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*Talk given by L. S. Petrosyan at the IX International Conference on Symmetry Methods in Physics, Yerevan, Armenia, July 3–8, 2001.

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Electronic states in parabolic quantum dot, taking into account boundary conditions, were studied. The threshold habit of level appearance inside the dot was discovered. Electron energy dependence on QD radius and confinement potential height was studied. The discussion of causes of removal of the random degeneration $U(3)$ was considered, as the consequence of modernization of the confinement potential.

Исследуются электронные состояния в параболической точке квантования с учетом граничных условий. Изучается пороговое поведение образования уровней в этой точке. Исследована зависимость энергии электрона от QD-радиуса и высоты потенциала конфайнмента. Представлено обсуждение исчезновения случайного вырождения $U(3)$ как следствия модернизации потенциала конфайнмента.

INTRODUCTION

The modern opportunities of nanotechnologies have made it possible to grow size-quantized structures of various dimensions and geometrical forms. One of the objects of this class under intensive research for today are the semiconductor quantum dots (QD) grown in various dielectric media. The important feature of QD is complete quantization of the charge carriers' (CC) energy taking place in them. They remind real atoms by this feature and consequently are frequently called «artificial atoms». Complete quantization of a CC spectrum in QD allows one to use them as a working body (active environment) for semiconductor lasers with unique properties (high stability, ultrahigh values of amplification of a material). For the theoretical description of physical processes occurring in QD there is a necessity of construction of QD mathematical model. Else, it is necessary to present maximum precisely the quantum-mechanichal model of a dot, in which is CC. Really, you see this term in the

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Schroedinger equation, for CC, defines symmetry of a concrete problem (effective mass is considered isotropic), so the degree of degeneracy of CC energy levels, too.

It is necessary to note that the shape of this potential in many respects depends on the method of QD growing, too [1]. The example of revealing of the generalization of Kohn's theorem is remarkable [2–4] in this respect in the case of QD. Especially due to correct mathematical model of confinement potential ($U_{\mathrm{conf}} = \gamma r^2$) it was possible to put theoretical basis under the generalization of this theorem on a case of size-quantized systems.

On the other hand, it is clear, that the shape of confinement potential $U_{\mathrm{conf}} = \gamma r^2$ can be used for the down levels. Coming near to a semiconductor-dielectric border, the trend of potential curve becomes distinct from parabolic. The simplest QD models taking into account this situation were considered in [5–7]. In the offered paper, the electronic levels in spherical QD of $\mathrm{GaAs}/\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ are investigated subject to the confinement potential curve trend deviation of a course of a curve of limiting potential from parabolic one of the semiconductor-dielectric border. At that it is supposed, that the distribution of Al concentration is chosen in such a manner that CC potential energy inside the dielectric is described by parabolic function but already with other parameters.

THEORY

Let us study electron energy levels in GaAs microcrystal, grown in $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$, with the following confinement potential

$$U(r) = \begin{cases} U_1(r) = \dfrac{\mu_1 \omega_1^2 r^2}{2}, & r < r_0, \\ U_2(r) = \dfrac{\mu_2 \omega_2^2 r^2}{2} + U_0 - \dfrac{\mu_2 \omega_2^2 r_0^2}{2}, & r \geqslant r_0, \end{cases} \tag{1}$$

where r_0 is dot radius; μ_1 is electron effective mass in microcrystal (for GaAs $\mu_1 = 0.067 m_e$); μ_2 is electron effective mass in the dielectric medium (for $\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ $\mu_2 = (0.067 + 0.083x)\, m_e$); $U_0 = 1.247 x Q_e$ eV is finite confinement potential barrier height ($Q_e = 0.6$ is the conduction-band discontinuity fraction); x is the Al concentration in the dielectric medium; ω_1 is confining frequency found from the continuity condition for $U(r)$ in $r = r_0$ point [8]

$$\omega_1 = \frac{1}{r_0} \sqrt{\frac{2U_0}{\mu_1}}. \tag{2}$$

For ω_2 we have considered two cases

a)

$$\frac{\mu_2\omega_2^2 r_0^2}{2} = \gamma U_0, \quad \omega_2 = \frac{1}{r_0}\sqrt{\frac{2\gamma U_0}{\mu_1}}, \tag{3}$$

b)

$$U_0 = \frac{\mu_1\omega_1^2 r_0^2}{2} = \frac{\mu_1\omega_1^2 a}{2} = \frac{\mu_2\omega_2^2 a}{2}, \quad \omega_2 = \frac{1}{a}\sqrt{\frac{2U_0}{\mu_2}} = \frac{r_0}{a}\sqrt{\frac{\mu_1}{\mu_2}}\omega_1, \tag{4}$$

where γ and a are new parameters of our problem.

