ELLIPSOIDAL AND LENS SHAPED QUANTUM DOTS

Eduard Kazaryan and Karen Dvoyan
Faculty of the Physics and Technology of Russian-Armenian University, Armenia

Keywords: ellipsoidal quantum dot, lens shaped quantum dot, electronic states, light absorption, adiabatic approximation, Lifshits-Slezov distribution, modified Pöschl-Teller potential.

Contents

Summary

Experimental realization of semiconductor quantum dots with nontrivial geometry induced a whole sequence of theoretical problems connected with the definition of specificity of energy spectrum and wave functions in similar systems. Ellipsoidal and lens-shaped quantum dots are remarkable systems which as limiting cases can transformed to either quantum wells or quantum wires. In suggested article the results of investigation of electronic and optical properties of strongly and weakly oblated (prolated) ellipsoidal quantum dots, two- and three dimensional quantum lenses as well as falciform quantum dots are presented. Thus, interband optical absorption of light in the ensemble of quantum dots with geometrical sizes dispersion Gaussian distribution in one case and within the framework of Lifshitz-Slezov model in another case is considered.

1. Introduction

Modern methods of growth of semiconductor nanostructures like MBE, MOCVD, gas epitaxy, Stranski-Krastanov growth method etc. have become basic methods for experimental realization of quantum dots (QDs) of various geometric shapes. Spherical (Figure 1), pyramidal, ellipsoidal (Figure 2), lens-shaped (Figure 3, 4 and 5), layered and other QDs are objects of great attention both theorists and experimentalists.

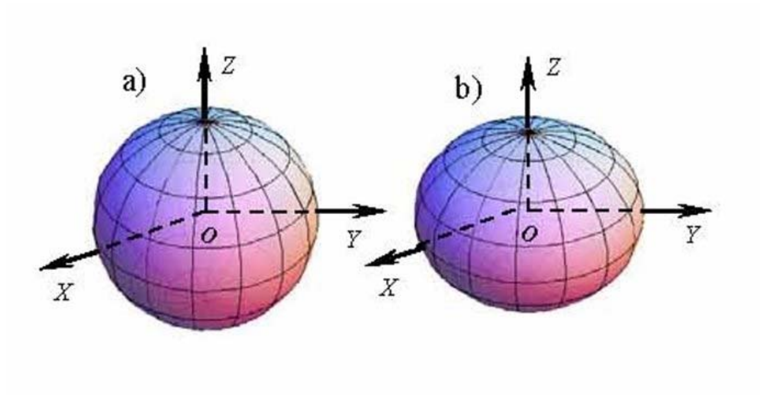

Figure 1. Deformation of the spherical QD into a spheroidal QD: a) spherical QD, b) spheroidal QD.

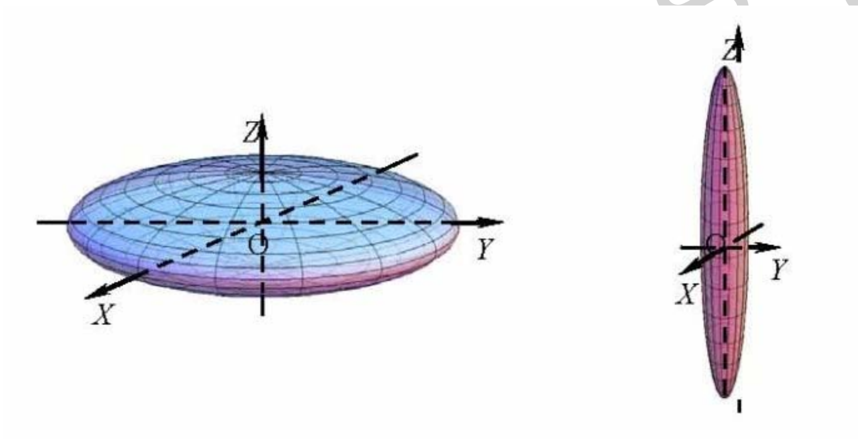

Figure 2. Strongly oblated and strongly prolated ellipsoidal QDs.

