Problem. Quantum wells (QWs), quantum wires (QWrs), and quantum dots (QDs) are basis objects of experimental, theoretical and computational physics of semiconductor nanostructures, characterized by one, two or three geometrical dimensions comparable with the effective de Broglie wavelength. Within the effective mass approximation the slow varying envelope wave functions, describing the electron (hole), Coulomb-impurity or exciton states in model QWs, QWrs and QDs are solutions of multidimensional boundary-value problems for Schrödinger-type equations with confining 1D, 2D, and 3D potentials, respectively [1, 2]. Conventional finite-difference and variational-projectional methods, as well as special analytic approximation methods that account for a particular structure geometry and a confining potential shape, are used to analyze the spectral, optical, and transport characteristics of the model.

Method. For solving the boundary-value problems with Schrödinger-type equations we developed a new universal computation scheme based on the generalization of Kantorovich method (KM), reducing the initial problem to a set of boundary problems for ordinary second-order differential equations [3]. Their discretization by the finite-element method is shown to provide appropriate accounting for both a particular structure geometry and a confining potential shape [4].

Solution. We developed symbolic-numerical algorithms (SNA) [5, 6] and elaborated a problem-oriented complex of programs, now available via the Computer Physics Communication and JINR Libraries. These programs, implementing the KM, have proved their efficiency in our studies of spectral and optical characteristics of electronic and impurity states of QWs, QWrs and QDs, and the problem of Coulomb scattering in the presence of the axially symmetric oscillator-type confining potentials, like those provided by a homogeneous magnetic field or QWrs induced by the axial channeling of ions in a crystal [4] and tunneling of coupled pairs of particles (or ions) through potential barriers [2].

Models of QDs. A computational scheme for solving elliptic boundary value problems with axially symmetric confining potentials using different sets of one-parameter basis functions is presented. The efficiency of the proposed symbolic-numerical algorithms implemented in Maple is shown by examples of spheroidal quantum dot models, for which energy spectra and eigenfunctions versus the spheroid aspect ratio were calculated within the conventional effective mass approximation. Critical values of the aspect ratio, at which the discrete spectrum of models with finite-wall potentials is transformed into a continuous one in strong dimensional quantization regime, were revealed using the exact and adiabatic classifications [5].

Within the effective mass approximation under the conditions of strong dimensional quantization, the Schrödinger equation for the slow envelope of the wave function \(\tilde{\Psi}(\tilde{r})\) of a charge carrier (electron \(e\) or hole \(h\)) in the models of QDs has the form [1]

\[
\{ (2\mu_p)^{-1} (\tilde{P} + \frac{e}{c} \tilde{A})^2 + (\tilde{F}, \tilde{r}) + \tilde{U}(\tilde{r}) - \tilde{E} \} \tilde{\Psi}(\tilde{r}) = 0,
\]

where \(\tilde{r} \in \mathbb{R}^3\) is the position vector of the particle having the effective mass \(\mu_p = \mu_e\) (or \(\mu_p = \mu_h\)), \(\tilde{P} = -i\hbar \nabla_{\tilde{r}}\) is the momentum operator, \(\tilde{A}\) is a vector potential of homogeneous magnetic field \(\tilde{H}\), \(\tilde{F}\) is electric fields, \(\tilde{E}\) is the energy of the particle, \(\tilde{U}(\tilde{r})\) is the axially-symmetric potential confining the particle motion in SQD, PSQD, or OSQD (see fig. 1).

