Direct interband absorption of light in the ensemble of cylindrical quantum dots' having strongly oblate elliptical cross-section

Karen G. Dvoyan*
[1]Russian-Armenian (Slavic) University, H. Emin 123, Yerevan 0051, Armenia

ABSTRACT

In the framework of adiabatic approximation the energy levels and direct interband absorption of light in the ensemble of cylindrical quantum dots' having strongly oblate elliptical cross-section are studied. Analytical expressions for the energy spectrum and wave functions of the electron are obtained. For the "slow" subsystem effective potential approximation, parabolic and modified Pöschl-Teller potentials are used. Low-energy levels in the energy spectrum are shown to be equidistant in both cases. Modified Pöschl-Teller potential approximation allows taking into account violation of equidistance of energy levels for higher exited states. Absorption coefficient and edge frequencies are obtained in the strong size quantization regime. Corresponding selection rules for quantum transitions are found.

Keywords: cylindrical quantum dot, ensemble, modified Pöschel-Teller potential, absorption of light

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, pyramidal, ellipsoidal, lens-shaped, layered and other QDs are objects of great attention both theorists and experimentalists[1-5]. It is caused by applied importance of the received results of the physical properties research of the specified systems in modern opto- and nanoelectronics. 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, it is interesting, 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[6]. 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. 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 cylindrical QD having strongly oblate elliptical cross-section.

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 with the high accuracy is approximated by parabolic potential in most cases. However, the effective parabolic potential can arise in QD also because of its external shape. Note that influence of QD shape on the formed potential is a result of application of geometrical adiabatic approximation. Further investigations have shown that for understanding and modeling of QD electronic properties for their potential applications, 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 on the external shape and the sizes of QD in many respects.

In this paper, the electron states and direct interband absorption of light in a cylindrical QD having strongly oblate elliptical cross-section at the strong SQ regimes is considered. For the "slow" subsystem, parabolic and modified Pöschl-Teller (MPT) effective potentials are used. Absorption edge and absorption coefficient are also considered. To facilitate

*dvoyan@gmail.com

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the comparison of obtained results with the probable experimental data, size dispersion distribution of growing QDs

by the small semiaxis by two experimentally realizing distribution functions have been taken into account. Distribution function of Lifshits-Slezov has been considered in the first model and Gaussian distribution function has been considered in the second case.

2. THEORY

2.1 Electronic states

Consider the motion of a charged particle (an electron, or a hole) in a cylindrical QD having strongly oblate elliptical cross-section (see Fig. 1). The particle potential energy can be written as

$$U(x,y,z)=\begin{cases}0, \dfrac{x^2}{a^2}+\dfrac{y^2}{b^2}\le 1, \cup|z|\le c \\ \infty, \dfrac{x^2}{a^2}+\dfrac{y^2}{b^2}>1, \cup|z|>c\end{cases}, a\ll b, \tag{1}$$

where a and b – are minor and major semiaxis of the cross-section of QD, respectively, $2c$ – is a cylinder height. In the regime of strong SQ, the energy of the Coulomb interaction between the electron and hole is much less than the energy caused by the SQ contribution. In this approximation, the Coulomb interaction can be neglected. Then, the problem is reduced to the determination of separate energy states of the electron and hole. The system Hamiltonian is

$$\hat{\mathrm{H}}=-\frac{\hbar^2}{2m_e^*}\left[\frac{\partial^2}{\partial X^2}+\frac{\partial^2}{\partial Y^2}+\frac{\partial^2}{\partial Z^2}\right]+U(X,Y,Z), \tag{2}$$

where m_e^* is an electron effective mass.

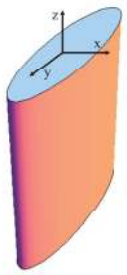

Fig. 1. Cylindrical QD having strongly oblate elliptical cross-section.

