THE ELECTRON ENERGY SPECTRUM IN AN ELLIPSOIDAL QUANTUM DOT WITH REGARD FOR FINITE BAND GAP AT THE INTERFACE

V.I. BOICHUK, V.B. HOL'SKYI, R.YU. KUBAY, R.I. LUKIN

Institute of Physics, Mathematics, and Computer Science,
Ivan Franko Drogobych State University
(3, Stryiska Str., Drogobych 82100, Ukraine; e-mail: lukin@drohobych.net)

UDC 539.184

We have developed the theory of the energy spectrum of a charge with regard for a real band gap for an ellipsoidal quantum dot (QD) with arbitrary oblateness. The dependence of the energy of bound states of a particle on both the volume of a QD and a degree of anisotropy of its shape is obtained. It is shown that the increase of the anisotropy of a QD results in a decrease of the ground-state energy of a particle, which is not observed in the model of infinite potential well. In addition, the growth of anisotropy causes the appearance of the first excited state in a nanocrystal.

1. Introduction

The research of low-dimensional structures opened new perspectives in the fabrication of semiconductor lasers, memory cells, and one-electron transistors. Quantum dots, in which particles are limited in three directions, are most interesting to study. These structures are characterized by a discrete spectrum, which gave them the name of "artificial" atoms [1–3]. Many theoretical works were devoted to the research of quantum dots modeled by quantum wells of spherical shape [4–9]. In an isolated cylindrical QD, a number of one- and two-electron problems are solved; in particular, the spin-orbital coupling is studied [10]. In the case of tunnel-linked QDs, the exciton ground state was found in [11], and the power spectrum of a charge was determined for QDs of cubic shape in [12]. In [13], the influence of a nanocrystal form on the quasiparticle energy levels was analyzed for spherical, cylindrical, and cubic QDs. The results showed that the nanocrystal shape significantly influences the particle energy spectrum.

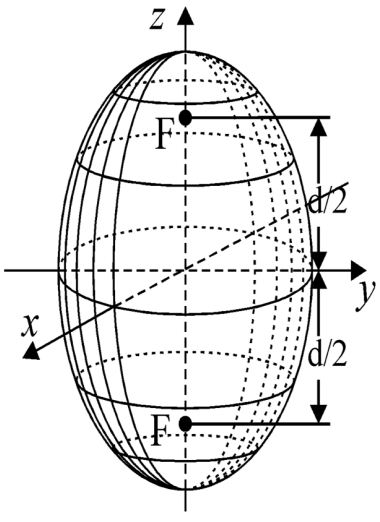

Fig. 1. Model of a nanocrystal

The shape of a QD is not always cubic, cylindrical, or spherical in real physical situations. The ellipsoidal shape is more general and can be considered under certain conditions as spherical or cylindrical. A theoretical research of ellipsoidal QDs was carried out in [14–17], where the energy spectra of a charged particle and an exciton were found, and the influence of polarization effects on the quasiparticle spectrum was studied. These calculations were performed for an infinite potential well which can be used either for a QD of a large volume or when the band gap at the interface is sufficiently large. In [18], ellipsoidal QDs were studied with regard for the real band gap at the boundary of media.

We will consider the dependence of the energy of confined particle states on the volume of a QD and the degree of its shape anisotropy. For this purpose, we introduce a quasispherical coordinate system, in which the complete separation of variables is possible. The results which are similar to those in the case of a cylindrical QD are obtained. However, the introduction of the orthogonal quasispherical coordinate system is valid only for a sufficiently large degree of oblateness (large eccentricity). In what follows, we will develop a theory to determine the energy spectrum of a charge by taking the real band gap for an ellipsoidal QD of arbitrary oblateness into account.