![Figure 1: (a) Strongly oblate ellipsoidal quantum dot. (b) Strongly prolate ellipsoidal quantum dot](image)
As a confinement potential $\tilde{U}(\mathbf{r})$, we choose the potential of a spherical or axially-symmetric well

$$\tilde{U}(\mathbf{r}) = \{0, S(\mathbf{r}) < 0; \tilde{U}_0, S(\mathbf{r}) \geq 0\},$$

bounded by the surface $S(\mathbf{r}) = 0$ with walls of finite or infinite height $1 \leq \tilde{U}_0 < \infty$. In Eq. (1) $S(\mathbf{r})$ depends on the parameters $\tilde{a}, \tilde{c}$, and $0 \leq \tilde{c}_1 \leq 1$

$$S(\mathbf{r}) = \frac{\tilde{a}^2 + \tilde{y}^2}{a^2} + \frac{(\tilde{z}^2 - c^2)(\tilde{z}^2 c_1^2 + 1 - c_1^2)^2}{c^2(\tilde{z}^2 c_1^2 + 1 - c_1^2)^2}.$$

At $c_1 = 0$ we get a spherical quantum dot model, at $0 < c_1 < 1$ it becomes a dumbbell QD with a symmetric double well, and at $c_1 > 1$ we get a triple-well model.

We use the reduced atomic units: $a_\text{B}^2 = \hbar^2/(2\mu_\text{e} c^2)$ is the reduced Bohr radius, $\kappa$ is the DC permittivity, $\tilde{E}_R \equiv Ry^* = \hbar^2/(2\mu_\text{e} a_\text{B}^2)$ is the reduced Rydberg unit of energy, and the following dimensionless quantities are introduced: $\Psi(\mathbf{r}) = a_\text{B}^{-3/2} \tilde{\Psi}(\mathbf{r})$, $2E = \tilde{E}/\tilde{R}^*$, $2\tilde{U}(\mathbf{r}) = \tilde{U}(\mathbf{r})/\tilde{R}^*$, $\mathbf{r} = \tilde{\mathbf{r}}/a_\text{B}$.

For an electron with the effective mass $\mu_\text{e} \equiv \mu_\text{e} = 0.067 m_0$ at $\kappa = 13.18$ in GaAs: $a_\text{B}^2 = a_\text{B}^2 = 104 \tilde{A}$ at $10.4$ nm and $Ry^* = \tilde{E}^* = 5.275$ meV. For a heavy hole with the effective mass $\mu_\text{h} = \mu_\text{e}/0.12 = 0.558 m_0$ the corresponding values are $a_\text{B}^2 = a_\text{B}^2 = 12.48 \tilde{A}$ at $1.248$ nm, and $E_b^* = \tilde{E}^*_b = 5.07$ meV.

In the region of parameters, where the effective mass approximation is valid, the efficiency of our SNA and combined programs was demonstrated in the analysis of spectral and optical characteristics of impurity states in QWs and electronic states in oblate or prolate spheroidal quantum dot models (OSQDs or PSQDs) with minor (c or a) and major (a or c) semiaxes, respectively. The results were used to estimate the energy boundary of photoabsorption $\lambda_1$ and the absorption coefficient $K/K_0$ for ensembles of OSQDs and PSQDs with random minor semiaxes at given average values $\tilde{c}$ or $\tilde{a}$ (in the units $\lambda = 104$ $\tilde{A}$ for electronic states in the bulk GaAs semiconductor) [7], that are shown in Figs. 2 and 3.

The set of quantum numbers relevant to nodal surfaces in the corresponding coordinate systems are given, namely, at $c/a = 1$ the exact set of $(n_r, l - |m|, m, \sigma = \sigma(-1)^m)$ in spherical coordinates, at $c/a < 1$ (or $a/c < 1$) the adiabatic sets of $(n_x, n_y, n_z, m, \sigma = (-1)^n_z)\|p$ for strongly oblate (or $(n_p, n_z, m, \sigma = (-1)^n_x)\|p$ for strongly prolate) shapes in cylindrical coordinates. The correspondence rules are $(n_x, n_p) = (l - |m|, m, \sigma = \sigma(-1)^m)$, $(n_z = 2n_r + (1 - \sigma)/2, n_p = (l - |m| - (1 + \sigma)/2)/2, m, |\sigma|)$, or $(n_x = n_y, n_z = l - |m|, m, |\sigma|)$.