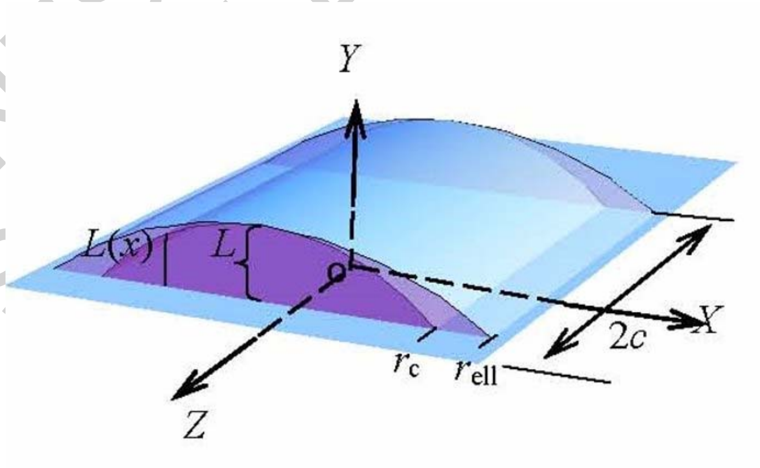

Figure 3. Cylindrical QD having thin lens-shaped cross-section.

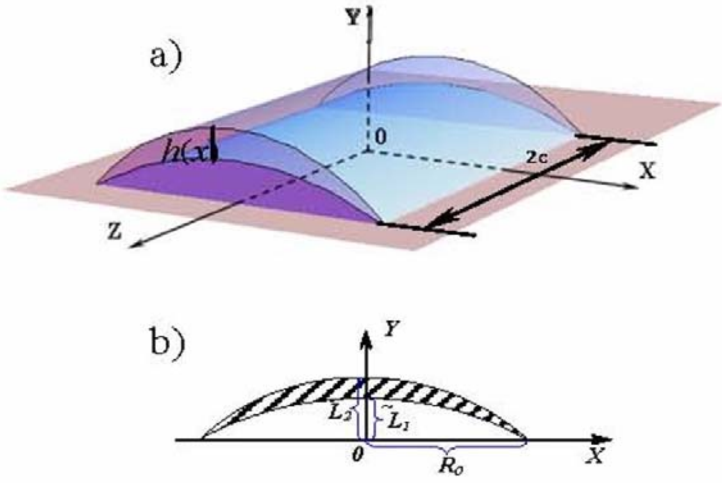

Figure 4. a) Cylindrical QD having thin falciform cross-section, b) cross-section of a cylindrical QD.

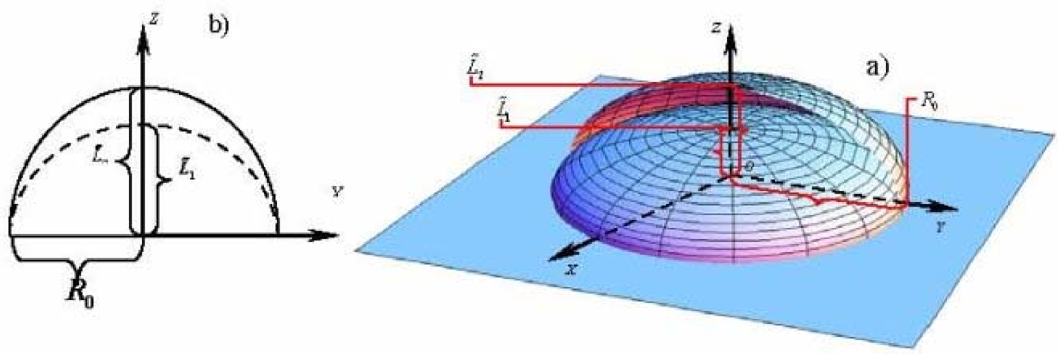

Figure 5. a) Thin ellipsoidal coated quantum lens, b) cross-section of a thin ellipsoidal coated quantum lens.

It is caused by applied importance of the received results of the physical properties research of the specified systems in modern opto- and nano-electronics. For the direct applications of these structures in semiconductor devices of new generation it is necessary to carry out the detailed analysis of physical processes occurring in them. The various analytical exact and approached methods are developed for the theoretical description of physical processes in QDs on the one hand, and numerical methods with another. Thus, there is an interesting situation connected with that circumstance that more complicated geometry of QD allows control its energy spectrum more flexibly by means of size quantization (SQ). However, non-triviality of QD geometry leads to complication of the analytical description of physical processes occurring in them. Thus, the description of properties of charge carriers (CCs) in QD with non-trivial geometry dictates application of specific methods of the approached analytical description of the specified systems. One of such effective methods is the adiabatic approximation.