Electron energy levels can be found from continuity condition of logarithmic derivatives of a wave function in $r = r_0$ point. We shall solve the Schroedinger equation in regions I ($r < r_0$) and II ($r \geqslant r_0$) to obtain the wave function.

For region I we have the following Schroedinger equation

$$-\frac{\hbar^2}{2\mu_1}\Delta\Psi_1 + \frac{\mu_1\omega_1^2 r^2}{2}\Psi_1 = E\Psi_1. \tag{5}$$

Not diverging solution of Eq. (5) in spherical coordinates is [9]

$$\Psi_1(r,\theta,\varphi) = C_1\,\mathrm{e}^{-\xi_1^2/2} r^\ell {}_1F_1\left[-\frac{1}{2}\left(\frac{E}{\hbar\omega_1} - \ell - \frac{3}{2}\right), \ell + \frac{3}{2}; \xi_1^2\right] Y_{\ell m}(\theta,\varphi), \tag{6}$$

where $\xi_1 = r\sqrt{(\mu_1\omega_1)/\hbar}$, $Y_{\ell m}(\theta,\varphi)$ are spherical functions; ℓ, m are orbital and magnetic quantum numbers, respectively; ${}_1F_1(a,b;x)$ is a degenerate hypergeometric function of the first order; C_1 is a normalization constant.

In region II the Schroedinger equation is the following

$$-\frac{\hbar^2}{2\mu_2}\Delta\Psi_2 + \left(\frac{\mu_2\omega_2^2 r^2}{2} + U_0 - \frac{\mu_2\omega_2^2 r_0^2}{2}\right)\Psi_2 = E\Psi_2. \tag{7}$$

The solution of equation, that is written in spherical coordinates and satisfies the standard conditions, has the form

$$\Psi_2(r,\theta,\varphi) = C_2\,\mathrm{e}^{-\xi_2^2/2} r^\ell U\left[-\frac{1}{2}\left(\frac{\varepsilon}{\hbar\omega_2} - \ell - \frac{3}{2}\right), \ell + \frac{3}{2}; \xi_2^2\right] Y_{\ell m}(\theta,\varphi), \tag{8}$$

where $\varepsilon = E - U_0 + \dfrac{\mu_2\omega_2^2 r_0^2}{2}$; $\xi_2 = r\sqrt{\dfrac{\mu_2\omega_2}{\hbar}}$; $U(a,b;x)$ is a degenerate hypergeometric function of the second order; C_2 is a normalization constant.

Finally for the Schroedinger equation in regions I ($r < r_0$) and II ($r > r_0$) we have the solution

$$\Psi(r,\theta,\varphi) = \\ = \begin{cases} \Psi_1(r,\theta,\varphi) = C_1\,\mathrm{e}^{-(a_1/2)r^2} r^\ell\,{}_1F_1\left[n_{1\ell}, \ell+\dfrac{3}{2}; a_1 r^2\right] Y_{\ell m}(\theta,\varphi),\ r < r_0, \\ \Psi_1(r,\theta,\varphi) = C_2\,\mathrm{e}^{-(a_2/2)r^2} r^\ell\, U\left[n_{2\ell}, \ell+\dfrac{3}{2}; a_2 r^2\right] Y_{\ell m}(\theta,\varphi), \quad r \geqslant r_0 \end{cases} \tag{9}$$

with the following notations:

$$a_1 = \frac{\mu_1\omega_1}{\hbar}, \quad a_2 = \frac{\mu_2\omega_2}{\hbar}, \quad n_{1\ell} = -\frac{1}{2}\left(\frac{E}{\hbar\omega_1} - \ell - \frac{3}{2}\right), \\ n_{2\ell} = -\frac{1}{2}\left(\frac{\varepsilon}{\hbar\omega_2} - \ell - \frac{3}{2}\right) = -\frac{1}{2}\left(\frac{E - U_0 + \dfrac{\mu_2\omega_2^2 r_0^2}{2}}{\hbar\omega_2} - \ell - \frac{3}{2}\right). \tag{10}$$