2. Statement of the Problem

Let us consider a problem of finding the electron energy spectrum in an ellipsoidal QD. The heterostructure is modeled by a quantum well which has the form of an elongated ellipsoid of rotation (Fig. 1). The problem will be solved in the prolate spheroidal coordinates [19]. The Hamiltonian of a charged quasiparticle in the effective mass approximation can be written as

$$\widehat{H} = -\frac{\hbar^2}{2}\nabla\frac{1}{m_e}\nabla + U(\xi), \tag{1}$$

$$U(\xi) = \begin{cases} U_0, & \xi \leqslant \xi_0, \\ 0, & \xi > \xi_0, \end{cases} \tag{2}$$

where m_e is the effective mass of an electron in the corresponding region, $U_0 > 0$, ξ_0 determines the region of a quantum dot in the spheroidal coordinates. The Laplacian in the spheroidal coordinates has the form

$$\nabla^2 = \frac{4}{d^2(\xi^2-\eta^2)}\left\{\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi} + \right.$$

$$\left. + \frac{\partial}{\partial\eta}(\eta^2-1)\frac{\partial}{\partial\eta} + \frac{\xi^2-\eta^2}{(\xi^2-1)(1-\eta^2)}\frac{\partial^2}{\partial\varphi^2}\right\}, \tag{3}$$

where d is the focal distance.

The Schrödinger equation in these coordinates allows one to present a wave function in the form

$$\Psi(\xi,\eta,\varphi) = A\,R(\xi)S(\eta)\Phi(\varphi), \tag{4}$$

where A is the normalization coefficient.

The functions $R(\xi)$, $S(\eta)$, and $\Phi(\varphi)$ are solutions of the following three equations:

$$\frac{d^2\Phi}{d\varphi^2} = -m^2\Phi(\varphi), \tag{5}$$

$$\frac{d}{d\eta}\left[\left(1-\eta^2\right)\frac{dS_{lm}(c,\eta)}{d\eta}\right] +$$

$$+ \left[\lambda_{lm} - c^2\eta^2 - \frac{m^2}{1-\eta^2}\right]S_{lm(c,\eta)} = 0, \tag{6}$$

$$\frac{d}{d\xi}\left[\left(1-\xi^2\right)\frac{dR_{lm}(c,\xi)}{d\xi}\right] -$$

$$- \left[\lambda_{lm} - c^2\xi^2 + \frac{m^2}{\xi^2-1}\right]R_{lm(c,\xi)} = 0, \tag{7}$$

where m, λ_{lm} are the constants of separation of the variables, $c = \dfrac{kd}{2}$, k depends on the chosen region: $k_1 = \sqrt{\dfrac{2m_{e1}}{\hbar^2}E}$, $k_2 = \sqrt{\dfrac{2m_{e2}}{\hbar^2}(E-U)}$ (the indices 1 and 2 correspond, respectively, to the region of a quantum well and the external medium) $n = 0, 1, 2, ...$, $m = 0, \pm1, \pm2, ..., \pm n$.

As is known, the solution of Eq. (5) is

$$\Phi(\varphi) = Ce^{im\varphi}. \tag{8}$$

The solution of (6) for either region is a linear combination of angular prolate spheroidal functions of the first and second kinds [20]:

$$S_{lm}(c,\eta) = C_1S^{(1)}_{lm}(c,\eta) + C_2S^{(2)}_{lm}(c,\eta). \tag{9}$$

The coordinate η ranges from -1 to 1, and the function $S^{(2)}_{lm}(c,\eta)$ has a discontinuity at the point $\eta = 1$. Thus, it is necessary to choose the coefficient $C_2 = 0$.

The solution of Eq. (7) is a linear combination of the prolate radial spheroidal functions of either the first and second or the third and fourth kinds [20]. In the region of a quantum well, we present the solution in the form

$$R^I_{lm}(c_1,\xi) =$$

$$= B_1R^{(1)}_{lm}(c_1,\xi) + B_2R^{(2)}_{lm}(c_1,\xi),\ 0 \leqslant \xi \leqslant \xi_0. \tag{10}$$

The function $R^{(2)}_{lm}(c_1,\xi)$ has a discontinuity at the point $\xi = 1$, that is why the coefficient $B_2 = 0$.