The method is used when QD geometry allows the specific separation of Hamiltonian to fast and slow subsystems. The similar situation arises in case of QD with the form of strongly oblated or prolated revolution ellipsoids. In the inverse case of ellipsoidal systems with the form a little different from spherical, the perturbation theory methods are effectively used, allowing reducing non-perturbated problem to spherical symmetric task, and the perturbation caused by QD spheroidicity − to consider as the small correction.

Further investigations have shown that for understanding and modeling of QD electronic properties and their potential application, the problem of CC energy finding taking into account SQ, and also knowledge of possible optical transitions in them is essential. The mentioned circumstance in its turn depends in many respects on the external form and the sizes of QD, as well as on presence of external quantizing fields. Let's notice that theoretical and numerical modeling of physical processes in QD can stimulate creation of new structures and reduce number of the experiments necessary for construction of optimal structure of devices. Combination of SQ to external influence factors on system, first of all, external electrical and magnetic fields and caused by them quantization, allows to control the system dimensionality during the process of given nanostructure functioning. By other words, modern solid state physics is in the process of solving an important task: creation of materials with given in advance physical properties. For the realization of the mentioned task three basic ways can be noted: controlling the external shape of QD during growth process, controlling the process of confinement potential forming on the boundary of QD, and application of external electrical and magnetic fields. It is obvious that different combination of the mentioned methods can lead to desired optimal results.

At present intensively investigated semiconductor nanostructures similar to $GaAs/Ga_{1-x}Al_xAs$ type structures. During QD growth as a result of diffusion the formed confinement potential in most cases with the high accuracy is approximated by parabolic potential. However, the effective parabolic potential can arise in QD also because of its external shape. In particular, it is related to both of strongly oblated (prolated) ellipsoidal QDs and thin quantum lenses (QL). Note that influence of QD shape on the formed potential is a result of application of geometrical adiabatic approximation. Adiabatic approximation application for theoretical calculations on the basis of significant difference of QD sizes in different geometrical directions is an effective method for obtaining analytical results and their comparison with experimental data.

2. Electronic States in a Weakly Oblated (Prolated) Ellipsoidal QD (Impermeable Walls)

In recent years there were many theoretical and experimental works devoted to ellipsoidal symmetry QDs, in particular, investigation of CC physical properties in QD with spheroidal shape (revolution ellipsoid a little different from sphere). For the first time the quantum mechanical problem of finding CC energy states in a weakly oblated (prolated) ellipsoidal quantum well in the framework of the first order perturbation theory is formulated and solved by Migdal for drop model of atomic nucleus. In the considered problem, the spherical quantum well with impermeable walls is exposed to a small deformation (without volume change), taking the shape of weakly prolated or oblated revolution ellipsoid with semiaxes $a=b$ and c (Figure 1). With development of the newest technologies of semiconductor nanostructures growth made it real an application of the solution of this problem for QD of the above mentioned spheroidal form. Let's notice that often in real structures during a spherical QD growth unavoidable deformation leads to the obtainment of exactly spheroidal QDs. Equation of QD boundary $\frac{x_0^2+y_0^2}{a^2}+\frac{z_0^2}{c^2}=1$ after change of variables

$$x \to \frac{ax_0}{R_0},\ y \to \frac{ay_0}{R_0},\ z \to \frac{cz_0}{R_0}, \tag{1}$$

is transformed to the sphere equation of radius R_0: $x^2+y^2+z^2=R_0^2$.

