RESEARCH OF THE ELECTRON STATE IN A PRISMATIC QUANTUM DOT WITH A SHELL

***Morozov M.V.*[1], *Domina N.A.*[1], *Khalanchuk L.V.*[1]**
[1] Dmytro Motornyi Tavria State Agrotechnological University,
B. Khmelnitskii av., 18, 72300, Melitopol, Ukraine;
E-mail: larysa.khalanchuk@tsatu.edu.ua

Low-dimensional quantum heterosystems are increasingly used in the elemental support of modern optoelectronic devices (lasers, monitors, modulators, etc.). Therefore, modeling the state of electrons at different quantum dots with a shell and without a shell of different shapes is an urgent task [1, 2]. Consider the simulation of the state of an electron in a rectangular prismatic quantum point, the dimensions of which are a, b, c with a shell of thickness d. The Schrödinger wave equation for steady states of S-electrons in the UD nucleus has the form:

$$\left(\frac{\partial^2\psi_1}{\partial x^2}+\frac{\partial^2\psi_1}{\partial y^2}+\frac{\partial^2\psi_1}{\partial z^2}\right)+k_1^2\cdot\psi_1(x,y,z)=0 \qquad (1)$$

where $k_1=\frac{\sqrt{2mE}}{\hbar}$ - wave number for the nucleus.

For the shell in the case where the potential energy U> E (total energy), the Schrödinger equation has the form:

$$\left(\frac{\partial^2\psi_2}{\partial x^2}+\frac{\partial^2\psi_2}{\partial y^2}+\frac{\partial^2\psi_2}{\partial z^2}\right)-k_2^2\cdot\psi_2(x,y,z)=0 \qquad (2)$$

where $k_2=\frac{\sqrt{2m(U_0-E)}}{\hbar}$ - wave number for the shell.

We use the Fourier method of separation of variables and look for a solution of the Schrödinger equation for the UD kernel in the case of an odd wave function in the form:

$$\psi_1(x,y,z) = A \cdot sink_{1,1}x \cdot sink_{1,2}y \cdot sink_{1,3}z \tag{3}$$

where $k_1^2 = k_{1,1}^2 + k_{1,2}^2 + k_{1,3}^2$

For the shell, the wave function $\psi_2(x,y,z)$ is equal to:

$$\psi_2(x,y,z) = B \cdot e^{-k_{2,1}x} \cdot e^{-k_{2,2}y} \cdot e^{-k_{2,3}z}. \tag{4}$$

Determine the eigenvalues of energy and the reduced amplitude B (for A = 1), using the boundary conditions - the wave function must be continuous and smooth. For x=a/2:

$$\psi_1\left(\frac{a}{2},y,z\right) = sin\left(k_{1,1} \cdot \frac{a}{2}\right) \cdot sin(k_{1,2} \cdot y) \cdot sin(k_{1,3} \cdot z) =$$

$$= \psi_2\left(\frac{a}{2},y,z\right) = B \cdot e^{-k_{2,1}\frac{a}{2}} \cdot e^{-k_{2,2}y} \cdot e^{-k_{2,3}z} \tag{5}$$

then

$$sin\left(k_{1,1} \cdot \frac{a}{2}\right) = B \cdot e^{-k_{2,1}\frac{a}{2}} \tag{6}$$

$$\psi_1'\left(\frac{a}{2},y,z\right) = \psi_2'\left(\frac{a}{2},y,z\right)$$

then

$$k_{1,1} \cdot \cos\left(k_{1,1} \cdot \frac{a}{2}\right) = -B \cdot k_{2,1} \cdot e^{-k_{2,1}\frac{a}{2}} \tag{7}$$

$$tg\left(k_{1,1} \cdot \frac{a}{2}\right) = -\frac{k_{1,1}}{k_{2,1}} \tag{8}$$

Similarly for y=b/2:

$$tg\left(k_{1,2} \cdot \frac{\mathrm{b}}{2}\right) = -\frac{k_{1,2}}{k_{2,2}} \tag{9}$$

for z=c/2:

$$tg\left(k_{1,3}\cdot\frac{c}{2}\right)=-\frac{k_{1,3}}{k_{2,3}} \qquad (10)$$

Equations (8)-(10) are solved by numerical methods of successive approximation (iterations). The model of absolutely opaque walls of a quantum dot is used to determine the initial zero approximation ($U\rightarrow\infty,\varphi_2\rightarrow 0$). Then the corresponding wave numbers are equal:

$$k_{1,1,0}=\frac{2\pi}{a}\cdot n_1;\ k_{1,2,0}=\frac{2\pi}{b}\cdot n_2;\ k_{1,3,0}=\frac{2\pi}{c}\cdot n_3,$$

where n_1, n_2, n_3 – integers: 1, 2, 3, …

Determine the eigenvalues of energy

$$E_{\mathrm{n1,n2,n3}}=\left(k_{1,1}^2+k_{1,2}^2+k_{1,3}^2\right)\cdot\frac{\hbar^2}{2m} \qquad (11)$$

Determine the reduced (A = 1) amplitude of the wave function for the shell:

$$B=sin\left(k_{1,1}\cdot\frac{a}{2}\right)\cdot e^{-k_{2,1}\frac{a}{2}} \qquad (12)$$

Then the probability density for the case $z_1=\frac{\pi}{2\cdot k_{1,3}}$ is equal to

$$\begin{cases}\rho_1(x,y)=sin^2k_{1,1}x\cdot sin^2k_{1,2}y, & |x|\le\frac{a}{2},|y|\le\frac{b}{2},\\ \rho_2(x,y)=B^2\cdot e^{-2k_{2,1}x}\cdot e^{-2k_{2,2}y}, & |x|>\frac{a}{2},|y|>\frac{b}{2}.\end{cases} \qquad (13)$$

The research results are used for an undergraduate laboratory workshop for students of "Computer Science" specialty from the course "Physical bases of modern information technologies" on the basis of mathematical and computer simulation (Scilab, MathCad).

REFERENCES

1. Lozovski V., Piatnytsia V. The Analytical Study of Electronic and Optical Properties of Pyramid-Like and Cone-Like Quantum Dots // Journal of Computational and Theoretical Nanoscience. № 8. P. 2335–2343. (2013).
2. Morozov M.V., Khalanchuk L.V. Modeling of the state of an electron in a cylindrical quantum dot with a shell // Visnyk of Zaporizhzhya National University. Physical and Mathematical Sciences. Zaporizhzhya: ZNU. № 2, pp. 117-123. (2019).

Key words:
Prismatic quantum dot, Schrödinger equation, wave function, eigen energy, mathematical computer simulation, discrete model.