For a particle outside the quantum well, we write a solution through a linear combination of the functions of the third and fourth kinds:

$$R^{II}_{lm}(c_2,\xi) =$$

$$= B_3R^{(3)}_{lm}(c_2,\xi) + B_4R^{(4)}_{lm}(c_2,\xi),\ \xi_0 \leqslant \xi \leqslant \infty. \tag{11}$$

The functions $R^{(3)}_{lm}(c_2,\xi)$ and $R^{(4)}_{lm}(c_2,\xi)$ for a spherical surface transform into the Hankel spheroidal functions of the third and fourth kinds. The function $R^{(4)}_{lm}(c_2,\xi)$ tends to $+\infty$ as $\xi \to \infty$; therefore, $B_4 = 0$.

Summarizing the above results, we write the electron wave function in a prolate spheroidal QD as

$$\Psi(\xi,\eta,\varphi) =$$

$$= \begin{cases} AS^{(1)}_{lm}(c_1,\eta)\cdot R^{(1)}_{lm}(c_1,\xi)e^{im\varphi}, & \xi \leqslant \xi_0, \\ BS^{(1)}_{lm}(c_2,\eta)\cdot R^{(3)}_{lm}(c_2,\xi)e^{im\varphi}, & \xi > \xi_0. \end{cases} \tag{12}$$

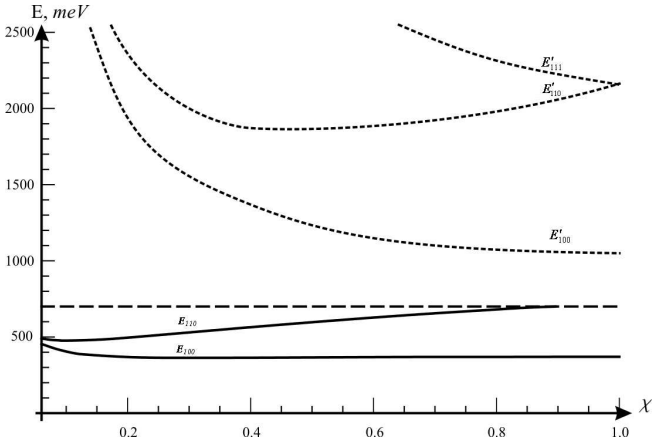

Fig. 2. Dependence of the electron energy in an ellipsoidal QD of the InAs/GaAs structure on χ at a constant volume $V = 200$ nm^3 (solid lines stand for the electron energies calculated within the finite band gap model, dotted lines stand for those calculated in the infinite band gap model, and a dashed line shows a quantum well depth)

Then we use the matching conditions for the wave function with regard for the continuity of $\Psi(\xi, \eta, \varphi)$ and that of the probability current density:

$$B_1 R^1_{lm}(c_1, \xi_0) = B_3 R^{(3)}_{lm}(c_2, \xi_0),$$

$$\frac{B_1}{m_{e1}} \left. \frac{d\left[R^1_{lm}(c_1, \xi)\right]}{d\xi} \right|_{\xi_0} = \frac{B_3}{m_{e2}} \left. \frac{d\left[R^3_{lm}(c_2, \xi)\right]}{d\xi} \right|_{\xi_0}. \qquad (13)$$

We get the dispersion equation to find the electron energy levels in a spheroidal QD. It shows that, in order to find a charged particle energy spectrum, it suffices to use the radial part of the wave function. While deriving the solutions of (13), we obtain the energies of the respective particle states, whose number is determined by the system's parameters and the quantum numbers l and m. Thus, the energy and the wave function $R(\xi)$ will depend not only on l and m, but also on the third quantum number n ($n = 1, 2, ...$) which numerates the roots of (13).

3. Analysis of Calculation Results

Numerical calculations were performed for the structures InAs/GaAs and CdSe/glass. In a first case, the band gap is $\Delta E_c = 700$ meV, and the electron effective mass is $m_{e1} = 0.027 m_0$ in indium arsenide and $m_{e2} = 0.065 m_0$ in gallium arsenide. In a second case, the band gap is $\Delta E_c = 1820$ meV, and the electron effective mass is $m_{e1} = 0.13 m_0$ in cadmium selenide and $m_{e2} = m_0$ in glass.

