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MODELING OF CYLINDRICAL QUANTUM DOTS WITH A SHELL

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The article deals with mathematical and computer modeling of electron states in a cylindrical quantum dot with a shell. Electron wave functions, eigenvalues of wave numbers and energy and their dependence on the geometrical parameters of a quantum dot (radius, height) and its shell (thickness, height of the potential barrier) are studied.

The Schrödinger equation for stationary states of S-electrons in a cylindrical coordinate system [1] has the next form:

$$\frac{\partial^2\psi_1}{\partial r^2}+\frac{1}{r}\cdot\frac{\partial\psi_1}{\partial r}+\frac{\partial^2\psi_1}{\partial z^2}+k_1^2\cdot\psi_1(r,z)=0. \quad (1)$$

The solution of equation [2] can be represented as:

$$\psi_1(r,z)=A\cdot\varphi_1(r)\cdot\varphi_2(z)=A\cdot J_0(k_3\cdot r)\cdot cos(k_4\cdot z). \quad (2)$$

The Schrödinger equation for shell of stationary states of S-electrons in a cylindrical coordinate system has the next form:

$$\frac{\partial^2\psi_2}{\partial r^2}+\frac{1}{r}\cdot\frac{\partial\psi_2}{\partial r}+\frac{\partial^2\psi_2}{\partial z^2}-k_2^2\cdot\psi_2(r,z)=0. \quad (3)$$

The solution of equation (3) can be represented as:

$$\psi_2(r,z)=B\cdot\varphi_3(r)\cdot\varphi_4(z)=B\cdot K_0(k_5\cdot r)\cdot e^{-k_6\cdot z}. \quad (4)$$

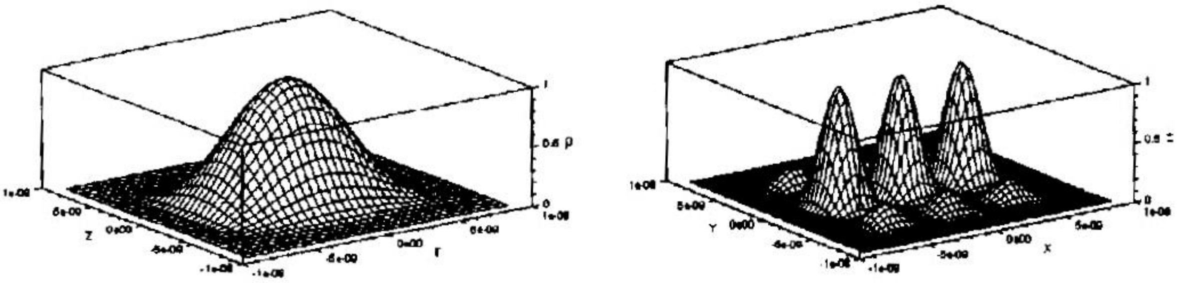
The Fourier method of separating the variables is used to obtain analytic solutions of the Schrödinger equation, as well as the numerical method of successive approximations (iterations) in determining the eigenvalues of the electron energy by means of boundary conditions. The wave functions are continuous and smooth unlike the boundaries of the shell of a cylindrical quantum dot.

The finite electron motion is considered in the effective mass approximation. The calculation results for eigen energy and wave numbers of the two electron states are presented: the ground state - axial and radial quantum numbers are equal to n = m = 1 and the excited state at n = m = 2.

The probability density of finding an electron in a given region of a cylindrical quantum dot with a shell can be represented as:

$$\rho(r,z)=|\psi(r,z)|^2=\begin{cases}|\psi_1(r,z)|^2, \text{якщо } |r|\le R \text{ та } |z|\le\frac{H}{2}\\ |\psi_2(r,z)|^2, \text{якщо } R<|r|<R+d \text{ або } \frac{H}{2}\le|z|\le\frac{H}{2}+d\end{cases} \quad (5)$$

Scilab, MathCad, discrete models of the solution of differential equations and discrete structured grids are used for mathematical computer modeling as well as for plotting of corresponding graphs of the wave function and the probability density of finding an electron in a given region of a cylindrical quantum dot (Fig. 1).



a) b)

Fig.1. The density of the probability of finding an electron in a cylindrical quantum dot with the shell for different axial and radial modes: a) n=1, m=1; b) n=2, m=2.

Thus, the state of the S-electron, which orbital moment is l = 0, is investigated in a cylindrical quantum dot with a shell and a limiting potential. Therefore, it is of high interest to simulate the electron states for other quantum dot geometry: spherical, conical, pyramidal.

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).

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

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