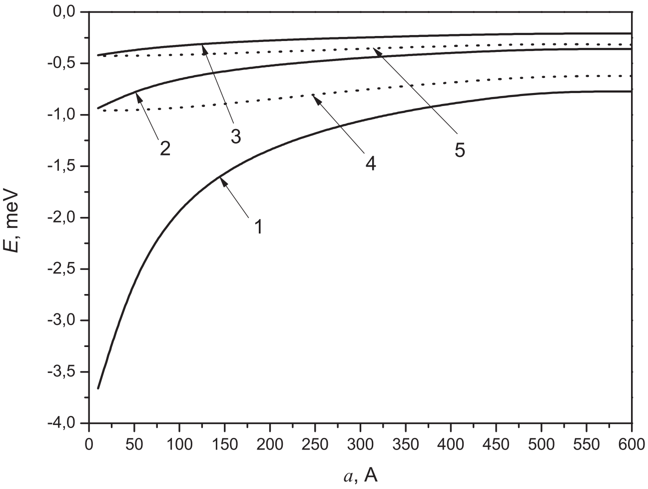

Fig. 2. Energy of a hydrogenic impurity electron in a spherical QAD

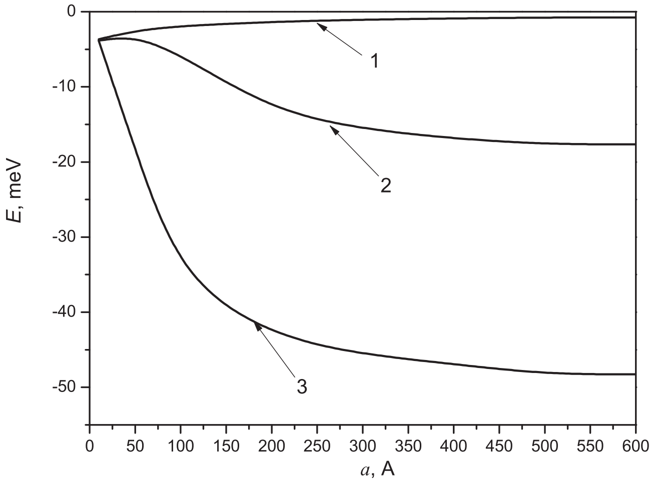

Fig. 3. Ground state energy of an impurity electron in a spherical QAD

we obtain another Coulomb equation similar to Eq. (17). The general solution of the Coulomb equation is a linear combination of two functions: the regular Coulomb function $F_l(\beta_2,\xi)$ and the logarithmic Coulomb function $G_l(\beta_2,\xi)$ [11]. In accordance with the irradiation condition, we have to select only an incident wave. The following reasonings are used at that. The behaviors of functions $F_l(\beta_2,\xi)$ and $G_l(\beta_2,\xi)$ at large distances ($\xi \to \infty$) are similar to those of the functions $\sin(\xi - l\pi/2 + \beta_l - \beta_2 \ln 2\xi)$ and $\cos(\xi - l\pi/2 + \beta_l - \beta_2 \ln 2\xi)$, respectively, where $\beta_l = \arg\Gamma(l+1+i\beta_2)$. Therefore, by analogy on the basis of Coulomb functions, we can construct two linearly independent functions [11]

$$Q_l^{+}(\beta_3,\xi) = G_l(\beta_3,\xi) + i\,F_l(\beta_3,\xi)\,, \tag{19}$$

$$Q_l^{-}(\beta_2,\xi) = G_l(\beta_2,\xi) - i\,F_l(\beta_2,\xi)\,, \tag{20}$$

which are also the solutions of the radial Coulomb equation in the given region. Hence, taking the analysis made above and the irradiation condition into account, we have to try a solution of the Coulomb equation in the form

$$\rho_2(\xi) = C_2 Q_l^{+}(\beta_2,\xi)\,. \tag{21}$$

The wave functions given by formulas (10), (11), (18), and (21), as well as the probability density flow, must be continuous at the heterostructure boundaries. From these conditions and the normalization one, we can determine discrete states, quasistationary states, and the mean lifetime of the particle in the given quasistationary state for a QAD with hydrogenic impurity, returning back to dimensional quantities:

$$\begin{aligned} &R_1(r)|_{r=a} - R_2(r)|_{r=a} = 0,\\ &\frac{1}{m_1^*}\frac{d}{dr}R_1(r)\bigg|_{r=a} - \frac{1}{m_2^*}\frac{d}{dr}R_2(r)\bigg|_{r=a} = 0,\\ &\int d\mathbf{r}\,|\psi(r,\theta,\varphi)|^2 = 1. \end{aligned} \tag{22}$$

5. Calculation Results and Their Analysis

The calculation of the electron energy spectrum was carried out for a spherical nanoheterosystem CdS/β-HgS with the following parameters: $m_1^* = 0.2$, $m_2^* = 0.036$, $\varepsilon_1 = 5.2$, $\varepsilon_2 = 11.3$, and $U_0 = 1200$ meV.

In Fig. 2, the dependences of the energies of the ground and excited stationary ($E < 0$) states on the QAD radius are depicted. The figure demonstrates that the growth of the QAD radius gives rise to an increase of the energy of both S- (solid curves) and P-states (dotted curves). The analysis testifies that, owing to a large band discontinuity for the given crystals, the electron with negative energy is located outside the QAD ($r \geq a$). As is seen from formula (3), an increase in the radius leads to a diminution of the well depth in this region, which results, in its turn, in the growth of the particle energy. To confirm this conclusion, in Fig. 3, we plotted the dependences of the impurity ground state energy in a spherical QAD on the QAD radius for various U_0. Curve *1* corresponds to the ground state of a hydrogenic impurity in the CdS/β-HgS heterosystem, curve *2* to $U_0 = 80$ meV,

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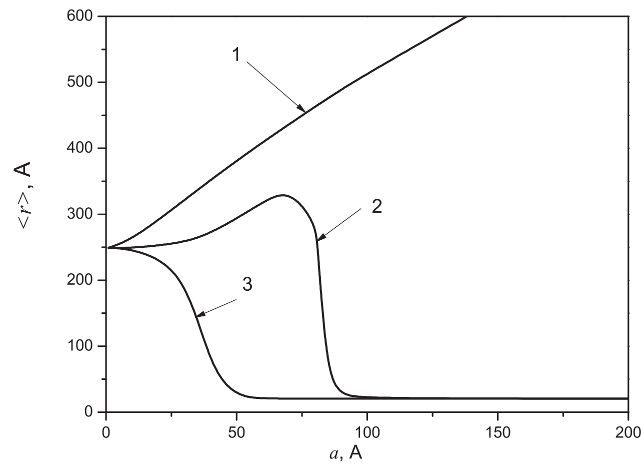

Fig. 4. Dependences of the average electron distances on the QAD radius at various $U_0 = 1200$ (*1*), 80 (*2*), and 50 meV (*3*)

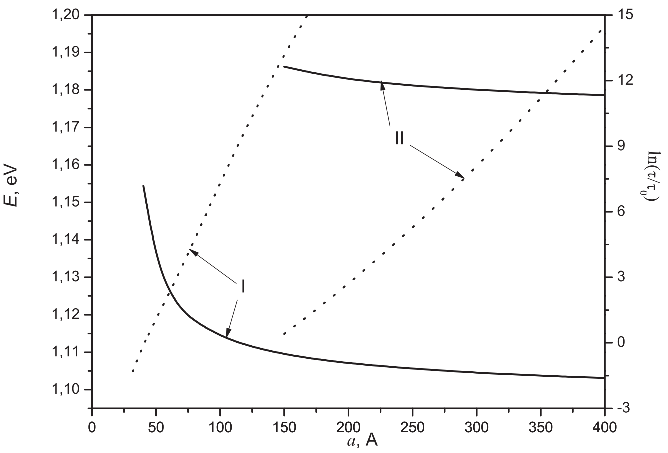

Fig. 5. Energies of quasistationary levels and mean lifetimes of an electron in them

and curve *3* to $U_0 = 50$ meV. The behavior of curves *2* and *3* testifies that, in the case of a small band discontinuity, the electron is located within the interval $r < r_0$ with a higher probability.