The particular shape of QD suggests that motion of an electron the X-direction should be faster than in Y-direction, a fact making possible adiabatic approximation. The system Hamiltonian (2) in this case can be represented as a sum of "fast" $\hat{H}_x$, "slow" $\hat{H}_y$ subsystems and Z-direction $\hat{H}_z$ Hamiltonians, being expressed through dimensionless quantities:

$$\hat{H}=\hat{H}_x+\hat{H}_y+\hat{H}_z, \tag{3}$$

with $\hat{H}_x = -\frac{\partial^2}{\partial x^2}$, $\hat{H}_y = -\frac{\partial^2}{\partial y^2}$, $\hat{H}_z = -\frac{\partial^2}{\partial z^2}$.Here $x = \frac{X}{a_B}$, $y = \frac{Y}{a_B}$, $z = \frac{Z}{a_B}$, $\hat{H} = \frac{\hat{\mathrm{H}}}{E_R}$ with $E_R = \frac{\hbar^2}{2m_e a_B^2}$ being an effective Rydberg energy, $a_B = \frac{\kappa\hbar^2}{m_e e^2}$ is an effective Bohr radius of electron, and κ is dielectric constant of the medium. The wave function (WF) can be sought in the form of

$$\Psi(x,y,z) = \chi(z) f(x;y) \Phi(y). \tag{4}$$

As a result of a cylindrical QD having strongly oblate elliptical cross-section problem symmetry, the motion of electron in the Z-direction is separated. The WFs and energy are given by the following expressions:

$$\chi(z) = \sqrt{\frac{1}{c}} \sin\left(\frac{\pi n_z}{2c} z + \frac{\pi n_z}{2}\right), \quad \varepsilon_z = \frac{\pi^2 n_z^2}{4c^2}, \quad n_z = 1,2,\ldots, \tag{5}$$

n_z – is quantum number (QN).

At a fixed value of the "slow" subsystem y coordinate, the electron motion is localized inside one-dimensional effective potential well $L(y)$ having a profile:

$$L(y) = 2a\sqrt{1 - \frac{y^2}{b^2}}. \tag{6}$$

The Schrödinger equation for the "fast" subsystem has the form

$$f''(x;y) + \varepsilon_x(y) f(x;y) = 0. \tag{7}$$

After simple transformations, one can obtain the following expressions for the "fast" subsystem WFs and the electron energy, respectively:

$$f(x;y) = \sqrt{\frac{1}{L(y)}} \sin\left(\frac{\pi n_x}{L(y)} z + \frac{\pi n_x}{2}\right), \tag{8}$$

$$\varepsilon_x(y) = \frac{\pi^2 n_x^2}{L^2(y)}, \tag{9}$$

where n_x – is QN of "fast " subsystem.

The expression (9) enters as a potential in the Schrödinger equation for the "slow" subsystem, but the Schrödinger equation with such effective potential is not analytically solvable one. That is why this problem has been solved using adiabatic approach. Two models for the "slow" subsystem effective potentials are used.

2.2 Parabolic Approximation

The "slow" subsystem potential energy is formed by elliptic geometry of the QD cross-section, which allows using of adiabatic approximation. Namely, we use the condition $|y| \ll b$, which means that for the lower levels of the spectrum the electron is localized in the domain near the geometric center of elliptical cross-section. This condition holds for the low energy states. For the higher excited energy states the adiabatic approximation is not applicable any more. Based on this, we expand expression (9) into a series

$$\varepsilon_x(y) = V_{Par}(y) \approx \varepsilon_0 + \beta^2 y^2, \tag{10}$$

where $\varepsilon_0 = \frac{\pi^2 n_x^2}{4a^2}$, $\beta = \frac{\pi n_x}{2ab}$. The expression (10) enters as an effective potential in the Schrödinger equation for the "slow" subsystem:

$$\Phi''(y) + \left(\varepsilon_{xy} - \varepsilon_0 - \beta^2 y^2\right)\Phi(y) = 0. \tag{11}$$

Solving this relation we obtain the expressions for the "slow" subsystem WFs and energy:

$$\Phi(y) = Exp\left(-\beta y^2/2\right) H_{n_y}\left(\sqrt{\beta} y\right) \tag{12}$$

$$\varepsilon_{xy} = \varepsilon_0 + 2\beta\left(n_y + \frac{1}{2}\right), \tag{13}$$

where $H_{n_y}\left(\sqrt{\beta} y\right)$ – are Hermite polynomials, n_y – is oscillatory QN of the "slow" subsystem.