In the regime of strong dimensional quantization the frequencies of the interband transitions between the levels $n_x = 1, n_{po} = 0, m = 0$ for OSQD or $n_p = 1, n_{zp} = 0, m = 0$ for PSQD in the BO1, at the fixed values $\tilde{a} = 2.5a_e$ and $\tilde{c} = 0.5a_e$ for OSQD or $\tilde{a} = 0.5a_e$ and $\tilde{c} = 2.5a_e$ for PSQD, are equal to $\omega_{100}^\text{ph} = 2.17 \times 10^{13}$ s$^{-1}$ or $\omega_{100}^\text{ph} = 3.32 \times 10^{13}$ s$^{-1}$ ($\omega_{100}^\text{ph} = h^{-1}\tilde{W}_{100,100}$ with the accuracy to $3\%$ and $0.5\%$, respectively), corresponding to the infrared spectral region [7]. The revealed difference in the spectra and the absorption coefficients allow verification of OSQD and PSQD models using the experimental data, e.g., photo-absorption, from which not only the energy level spacing, but also the mean geometric dimensions of QDs can be derived. The adiabatic approximations implemented in an analytic form can be applied also to treat a lower part of spectra of models of strongly deformed nuclei.

![Figure 2: Absorption coefficient $K/K_0$ consists of sum of the first partial contributions vs the energy $\lambda = \lambda_1$ of the optc interband transitions for the Lifshits-Slezov distribution in third Born Oppenheimer approximation for ensemble of OSQDs $\tilde{c} = 0.5$, $a = 2.5$ (summation by $n_{po} = 1, 2, 3, n_{po} = 0, 1, 2, 3, 4, 5$, $m = 0$) and the schematic plots of interband transition](image)
of basis functions. Symbolic algorithms for evaluation of asymptotics of the basis functions, effective potentials and linear independent solutions of the ODEs in the form of inverse power series of independent variable at large values are given, by using appropriate etalon equations. Benchmark calculation of quantum tunneling problem of coupled pair of identical ions through Coulomb-like barrier is presented [6].

Wave function $\Psi(x, y)$ of the model of heavy ion pair connected with oscillator potential scattering in the center mass coordinate system through Coulomb barriers satisfies the 2D Schrödinger equation [2]:

$$\left\{ -\frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial x^2} + x^2 + 2(U(x, y) - E) \right\} \Psi(x, y) = 0,$$

where $x_1 = s_2 y + s_1 x$, $x_2 = s_2 y - s_3 x$ are variables in the laboratory system of coordinates, parameters $s_2 = \left(\frac{m_1 \alpha}{M}\right)^{1/2}$, $s_1 = \frac{\alpha}{M}$, $s_3 = \frac{\alpha}{M}$ are defined via masses of ions $m_1$ and $m_2$ and total mass $M = m_1 + m_2$ and reduced mass $\mu = \frac{m_1 m_2}{m_1 + m_2}$ in the oscillator units of length $x_{osc} = \sqrt{\frac{\hbar}{\mu \omega}}$ and energy $E_{osc} = \hbar \omega$ ($\omega$ is oscillator frequency), $U(x, y) = U_1(x_1) + U_2(x_2)$ is two-center potential. We choose barrier potential $U_i(x_i)$ of ions labeled by $i = 1, 2$ with charges $\tilde{Z}_i > 0$ in the form of the truncated Coulomb potential cut off on small $0 < \bar{x}_{\text{min}} < 1$ and large $\bar{x}_{\text{max}} > 1$ distances from origin,

$$U_i(x_i) = \begin{cases} \tilde{Z}_i - \frac{\tilde{Z}_i}{\bar{x}_{\text{min}}}, & |x_i| > \bar{x}_{\text{min}} \text{; } 0, |x_i| > \bar{x}_{\text{max}} \end{cases},$$

or the Coulomb-like potentials that depend on the integer parameter $s \geq 2$ and truncation parameter $\bar{x}_{s_{\text{min}}} > 0$ and defined as

$$U_i(x_i) = \tilde{Z}_i(|x_i|^s + \bar{x}_{s_{\text{min}}}^s)^{-1/s}.$$

In both cases the sum of barrier potential functions $U(x, y) = U_1(x_1) + U_2(x_2)$ has asymptotic form

$$U(x, y) \rightarrow \sigma_y \frac{Z_{12}}{y} + O(y^{-3}), \quad y \rightarrow \pm \infty,$$

where $\sigma_y = 1$ if $y > 0$ and $\sigma_y = -1$ if $y < 0$; $Z_{12} = 0$ for Eq. (4) and $Z_{12} = (\tilde{Z}_1 + \tilde{Z}_2)/s_2$ for Eq. (5).