This result is also confirmed by the dependence of the average distance $\langle r \rangle$ on the QAD radius. Such dependences are exhibited in Fig. 4 for the ground state of the system at various U_0-values. For a real CdS/β-HgS nanoheterostructure ($U_0 = 1200$ meV), an increase of the QAD radius leads to a proportional growth of $\langle r \rangle$. For instance, the average distance $\langle r \rangle = 1484$ Å at $a = 600$ Å. However, if $U_0 = 80$ meV, the dependence of $\langle r \rangle$ on the QAD radius is nonmonotonous, and $\langle r \rangle \to 20.6$ Å in the region $r > 100$ Å. At the same time, if $U_0 = 50$ meV, $\langle r \rangle \to 20.6$ Å, provided $r > 50$ Å.

We also calculated the energies of impurity quasistationary states and the mean lifetimes of an electron in those states. For this purpose, we used the method different from that of work [12]. We obtained a complex equation for the complex unknown $\tilde{E} = E - i\hbar\delta/2$. Numerically, the real and imagine parts of this equation were separated. Thus, we obtained a system of equations for the energy of a quasistationary level and the corresponding mean lifetime of electron, which is reciprocal of δ. The execution of the indicated calculation program demands carrying out rather complicated numerical calculations aimed at separating the system into the real and imaginary parts, and finding the solutions, provided that the entering quantities are the integrals of complicated special functions.

In Fig. 5, the dependences of the energies of first two quasistationary S-states (solid curves) and the corresponding mean lifetimes of electron in those states (dotted curves) on the QAD radius a are shown. For convenience, the time $\tau_0 = 2.06$ ps is introduced, which is the mean lifetime of an electron in the first quasistationary S-state in the case $a = 40$ Å. The plots testify that the growth of the QAD radius leads to a reduction of the electron energy and an increase of the particle lifetime in the states concerned. This result stems from a reduction of the spatial confinement. At lower energies, the barrier is wider and higher, which increases the lifetime of the electron in the corresponding states. For example, for the radius $a = 150$ Å, the lifetime in the first quasistationary S-state $\tau = 1.35\,\mu$s. The figure also demonstrates that the second quasistationary level is expelled out of the range $0 < E < U^*(a) - e^2/\varepsilon_1 a$ at $a < 150$ Å, i.e. it transits into the continuous spectrum.

Hence, in this work, on the basis of the exact solution of the Poisson equation for a donor hydrogenic impurity located in the middle of QAD, the general formula for the total potential energy of an electron is obtained, and the effective potential barrier for an electron in the heterostructure is introduced. The Schrödinger equation with the potential energy obtained is solved exactly for the stationary states of the hydrogenic impurity. The dependences of the electron energy levels and the lifetime on the QAD radius and the potential barrier height are analyzed. The average distances for an electron in the heterostructure are determined.

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СТАЦІОНАРНІ ТА КВАЗІСТАЦІОНАРНІ СТАНИ ВОДНЕВОПОДІБНОЇ ДОМІШКИ У СФЕРИЧНІЙ КВАНТОВІЙ АНТИТОЧЦІ

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Р е з ю м е

Для сферичної наногетероструктури CdS/β-HgS в наближенні ефективної маси на основі точних розв'язків рівнянь Пуассона та Шредінгера визначено дискретні стани водневоподібної домішки для різних розмірів квантової антиточки. Розглянуто залежність дискретних енергетичних рівнів від величини потенціального бар'єра. Знайдено і проаналізовано середні значення відстані електрона у структурі. Проведено дослідження квазістаціонарних станів домішки, що дозволило визначити квазістаціонарні енергетичні рівні та обчислити середній час життя електрона у цих станах.