By the same change the Hamiltonian of the particle $\hat{H}=-\frac{\hbar^2}{2\mu_0}\Delta$ is transformed to $\hat{H}=\hat{H}_0+\hat{V}$, where

$$\hat{H}_0=-\frac{\hbar^2}{2\mu_0}\Delta, \tag{2}$$

$$\hat{V}=-\frac{\hbar^2}{2\mu_0}\left(\left(\frac{R_0^2}{a^2}-1\right)\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+\left(\frac{R_0^2}{c^2}-1\right)\frac{\partial^2}{\partial z^2}\right), \tag{3}$$

μ_0 is effective mass of the particle, and Δ is Laplace operator. Thus, the problem of motion in the ellipsoidal well is reduced to the problem of motion in the spherical well. If the ellipsoid is a little differed from the sphere of radius $R_0=\left(a^2c\right)^{1/3}$, then $\hat{V}$ can be considered as a small perturbation. Introducing the parameter of ellipsoidality $\beta=\frac{c-a}{c}\ \left(|\beta|\ll 1\right)$, change of the energy levels of the particle in the first order of perturbation theory in comparison with the levels in the spherical well are sets as

$$\Delta E_{n,l,m}=4\beta\frac{l(l+1)}{(2l-1)(2l+3)}\left(\frac{m^2}{l(l+1)}-\frac{1}{3}\right)E_{n,l}^0. \tag{4}$$

where n,l,m are main, orbital and magnetic quantum numbers (QN), correspondingly, $E_{n,l}^0=\frac{\hbar^2\alpha_{n,l}^2}{2\mu_0R_0^2}$ is CC energy in a spherical QD, $\alpha_{n,l}$ are the roots of the first order Bessel function.

Distinctive result of CC spectrum in a QD with weakly expressed ellipsoidality is that the center of gravity of multiplet of energy states is not changed

$$\frac{1}{2l+1}\sum_{m=-l}^{l}E_{n,l,m}=E_{n,l}^0, \tag{5}$$

in case of spherical QD deformation without volume change. By other words, corrections to the energy for different values of QNs are entered with different signs, in the result of which spectrum is rearranged and the center of gravity of multiplet is not shifted. It should be noted that the situation is dramatically changed in case of the presence of hydrogen-like impurity in the center of a spheroidal QD. In that case the correction to the CC energy in the first order of perturbation theory equals to zero. Nonzero correction is arises only in the second order of perturbation theory, which is the result of size and Coulomb quantizations concurrence.

3. The model of finite deep rectangular ellipsoidal well

As it has been mentioned above the considered ellipsoidal QD is actual by the fact that as a result of deformation during the QD growth small deviations of QD external shape purely spherical are inevitable. From the geometrical point of view, revolution ellipsoids possess two parameters (semiaxes a and c), which represent itself as control levers for CC spectrum instead of one (radius R_0) in case of sphere. It is necessary to take into account potential difference finiteness inside and outside of QD to make the task closer to the real one. The first step towards the mentioned direction is consideration of a finite potential well case, which confinement has the following form

$$U(r)=\begin{cases}0; & r\le R_0\\ U_0; & r>R_0\end{cases} \tag{6}$$

where U_0 is the height of the well. In this case the energy correction in the first order of perturbation theory is defined by the following formula,

$$\begin{aligned}\Delta E_{n,l,m} &= 4\beta\left(E_{n,l}^0-\bar{U}_{nl}\right)\frac{l(l+1)}{(2l-1)(2l+3)}\left(\frac{m^2}{l(l+1)}-\frac{1}{3}\right)+\\ &\quad+3\hbar^2(\alpha_1-\alpha_2)\frac{6m^2-2l(l+1)}{4l(l+1)-3}R_{1nl}^2(R_0)R_0,\end{aligned} \tag{7}$$

where $\bar{U}_{nl}=U_0\int_{r_0}^{\infty}R_{2nl}^2r^2dr$, $\alpha_{1,2}=\dfrac{\beta}{3\mu_{1,2}}$, R_{1nl} and R_{2nl} are radial parts of wave function (WF), inside and outside of QD, correspondingly.