From the conditions of normalization and continuity for eigenfunction, C_1 and C_2 constants are

$$C_1 = C_\ell, \quad C_2 = C_\ell A_\ell, \\ A_\ell = \exp\left(-\frac{a_1 - a_2}{2} r_0^2\right) \frac{{}_1F_1[n_{1\ell}, \ell+3/2; a_1 r_0^2]}{U[n_{2\ell}, \ell+3/2; a_2 r_0^2]}, \quad C_\ell^2 = \frac{1}{I_{1\ell} + A_\ell^2 I_{2\ell}}, \\ I_{1\ell} = \int\limits_0^{r_0} \mathrm{e}^{-a_1 r^2} r^{2\ell+2} \left({}_1F_1\left[n_{1\ell}, \ell+\frac{3}{2}; a_1 r^2\right]\right)^2 dr, \\ I_{2\ell} = \int\limits_{r_0}^{\infty} \mathrm{e}^{-a_2 r^2} r^{2\ell+2} \left(U\left[n_{2\ell}, \ell+\frac{3}{2}; a_2 r^2\right]\right)^2 dr. \tag{11}$$

The condition of continuity for logarithmic derivatives $\Psi_1(r,\theta,\varphi)$ and $\Psi_2(r,\theta,\varphi)$ in point $r = r_0$ has the form

$$\frac{1}{\mu_1}\frac{\Psi_1'}{\Psi_1}\bigg|_{r=r_0} = \frac{1}{\mu_2}\,\frac{\Psi_2'}{\Psi_2}\bigg|_{r=r_0}. \tag{12}$$

Using the differential formulas for ${}_1F_1(a,b;x)$ and $U(a,b;x)$ functions the condition (12) can be written as

$$\frac{\mu_2}{\mu_1}\left\{\frac{1}{2}(\ell - a_1 r_0^2) + a_1 r_0^2 \frac{n_{1\ell}}{\ell+3/2}\frac{{}_1F_1[n_{1\ell}+1,\ell+5/2;a_1 r_0^2]}{{}_1F_1[n_{1\ell},\ell+3/2;a_1 r_0^2]}\right\} =$$

$$= \left\{\frac{1}{2}(\ell - a_2 r_0^2) - a_2 r_0^2 n_{2\ell}\frac{U[n_{2\ell}+1,\ell+5/2;a_2 r_0^2]}{U[n_{2\ell},\ell+3/2;a_2 r_0^2]}\right\}. \quad (13)$$

And for ground state ($\ell = 0$, $m = 0$) we have

$$\frac{\mu_2}{\mu_1}\frac{a_1}{a_2}\left\{1 - \frac{4n_{10}}{3}\frac{{}_1F_1\left[n_{10}+1,5/2;a_1 r_0^2\right]}{{}_1F_1\left[n_{10},3/2;a_1 r_0^2\right]}\right\} =$$

$$= 1 + 2n_{20}\frac{U\left[n_{20}+1,5/2;a_2 r_0^2\right]}{U\left[n_{20},3/2;a_2 r_0^2\right]}. \quad (14)$$

Solving transcendental equations (13) and (14) we obtain the dependence $E = E(x, r_0)$. Fixing the value x of Al concentration we will find the energy dependence on the frequency, i.e., from the dot radius. If $r_0 = \mathrm{const}$, we will find the dependence $E = E(x)$.