For the total WFs and energy of the electron we obtain, respectively:

$$\Psi(x,y,z) = \sqrt{\frac{1}{c}}\sin\left(\frac{\pi n_z}{2c} z + \frac{\pi n_z}{2}\right)\sqrt{\frac{1}{L(y)}}\sin\left(\frac{\pi n_x}{L(y)} z + \frac{\pi n_x}{2}\right)\times$$
$$\times\left(\frac{\beta}{\pi}\right)^{1/4}\frac{1}{\sqrt{2^{n_y} n_y!}} Exp\left(-\beta y^2/2\right) H_{n_y}\left(\sqrt{\beta} y\right), \tag{14}$$

$$\varepsilon = \frac{\pi^2 n_z^2}{4c^2} + \frac{\pi^2 n_x^2}{4a^2} + \frac{\pi n_x}{ab}\left(n_y + \frac{1}{2}\right). \tag{15}$$

It is interesting to note that the localization radius of the electron, $r_{loc} \sim (\beta)^{-1/2}$, depends only on the geometrical parameters of QD, and does not depend on the electron mass, as in the case of the ordinary oscillator.

2.3 Modified Pöschl-Teller Potential Approximation

As it was mentioned above, the adiabatic approximation is applicable only for obtaining the expressions for lower levels of the energy spectrum. Parabolic potential obtained by Taylor series of the energy expression for the "fast" subsystem creates a family of equidistant levels in the energy spectrum. One should observe that each energy level of the "fast" subsystem has its own family of equidistant levels with gaps depending on the QN of the particular "fast" subsystem. Actually, however, only two or three lower energy levels are split into equidistant level subsystems; for higher levels of the "fast" subsystem the sublevels are not more equidistant.

We suggest more realistic model of one-dimensional effective potential in form of MPT potential[7] (see Fig.2). In dimensionless quantities this potential has the following form:

$$\varepsilon_x(y) = V_{PT}(y) \approx \frac{\pi^2 n_x^2}{4a^2} - \frac{U_0}{\left(\mathrm{c}\,h\left(y/\gamma\right)\right)^2} + U_0. \tag{16}$$

Here U_0 and γ are parameters depending on the QN n_x of the "fast" subsystem, respectively describing the depth and width of corresponding quantum well. Selection of this potential is explained by the fact that Taylor expression of (16) potential is parabolic for small values of y, as in (10). On the other hand, at higher values of y coordinate the

discrepancy of MPT potential from parabolic is increased. Thus, violation of equidistance for "slow" subsystem of energy levels may be taken into account.

Solving Schrödinger equation of the "slow" subsystem with the MPT potential, after some transformations one can obtain for the electron total energy:

$$\varepsilon_{PT} = \frac{\pi^2 n_z^2}{4c^2} + \frac{\pi^2 n_x^2}{4a^2} + \frac{U_0}{4\gamma^2}\left(-1 - 2n_y + \sqrt{1 + 4U_0\gamma^2}\right)^2. \tag{17}$$

For small values of coordinate y the potential (16) assumes a form of approximated parabolic potential:

$$V_{AP}^{P}(y) \approx \frac{\pi^2 n_x^2}{4a^2} + \frac{U_0 y^2}{\gamma^2}. \tag{18}$$

Further solution of the Schrödinger equation for the "slow" subsystem with the potential (18) leads to the following expression for the electron energy:

$$\varepsilon_{AP}^{P} = \frac{\pi^2 n_z^2}{4c^2} + \frac{\pi^2 n_x^2}{4a^2} + \frac{2\sqrt{U_0}}{\gamma}\left(n_y + \frac{1}{2}\right), \tag{19}$$

which fully agrees with the result (15).

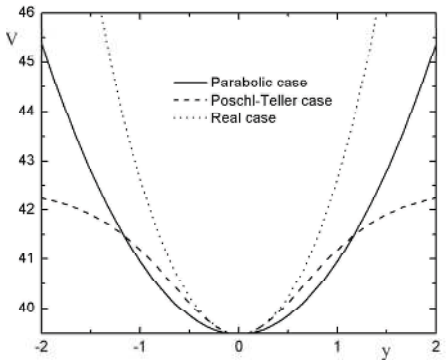

Fig. 2. Dependences of a real, parabolic and MPT potentials on coordinate.