Figure 2 shows the electron energy levels of the InAs/GaAs nanocrystal structure as a function of the nanocrystal anisotropy form which is determined by the expression

$$\chi = \frac{b}{a}, \qquad (14)$$

where b is the minor half-axis, and a is the major half-axis. Let the volume of nanocrystal be 200 nm^3 which corresponds to the volume of a spherical QD with a radius of 6 lattice constants. At $\chi = 1$ (a spherical QD), there is one energy level for this volume, i.e. the QD under consideration is ideal. With decrease in χ, the ground state energy E_{100} decreases. At $\chi = 0.85$, the first excited state appears in the nanocrystal, and its energy also reduces with decrease in χ. However, both energies E_{100} and E_{110} show an insignificant growth at $\chi = 0.25$ and $\chi = 0.1$, respectively. The obtained nonmonotonic dependence $E = E(\chi)$ is related to the influence of two competing factors on the particle energy: the reduction of χ at a constant volume leads to the enhancement of the particle motion limitation in the plane XOY and a decrease of the motion confinement in the perpendicular direction. The result mentioned is in good qualitative agreement with the particle energy behaviour in a quantum wire (QW) with elliptic cross-section [21–23]. For this nanocrystal, the infinite bandgap used in [14–17] (E'_{100}, E'_{110}, and E'_{111}) leads to a great mismatch in the results on particle energy values, as is seen from the figure. At small χ, the difference in the energies of analogous states for various quantum well models exceeds 800 meV and rises with increase in the ellipsoid prolateness χ.

In the structure CdSe/glass with higher band gap for a QD even with volume of 20 nm^3, there exist more energy levels (Fig. 3). The ground state (E_{100}), which is called s-state ($l = 0$ and $m = 0$) for the spherical surface, has its minimum at $\chi = 0.5$. The first (E_{110}) and second (E_{111}) excited states of the nanostructure in question arose from the splitting of the threefold degenerate p-state of a spherical quantum dot. In addition, state E_{111} is twofold degenerate ($m = 1$). Level E_{110} falls with increase in the nanocrystal surface anisotropy, while that of E_{111} gains in growth. The transition to the spheroidal symmetry lifts also the degeneracy of the quasiparticle d-state giving rise to non-degenerate state E_{120} and two twofold degenerate ones E_{121} ($m = 1$) and E_{122} ($m = 1$). The functions $E = E(\chi)$ for these states are similar to

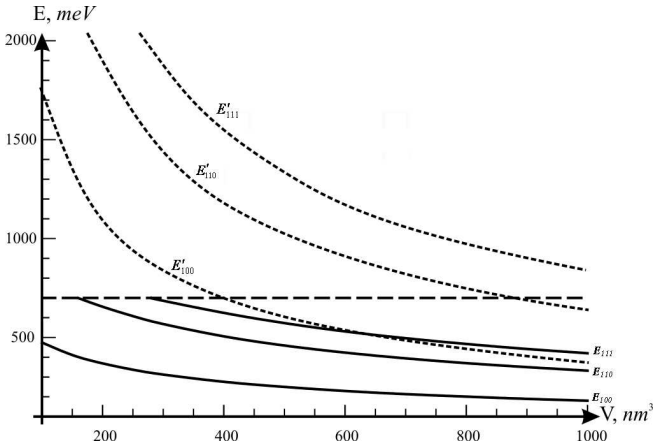

Fig. 3. Dependence of the electron energy in an ellipsoidal QD of the CdSe/glass structure on χ at a constant volume $V = 200$ nm^3. Notation of lines is analogous to that of Fig. 2