As it has already been mentioned above, the correction to the energy levels is linearly depends on the parameter of ellipsoidality β. The sign of correction depends not only on the sign of β but also on concrete QNs and more likely on their combination. It should be noted that as in the case of infinity deep well, correction to the ground state energy ($l=m=0$) is turned out zero. Also note that consideration of small ellipsoidality leads to the incomplete removal of energy degeneracy by QN m (double degeneracy of energetic levels remains the same). Numerical calculations for $GaAs/Ga_{1-x}Al_xAs$ structure are represented, where x is Al concentration: $\mu_1=0.067m_0$, $\mu_2=(0.067+0,083x)m_0$, m_0 is free electron mass. The considered calculations are presented in the units of effective Rydberg energy $E_{\mathrm{R}} = \dfrac{\hbar^2}{2\mu_1 a_{\mathrm{B}}^2}$, where a_{B} is the Bohr effective radius. For the selected structure the mentioned quantities are $E_{\mathrm{R}} = 5.275\mathrm{meV}$, $a_{\mathrm{B}} = 104\text{Å}$. Figure 6 represents the dependence of correction ΔE_{11} on the radius of QD in case of parameters of ellipsoidality $\beta = 0.1$ and $\beta = 0.25$. It can be seen from figure that for large values of radius ΔE_{11} tends to zero.

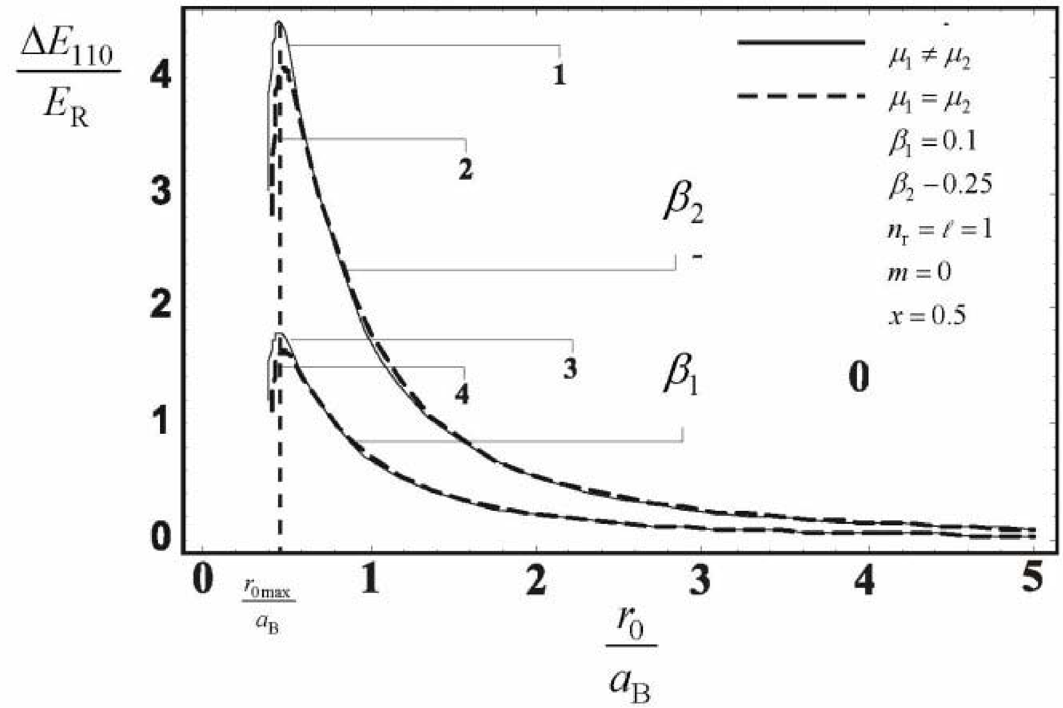

Figure 6. Dependence of the energy correction ΔE_{110} on the QD radius for various values of parameter of ellipsoidality β.

Decreasing of QD radius leads to correction increasing, and after getting its maximal value, it dramatically decreases. Note, that $\Delta E_{11,\max}(\beta = 0.25) = 4.469 E_{\mathrm{R}}$, $\Delta E_{11,\max}(\beta = 0.1) = 1.787 E_{\mathrm{R}}$ is corresponding to the radius value $r_{0,\max} = 0.454 a_{\mathrm{B}}$. It is explained by the fact that in case of large values of radius the particle is localized far away from the walls of QD, which influence is weak. In case of smaller values of radius, ellipsoidality contribution increases.

However, further decreasing of radius leads to the localization of the particle outside of QD and, naturally, boundary ellipsoidality weaker affected the CC energy. Similar situation arises in QD in case of solving the problem of finding binding energy in the Coulomb field.

Note that in case of $\mu_1 \neq \mu_2$ the same results are obtained with shifted to top curves, which is explained by the contribution of CC effective masses difference.