2.4 Direct Interband Light Absorption

Let us proceed to consideration of the direct interband absorption of light in a cylindrical QD having strongly oblate elliptical cross-section in the regime of strong SQ. Consider the case of a heavy hole, $m_e^* \ll m_h^*$. The absorption coefficient is defined by the expression[8]

$$K = A\sum_{\nu,\nu'}\left|\int \Psi_\nu^e \Psi_{\nu'}^h d\vec{r}\right|^2 \delta\left(\hbar\Omega - E_g - E_\nu^e - E_{\nu'}^h\right), \tag{20}$$

Where ν and ν' are sets of QNs corresponding to the electron and heavy hole, E_g is the forbidden gap width in the bulk semiconductor, Ω is the incident light frequency, and A is a quantity proportional to the square of matrix element in decomposition over Bloch functions[9].

In the regime of strong SQ, for the absorption edges $W_{110}^{P(PT)} = \dfrac{\hbar\Omega_{110}}{E_g}$ in the cases of parabolic and MPT potentials, we obtain, respectively:

$$W_{110}^{P}=1+\frac{M}{\mu}\frac{d^2}{a_B^2}\left(\frac{\pi^2}{4c^2}+\frac{\pi^2}{4a^2}+\frac{\pi}{2ab}\right). \tag{21}$$

$$W_{110}^{PT}=1+\frac{M}{\mu}\frac{d^2}{a_B^2}\left(\frac{\pi^2}{4c^2}+\frac{\pi^2}{4a^2}+\frac{U_0}{4\gamma^2}\left(-1+\sqrt{1+4U_0\gamma^2}\right)^2\right). \tag{22}$$

Here as a length unit we use the expression $d=\frac{\hbar}{\sqrt{2\mu E_g}}$, $\mu=\frac{m_e^* m_h^*}{m_e^*+m_h^*}$ – is the reduced mass of electron and hole, $M=m_e^*+m_h^*$.

For comparison of the obtained results with experimental data, one has to take into account the random character of cylindrical QDs having strongly oblate elliptical cross-section dimensions (or semiaxis) obtained in the growth process. The absorption coefficient should be multiplied by concentration of QDs. Instead of distinct absorption lines, taking into account of size dispersion will give a series of fuzzy maximums. In the first model, we use the Lifshits–Slezov distribution function[10]:

$$P(u)=\begin{cases}\dfrac{3^4 eu^2 Exp\left(\left(-1/(1-2u)/3\right)\right)}{2^{5/3}(u+3)^{7/3}(3/2-u)^{11/3}} & u<3/2\\ 0 & u>3/2\end{cases},\quad u=\frac{a}{\overline{a}}\quad , \tag{23}$$

where $\overline{a}$ – is some average value of the semiaxis. In the second model, the Gaussian distribution function is used[11]:

$$P(u)=A_0 Exp\left(-\frac{(u-1)^2}{\sigma/\overline{a}}\right). \tag{24}$$

3. DISCUSSION OF RESULTS

As one can see from the electron energy spectrum expressions (15) and (19), the energy levels inside the cylindrical QDs having strongly oblate elliptical cross-section are equidistant. More correctly, each level of the "fast" subsystem has its own family of equidistant energy levels created by the "slow" subsystem. The obtained result is valid only for the low spectrum levels (i.e. small QNs), which is a consequence of the adiabatic approximation. It is important that approximation of one-dimensional energy expression by a MPT potential makes possible taking into account the energy levels non-equidistance at higher energy values. One can see from Fig. 2. that the effective one-dimensional potential is well approximated by the MPT potential for the small values of coordinate. As the y-coordinate grows, the difference between the course of real and approximated potentials becomes evident, both for the MPT and parabolic potentials.

Numerical calculation results were made for a QD consisting of $GaAs$ with the following parameters: $m_e^*=0.067m_0, m_e^*=0{,}12m_h^*$, $E_R=5.275meV$, $a_B=104$ Å, $E_g=1.43eV$, m_0 – is a free electron mass.

Fig. 3. represents the dependence of the first two equidistant families of electron energy in a cylindrical QD on the minor semiaxis a of the QD elliptical cross-section at a fixed value of the other geometrical parameters of QD for the case of parabolic approximation. The energy spectrum is equidistant, as expected. Grow in the parameter a results in a width increase of elliptical cross-section of the cylindrical QD, which in its turn decreases the electron energy due to SQ.