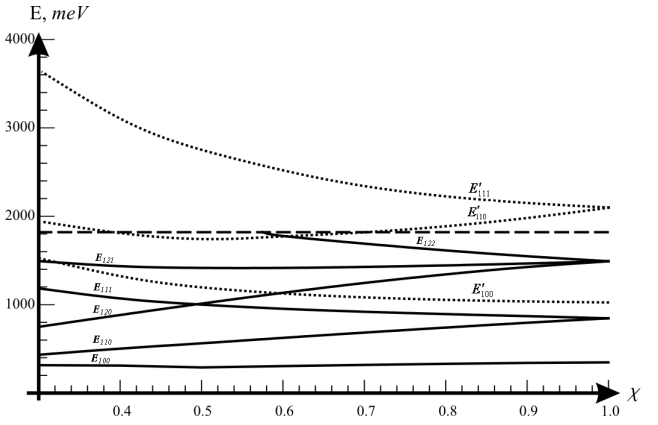

Fig. 4. Dependence of the electron energy in an ellipsoidal QD of the InAs/GaAs structure on the volume at a constant anisotropy coefficient ($\chi = 0.7$). Notation of lines is similar to that of Fig. 2

those calculated within the model of $U_0 = \infty$: E_{120} decreases, E_{121} has a minimum (at $\chi = 0.55$), while E_{122} grows and, at $\chi = 0.6$, exceeds the limits of a QW. For this QD, the difference between the ground energy levels in models of finite and infinite band gap is also more than 800 meV. As is seen from the figure, only state E'_{110} of all excited states of the model with finite potential U_0 fits into the real potential well region, though for $0.4 \leq \chi \leq 0.7$.

The results of calculations of the electron energy confined states depending on the nanocrystal volume at a given value of anisotropy are presented in Fig. 4 (InAs/GaAs) and in Fig. 5 (CdSe/glass). They show that if the volume rises, the electron energy falls monotonously for all energy levels irrespective of the type of a heterostructure and the quantum well model. At the given volume value, the electron energy values E_{nlm} in the model with finite U_0 are always less than E'_{nlm} of the model $U_0 = \infty$. Two physical quantities in the $E_{nlm} - E'_{nlm}$ value play an important role: the effective mass and the real band gap. In this connection, the model $U_0 = \infty$ in the region of medium-sized QDs ($V > 20$ nm^3) gives a rather good description of the CdSe/glass heterostructure due to the relatively large electron effective mass and the significant band gap. In the case of the InAs/GaAs heterostructure, even if the volume is greater by one order, such a model fits less. It is testified by the fact that, for $V \leq 400$ nm^3, the ground state energy E'_{100} ($U_0 = \infty$) is bigger than the real band gap.

The heterostructure has one more characteristic. The calculations show that, in a sufficiently large volume range, there exists an ideal QD: there is only one

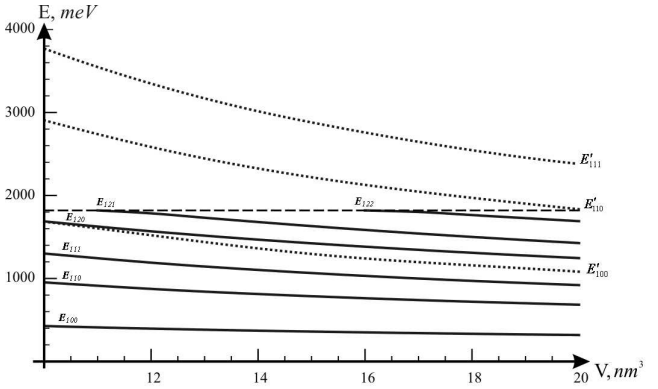

Fig. 5. Dependence of the electron energy in an ellipsoidal QD of the CdSe/glass structure on the volume at a constant anisotropy coefficient ($\chi = 0.7$). Notation of lines is similar to that of Fig. 2

confined state. In particular, at $\chi = 0.7$ (Fig. 4), this physical situation is realized provided 20 nm^3 $\leq V \leq$ 150 nm^3.

4. Conclusions

We have developed the theory of electron energy states in an ellipsoidal QD with regard for a finite gap at the interface. We considered two heterosystems which significantly differ in their band gaps and electron effective masses: InAs/GaAs and CdSe/glass. By the example of these heterosystems, we have studied the dependence of the ground-state energy, as well as those for some excited states of an electron, on the ellipsoid oblateness $\chi = \dfrac{b}{a}$ and a QD volume. We have analyzed

the results for a QD model with the real band gap U_0 and a model with $U_0 = \infty$. We also made comparison of the obtained data with those derived by other authors.