The asymptotic boundary conditions for the solution $\Psi(y, x) = \{\Psi_{i_o}(y, x)\}_{i_o=1}^{N_o}$ with direction $v = \pm \infty$ can be written in the obvious form

$$\Psi_{i_o}(y \rightarrow -\infty, x) \rightarrow B_{i_o}^{(0)}(x) \exp(i(p_{i_o} y - \sigma_y \tilde{Z}_{i_o} \bar{x}_{i_o}(\ln(2p_{i_o} |y|)))) \sqrt{p_{i_o}}$$

$$+ \sum_{j=1}^{N_o} B_{j}^{(0)}(x) \exp(-i(p_j y - \sigma_y \tilde{Z}_{j} \bar{x}_{j}(\ln(2p_j |y|)))) \sqrt{p_j} R_{j,i_o},$$

$$\Psi_{i_o}(y \rightarrow +\infty, x) \rightarrow \Psi_{i_o}(y, x \rightarrow +\infty) \rightarrow 0.$$

Here $N_o$ is the number of open channels at fixed energy $2E = p^2 + \varepsilon_j^{(0)} > 0$, $T_{j,i_o}$ and $R_{j,i_o}$ are unknown transition and reflections amplitudes, $B_{j}^{(0)}(x)$ are the basis functions of oscillator with energy $\varepsilon_j^{(0)} = 2n + 1$ at $n \geq 0$, $j = n + 1$

$$\left\{ -\frac{\partial^2}{\partial x^2} + x^2 - \varepsilon_j^{(0)} \right\} B_{j}^{(0)}(x) = 0,$$

$$\int_{-\infty}^{+\infty} B_{j}^{(0)}(x) B_{j'}^{(0)}(x) dx = \delta_{jj'}.$$

The total probabilities $T \equiv T_{11} = \sum_{j=1}^{N_o} |T_{j1}|^2$ of penetration through truncated Coulomb (4) and Coulomb-like (5) potential barriers are shown in Fig. 4. The first of them is in a good agreement with results obtained by solving BVP (3), (4), (7), (8) in a 2D domain using Numerov method and close-coupling method in the basis of asymptotic states (8). These pictures illustrate the important peculiarity that a more realistic nontruncated Coulomb-like barrier, having a more wide than truncated one, leads to a set of the probability maximums having a bigger half-width. It can
Figure 4: The total probabilities $T \equiv T_{11} = \sum_{N=1}^{\infty} |T_{1j}|^2$ of penetration through truncated Coulomb (4) at $x_{\text{max}} = 5$ (upper panels), and Coulomb-like (5) (lower panels), potential barriers be used for verification of the models and quantum transparency effect, for example, see Fig. 5.

Prospects. The computational scheme, the SNA, and the complex of programs allow extension for the analysis of spectral and optical characteristics of the exciton states in finite-dimensional quantum models at the different geometry of structure, shape of confining potential, and external fields, and developing quantum transparency and diffusion models, employment of MPI and Grid technologies.

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Figure 5: Profiles $|\Psi_{Em-\text{-}1}^{(-)}|$ of the total wave functions of the continuous spectrum in the $yx$ plane with $Z_1 = Z_2 = 0.5$, $m_1 = m_2 = 1$ at resonance energies $2E = 8.1403$ a.u. and $2E = 9.4748$ a.u., demonstrating resonance transmission and total reflection, respectively, from third panel of Fig. 4

References