Fig.4 illustrates the dependence of the electron energy of "slow" subsystem in a cylindrical QD on the elliptical cross-section minor semiaxis at a fixed value of the major semiaxis for both MPT potential approximated by parabolic and

parabolic potential cases. In other words, we compare results obtained from relations (19) with those from (15). From Fig. 4. it is easily seen that the energy levels are equidistant in both cases, since for small values of the y -coordinate it is sufficient to keep only quadratic terms in the Taylor series of the MPT potential, what leads to practical coincidence with parabolic potential.

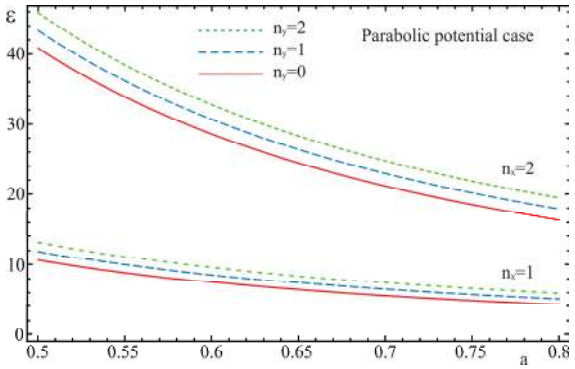

Fig. 3. The first two equidistant energy families dependences on the minor semiaxis a of the cylindrical QD elliptical cross-section.

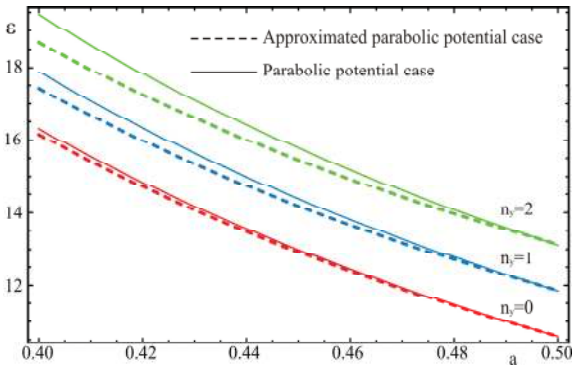

Fig. 4. The energy dependence on the minor semiaxis a at a fixed value of the major semiaxis b .

The electron energy dependence on the parameter γ, describing the quantum well width of MPT potential, is represented on the Fig. 5. Note that the energy levels are not more equidistant. Increase in parameter γ (quantum well width) leads to decrease of the electron energy as a consequence of confinement reduction. As it is seen from the figure, curves corresponding to the cases of the MPT and approximated parabolic potentials, are merged with γ increasing. This explains by the fact that the electron energy becomes less "sensitive" to the confinement potential profile for the wider potential well.

The electron energy dependence on the quantum well depth parameter U_0 in the cases of the MPT potential and approximated parabolic potentials is represented on the Fig. 6. With potential well depth increasing, the electron energy increases, which is also explained by SQ impact increase.

The difference between the electron energy on the parameter U_0 obtained for the approximated parabolic potential and MPT potential cases is shown on the Fig. 7. The curve corresponding to the approximated parabolic potential is

positioned higher than the MPT potential curve (see inset in Fig. 7.). As a result, the mentioned difference of energies increases with parameter U_0 increase.

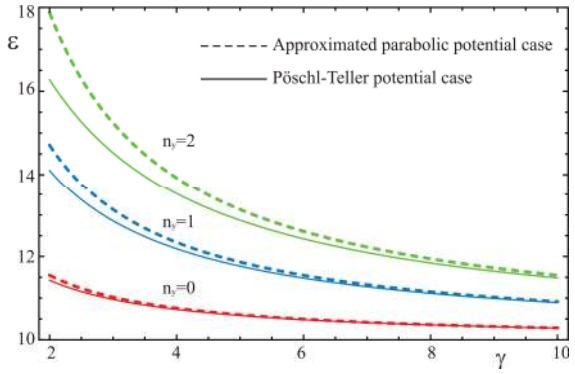

Fig. 5. The energy dependence on the quantum well width parameter γ.