1. M.A. Kastner, Phys. Today **46**, 24 (1993).
2. A.D. Yoffe, Adv. Phys. **42**, 173 (1993).
3. A.D. Yoffe, Adv. Phys. **50**, 1 (2001).
4. A.I. Ekimov and A.A. Onushchenko, Pis'ma Zh. Eksp. Teor. Fiz. **34**, 363 (1981).
5. Al.L. Efros and A.L. Efros, Fiz. Tekhn. Polupr. **16**, 1209 (1982).
6. N.E. Kaputkina and Yu.E. Lozovik, Fiz. Tekhn. Polupr. **40**, 2134 (1998).
7. B. Szafran, J. Adamowski, and S. Bednarek, Physica E **4**, 1 (1999).
8. S. Bednarek, B. Szafran, and J. Adamowski, Phys. Rev. B **59**, 13036 (1999).
9. V.I. Boichuk and V.B. Holskyi, Zh. Fiz. Dosl. **8**, 122 (2004).
10. Y. Li, O. Voskoboynikov, C.P. Lee, S.M. Sze, and O. Tretyak, Eur. Phys. J. B /bf 28, 475 (2002).
11. V.I. Boichuk and V.B. Holskyi, Nauk. Zapysky NaUKMA **23**, 50 (2004).
12. V.I. Boichuk, I.V. Bilynskyi, and V.B. Holskyi, Ukr. Fiz. Zh. **48**, 56 (2003).
13. V.I. Boichuk and V.B. Holskyi, Fiz. Khim. Tverd. Tila **1**, 82 (2007).
14. G. Cantele, D. Ninno, and G. Iadonisi, J. Phys.: Condens. Matter. **12**, 9019 (2000).
15. G. Cantele, D. Ninno, and G. Iadonisi, Nano Lett. **1**, 121 (2001).
16. G. Cantele, D. Ninno, and G. Iadonisi, Phys. Rev. B **64**, 125325 (2002).
17. H. Leon, J.L. Marin, and R. Riera, Physica E **27**, 385 (2005).
18. G.G. Zehrya, O.V. Konstantinov, and A.V. Matvyeyevtsev, Fiz. Tekhn. Polupr. **37**, 334 (2003).
19. G.A. Korn and T.M. Korn, *Mathematical Handbook for Scientists and Engineers* (McGraw-Hill, New York, 1961).
20. Le-Wei Li, Xiao-Kang Kang, and Mook-Seng Leong, *Spheroidal Wave Functions in Electromagnetic Theory* (Wiley, New York, 2002).
21. V.A. Holovatsky and V.I. Gutsul, Zh. Fiz. Dosl. **10**, 108 (2006).
22. V.A. Holovatsky and V.I. Gutsul, Izv. Vuzov. Fiz. **12**, 55 (2006).
23. V.A. Holovatsky and V.I. Gutsul, Condens. Matter Phys. **10**, 61 (2007).

Received 03.07.07

ЕНЕРГЕТИЧНИЙ СПЕКТР ЕЛЕКТРОНА В КВАНТОВІЙ ТОЧЦІ ЕЛІПСОЇДАЛЬНОЇ ФОРМИ З ВРАХУВАННЯМ СКІНЧЕННОГО РОЗРИВУ ЗОН НА МЕЖІ СЕРЕДОВИЩ

В.І. Бойчук, В.Б. Гольський, Р.Ю. Кубай, Р.І. Лукін

Р е з ю м е

Розвинуто теорію для визначення енергетичного спектра заряду з врахуванням реального розриву зон для еліпсоїдальної квантової точки (КТ) довільного ступеня сплюснутості. Отримано залежності енергії зв'язаних станів частинки як від об'єму КТ, так і від ступеня анізотропії її форми. Показано, що із збільшенням анізотропії КТ енергія основного стану частинки зменшується, що не спостерігається в моделі нескінченної потенціальної ями. Також зростання анізотропії зумовлює появу першого збудженого стану в нанокристалі.