DISCUSSION

In Fig. 1, *a* the dependences of the electron energy E (in $E_{R1} = 5.24772$ MeV effective Rydberg energy units, corresponding to first medium) on QD radius r_0 for GaAs/$\mathrm{Ga}_{1-x}\mathrm{Al}_x\mathrm{As}$ (in $a_{B1} = 104$ Å effective Bohr radius units) are plotted for the first model of confinement potential for the fixed parameters $x = 0.4$, $\gamma = 0.01$ and in $\ell = 0$ case. As follows from this picture, the electron energy increases with the decrease of r_0. It was expected, because according to (3) correlation $r_0 \to 0$ at $\omega_2 \to \infty$. The inverse situation is observed at $r_2 \to \infty$. It should be noted, that levels in QD appear starting from some threshold value of r_0, for instance, in case of the ground level $r_0 \approx 0.3a_{B1}$. The occurrence of new levels in QD is accompanied by the change of $E(r)$ dependence curve monotonous trend rate.

In Fig. 1, *b* the plots of $E(r)$ dependences (in the same units) for the second model of confinement potential at $x = 0.3$, $a = 2$ values of parameters, in $\ell = 0$ case, are presented. Unlike the first case now the levels of the electron energy at $r_0 \to 0$ tend to constant values. This values correspond to energy levels of an oscillator with ω_2 frequency. From this figure it is clear, that the levels become equidistant at $r_0 \to 0$. In other respects $E(r)$ behavior is analogous to the first case.

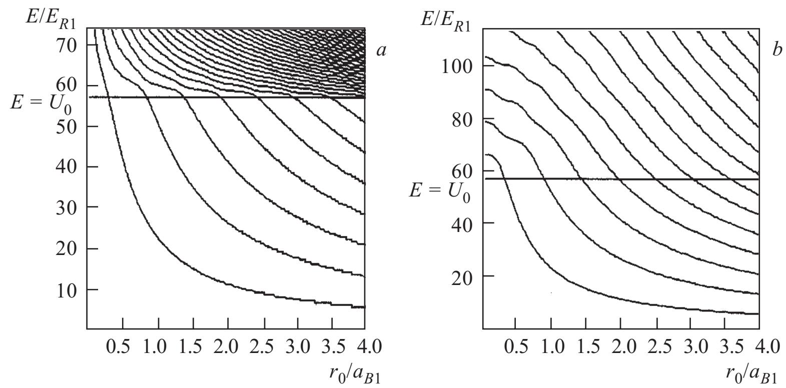

Fig. 1. Electron energy dependences on radius of QD $\mathrm{GaAs/Ca_{1-x}Al_xAs}$ for the fixed parameters $x = 0.4$, $\gamma = 0.01$ (*a*) and $x = 0.3$, $a = 2$ (*b*), and in $\ell = 0$ case

At last, in Fig. 2 the plots of electron energy dependences on Al concentration x for $r_0 = 1$, $a = 2$, in $\ell = 0$ case are presented. According to this picture, the electron energy increases with the increase of x (with the increase of potential height). In this case levels appear in QD from some threshold value of x.

As follows from expressions (13), (14), that define the electron energy spectrum in QD, the values of these levels explicitly depend on orbital quantum number ℓ. Thus the spontaneous degeneration removal takes place because of the account of boundary conditions. In other words, the Hamiltonian of this problem doesn't have high symmetry $U(3)$ any more. Another relevant circumstance of the boundary condition account is the fact, that the given Hamiltonian isn't strictly diagonalizable and, therefore, the violation of the generalized Kohn theorem takes place in such a QD.

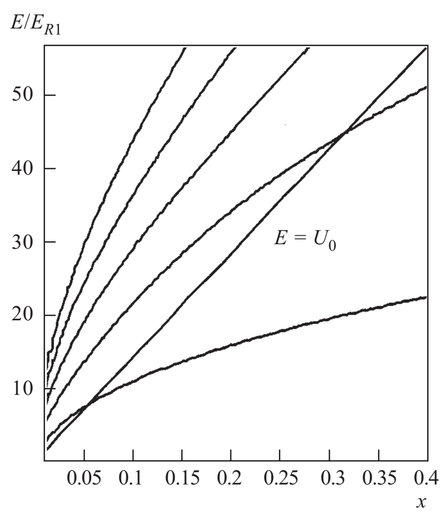

Fig. 2. Electron energy dependence on concentration x of Al (i. e., on U_0) for the fixed parameters $r_0 = 1$, $a = 2$, and in $\ell = 0$ case

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