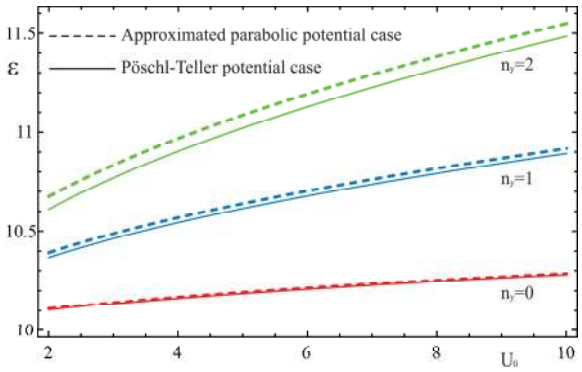

Fig. 6. The energy dependence on the potential well depth parameter U_0.

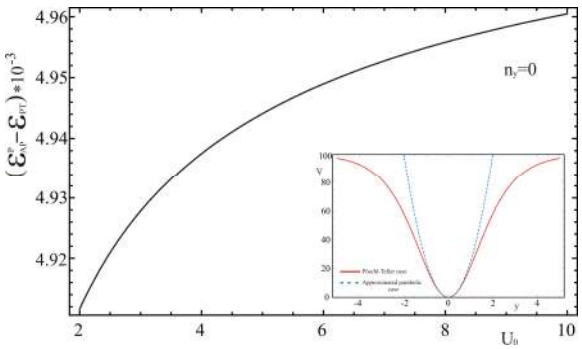

Fig. 7. The dependence of the electron energy difference on the potential well depth parameter U_0 for the cases of approximated parabolic potential and MPT potential.

Consider now the selection rules for transitions between the levels with different QNs. For parabolic approximation for the Z-direction QN the transitions between the levels with $n_z = n_z'$ are allowed, while for the QN of the fast subsystem – the transitions with $n_x = n_x'$. For the oscillatory QN the transitions for the levels with $n_y = n_y'$ are allowed. For MPT

potential approximation case the selection rules are the following: $n_z = n_z'$. For other QNs transitions between energy levels are admissible.

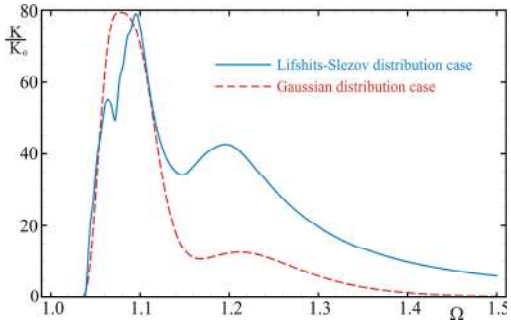

Fig. 8. Dependence of the absorption coefficient on the incident light frequency.

Finally, Fig. 8. illustrates the dependence of absorption coefficient K on the frequency of incident light, for the ensemble of cylindrical QDs having elliptical cross-section in strong SQ regime. As it mentioned above, instead of distinct absorption lines, the size dispersion consideration will give a series of fuzzy maximums. Note that both in the model of Gaussian and in the model of Lifshits-Slezov distributions a single distinctly expressed maximum of absorption is observed. When the light frequency increased, the second weakly expressed maximum is seen. Further increase of the incident light frequency results in a fall of absorption coefficient. As it is seen from the figure, on the curve corresponding to the Lifshits-Slezov distribution, the relatively small maximum is observed. This is a result of distribution asymmetry by geometrical size dispersion.

4. CONCLUSION

In this paper we have theoretically obtained that the energy spectrum inside the cylindrical QD having strongly oblate elliptical cross-section is equidistant for low levels. The "slow" subsystem effective potential is successfully approximated with parabolic and MPT potentials. Absorption coefficient for QD's ensemble is obtained for MPT potential approximation for the two types of experimentally realizing distributions by geometrical size dispersion: Lifshits-Slezov and Gaussian. The absorption edge frequencies are obtained in the strong size quantization regime for the QD in the cases both parabolic and MPT potential approximations. Corresponding selection rules for quantum transitions are also found. This theoretical investigation of cylindrical QD's ensemble having strongly oblate elliptical cross-section be used for applications in photonics.

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