-
-
-

Bibliography

Abramovitz M., Stigan I. (1979). *Handbook on Special Functions*, 830 pp. Nauka, Moscow. [A comprehensive description of properties of various classes of special functions].

Alferov Zh. (1998). The history and future of semiconductor heterostructures. *Semiconductors* **32**, pp. 1-14. [A comprehensive review of the physical properties, growing methods and applications of semiconductor heterostructures].

Askerov B. M. (1985). *Electronic transport phenomena in semiconductors*, 394 pp. Nauka, Moscow. [This book presents the kinetic phenomena in bulk semiconductors].

Bimberg D., Grundman M.and Ledentsov N. (1999). *Quantum dot heterostructures*, 328 pp. Wiley, New-York. [A comprehensive discussion of electronic, optical, kinetic, thermal etc. properties of semiconductor quantum dots].

Bimberg D., Grundmann M., and Ledentsov N. (1998). Growth, spectroscopy and laser application of self-ordered III-V quantum dots. *MRS Bulletin* **23**, pp. 31-34. [A famous article of self-ordered III-V quantum dots based lasers].

Chakraborty T. (1999). *Quantum dots*, 348 pp. Elsevier, Amsterdam. [A comprehensive discussion of quantum confinement effects, impurity and excitonic states as well as many-electron states in semiconductor quantum dots].

Chanchapanyan (Tshantshapanyan) A.A. (2005). Light absorption in a cylindrical quantum dot with lens-shaped creoss-section. Proceedings of the Fifth International Conference *"Semiconductor Micro- and Nanoelectronics"*. Aghveran, Armenia, 2005, pp.189-192.[A paper devoted to the electronic and optical properties of a lens-shaped geometry quantum dot].

Dvoyan K.G., Kazaryan E.M., and Petrosyan L.S. (2005). Electronic states in quantum dots with ellipsoidal symmetry. *Physica E: Low-dimensional Systems and Nanostructures*, Vol. **28**, issue 4, pp. 333-338. [A paper devoted to the electronic properties of the ellipsoidal quantum dot with a finite potential].

Dvoyan K.G., Hayrapetyan D.B., Kazaryan E.M., Tshantshapanyan A.A. (2007). Electron States and Light Absorption in Strongly Oblate and Strongly Prolate Ellipsoidal Quantum Dots in Presence of Electrical and Magnetic Fields. *Nanoscale Research Letters*, Vol. **2**, Issue 12, pp. 601-608. [A manuscript about the electronic properties and light absorption of the ellipsoidal geometry quantum dots under influence of electrical and magnetic fields].

Dvoyan K.G., Kazaryan E.M.,. Tshantshapanyan A.A. (2009). Light absorption in coated ellipsoidal quantum lenses. *Journal of Materials Science: Materials in Electronics* Vol. **20**, Number 6, pp. 491-498. [Discussion of the electronic properties and light absorption of the coated lens shaped quantum dots].

Dvoyan K.G., Hayrapetyan D.B., Kazaryan E.M., Tshantshapanyan A.A. (2009). Electronic states and light absorption in a cylindrical quantum dot having thin falciform cross section. *Nanoscale Research Letters* **4**, pp. 130-137. [This presents the electronic states and interband transitions in cylindrical quantum dot with falciform cross section].

Efros Al. and. Efros A (1982). Interband light absorption in semiconductor sphere. *Semiconductors* **16**, pp. 1209-1214. [Pioneering paper about optical absorption in spherical quantum dots for various regime of size-quantization].

Ehrenberg W.,. Siday R. E (1949). The Refractive Index in Electron Optics and the Principles of Dynamics. *Proc. Phys. Soc. London Sect. B* **62**, pp. 8-21. [Pioneering paper related to the role of electromagnetic potentials in quantum theory].

Flugge S. (1971). *Practical Quantum Mechanics Part 2*, 287 pp. Springer, Germany. [Remarkable collection of quantum mechanical problems].

Galitsky V.M., Karnakov B.M., Kogan V.I. (1981). *Practical quantum mechanics*, 369 pp. Nauka, Moscow. [Well known collection of quantum mechanical problems].

Gasparyan A.S., Kazaryan E.M. (1997). To the theory of impurity states in ellipsoidal microcrystals. Journal of Contemporary Physics, vol. **32**, pp. 130-136. [This presents the electronic and impurity states of the ellipsoidal quantum dot].

Han D., Asryan L. (2008). Characteristic temperature of a tunneling-injection quantum dot laser: Effect of out-tunneling from quantum dots. Solid-State Electronics, vol. **52**, issue 10, pp. 1674-1679. [This studies the temperature dependence of a tunneling-injection quantum dot laser].

Harrison P. (2005). *Quantum Wells, Wires and Dots: Theoretical and Computational Physics*, 482 pp. University of Leeds, Leeds, United Kingdom [A famous book devoted to the electronic, optical, kinetic, thermal etc. properties of semiconductor quantum dots].

Juharyan L.A., Kazaryan E.M., Petrosyan L.S. (2006). Electronic states and interband light absorption in semi-spherical quantum dot under the influence of strong magnetic field. *Solid State Communications* **139**, pp. 537-540. [This is a case study reporting on the electronic states and interband transitions in a semispherical quantum dot].

Kazaryan E.M., Petrosyan S.G. (2005). *Physical principles of semiconductor nanoelectronics*, 424 pp. Izd. “RAU”. [A comprehensive discussion of the electronic, optical, kinetic, etc. properties of low dimensional semiconductor structures].

Lifshits I.M., Slezov V.V. (1958). About kinetics of supersaturated solid solution diffusion disintegration. *JETP*, V. **35**, pp. 479-488. [Pioneering paper about size dispersion influence on supersaturated solid solution quantum dots growth].

Landau L. D., Lifshits E. M. (1989), *Quantum Mechanics*, 689 pp. Nauka, Moscow. [Fundamental textbook of quantum mechanics].

Lew Yan Voon L.C., Willatzen M. (2004). On triaxial ellipsoidal quantum dots. *J. Phys.: Condens. Matter* **16**, pp. 1087–1093, 2004. [This studies the electronic states of triaxial ellipsoidal quantum dots].

Rosencher E., Bois P. (1991). Model system for optical nonlinearities: Asymmetric quantum wells. *Physical Review B*, **44**, pp. 11315-11327. [This studies the generation of a second harmonic in the asymmetric quantum wells].

Trallero-Herrero C., Trallero-Giner C., Ulloa S.E.,. Perez-Alvarez R. (2001). Electronic states in a cylindrical quantum lens: Quantum chaos for decreasing system symmetry. *Physical Review E*, Volume **64**, Issue 5, November, p.056237. [A paper devoted to the electronic properties of a lens-shaped quantum dots].

Biographical Sketches

Eduard Kazaryan is deputy rector of Russian-Armenian (Slavic) University, head of the chair of the General and theoretical physics of the department of Physics and technology, Doctor of physical and mathematical sciences, professor. He graduated from the Moscow State University in 1965. The PhD thesis defended in 1971, and the doctoral thesis – in 1981. Received the rank of professor in 1983. Elected as the full member of National Academy of Science of Armenia in 1996. Scientific researches are devoted to the solid state physics, physics of exciton, low-dimensional semiconductor physics. He is coauthor of monograph “Physical foundations of nanoelectronics” (2005, in Armenian). He is author of more than 140 articles devoted to the above mentioned subject area. Prof. Kazaryan is awarded by the Republic of Armenia Presidents’ Award in the field of Physics for papers’ series of the theory of electronic and optical properties of nanostructures in 2008.

Karen Dvoyan is assistant professor at the chair of the General and theoretical physics of the department of Physics and technology of the Russian-Armenian (Slavic) University, candidate of the physical and mathematical sciences (PhD). He graduated from the Yerevan State University in 1997. The PhD thesis defended in 2001. Scientific interests' field includes the theory of electronic and optical properties of the semiconductor nanostructures. Researches are devoted to the theory of electronic, excitonic and impurity states and also optical absorption in the ellipsoidal, cylindrical and lens shaped quantum dots both in the presence and in the absence of the external fields. He is author of more than 30 articles devoted to the above mentioned subject area. Dr. Dvoyan is awarded by the Republic of Armenia Presidents' Award in the field of Physics for papers' series of the theory of electronic and optical properties of nanostructures in 2008.