ISSN 1063-7788, Physics of Atomic Nuclei, 2010, Vol. 73, No. 2, pp. 331–338. © Pleiades Publishing, Ltd., 2010.

ELEMENTARY PARTICLES AND FIELDS
Theory

Adiabatic Approach to the Problem of a Quantum Well with a Hydrogen-Like Impurity*

A. A. Gusev[1)**], O. Chuluunbaatar[1)], S. I. Vinitsky[1)***], V. L. Derbov[2)], E. M. Kazaryan[3),4)], A. A. Kostanyan[3),4)], and H. A. Sarkisyan[3),4)****]

Received April 17, 2009

Abstract—An adiabatic method is presented for solving a boundary discrete spectrum problem for a parabolic quantum well and a rectangular quantum well with infinitely-high walls in the presence of a hydrogen-like impurity. The upper and lower bounds for the energy of the ground state of the systems are obtained under the conditions of the shift of the Coulomb center in a given range of the parameter with respect to earlier variational estimates. The comparison of the rate of convergence of the adiabatic expansion of the solution in parametric bases in the cylindrical and spherical coordinates is carried out.

DOI: 10.1134/S1063778810020201

1. INTRODUCTION

In [1, 2] the optical absorption into the ground state of GaAs parabolic quantum well and rectangular quantum well with infinitely high walls in the presence of a hydrogen-like impurity was considered. The calculations of the ground state of these quantum wells were carried out using a single-parameter variational functions in the cylindrical coordinate system. The upper bounds of these energies were obtained depending on the shift of the Coulomb potential center. The analysis of more complex quantum-mechanical models leads to boundary problems in nonstandard domain of the configuration space with complex boundary, solved using multiparameter variational functions [3], finite-element method [4, 5], or by means of reducing the problem to ordinary differential equations following Kantorovich method [6], known in physics as the adiabatic approach of quantum-mechanical problems with slow and fast variables [7]. In the Kantorovich method the basis functions depend upon the slow variables as parameters and obey the boundary conditions that account for all specific features of the original problem, which provides the efficiency of the method for solving boundary problems in a nonstandard domain, e.g., in a sector of a circle with mixed boundary conditions [7], as well as in the presence of singular potential against the background of confining potentials of the oscillator type with respect to some of the independent variables [8]. This determines the potentialities of using the method in the analysis of low-dimensional quantum-mechanical models of semiconductor nanostructures [9].

Here we present a scheme for solving the discrete-spectrum boundary problem for a parabolic quantum well and rectangular quantum well with infinitely high walls in the adiabatic representation in the cylindrical and spherical coordinates. The upper and lower bounds are obtained for the ground-state energies of the systems under the conditions of the shift of the Coulomb potential center in a given range of the parameter with respect to earlier variational estimates. It is shown that the rate of convergence of the solution expansion depends upon the choice of the adiabatic basis representation with the specific features of the problem taken into account.

2. ADIABATIC REPRESENTATION FOR A QUANTUM WELL IN THE CYLINDRICAL COORDINATES

For a quantum well the Schrödinger equation governing the discrete-spectrum wave function $\psi(z,\rho,\phi) = \psi_{m_z}(z,\rho)\exp(im_z\varphi)/\sqrt{2\pi}$ with the fixed magnetic quantum number m_z in the cylindrical coordinates $(z,\rho,\phi) \in \mathbf{R}^3$ has the form [1]

$$\left[-\frac{\hbar^2}{2m^*}\left(\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho} - \frac{m_z^2}{\rho^2} + \frac{\partial^2}{\partial z^2}\right) \right. \qquad (1)$$

*The text was submitted by the authors in English.

1)Joint Institute for Nuclear Research, Dubna, Russia.
2)Saratov State University, Russia.
3)Russian–Armenian (Slavonic) University, Yerevan, Armenia.
4)Yerevan State University, Armenia.
**E-mail: gooseff@jinr.ru
***E-mail: vinitsky@theor.jinr.ru
****E-mail: shayk@ysu.am

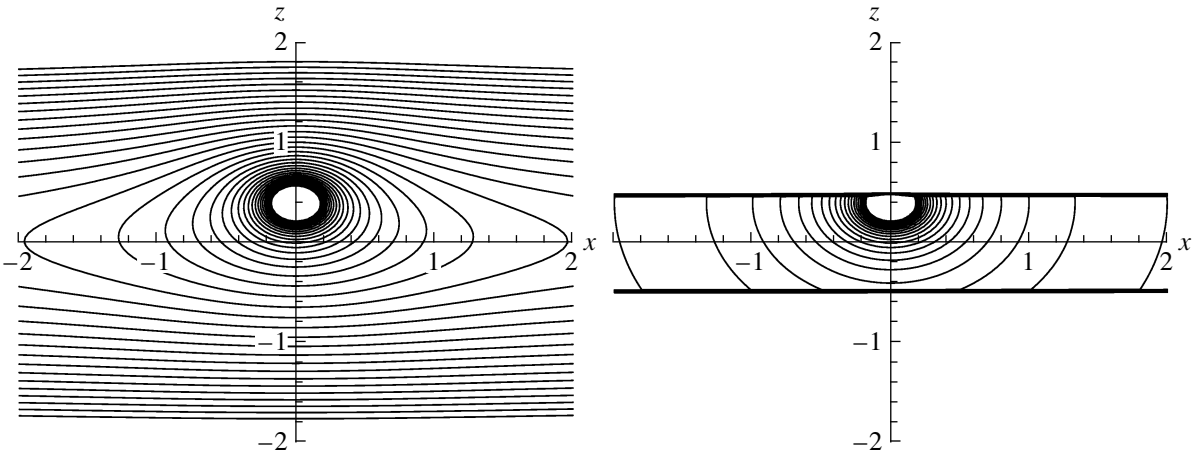

Fig. 1. Isolines of potential energy surface as function of two independent variables $\bar{\rho}$, $\bar{z}$ with shift of center of Coulomb potential along variable $\bar{z}$ on $\bar{z}_c = 0.4$. Left panel: Model A for values of parameters $m_z = 0$, $Z = 1$ and $\bar{\omega} = 3$. Right panel: Model B for values of parameters $m_z = 0$, $Z = 1$, and $\bar{L} = 1$.

$$+ U(z,\rho)\Big]\psi_{m_z}(z,\rho) = E\psi_{m_z}(z,\rho).$$

Here, E is the energy of the discrete spectrum, $U(z,\rho)$ is the quantum well potential taken as the sum of the confining potential $V_{\text{conf}}(z)$, depending on the longitudinal coordinate z, and the Coulomb potential (see Fig. 1)

$$U(z,\rho) = V_{\text{conf}}(z) - \frac{Ze^2}{\varepsilon_d\sqrt{(z-z_c)^2+\rho^2}},$$

where $m^* = \beta m_e$ is the reduced mass, Z is the reduced Coulomb charge, z_c is the shift of the Coulomb center along z, ε_d is the relative dielectric constant. The confining potential is chosen as the potential $V_A(z)$ of a harmonic oscillator having the frequency ω (Model A):

$$V_{\text{conf}}(z) = V_A(z) = \frac{m^*\omega^2}{2}z^2$$

or as an infinitely deep potential well with vertical wall $V_B(z)$ (Model B):

$$V_{\text{conf}}(z) = V_B(z) = \begin{cases} 0, & |z| < L/2, \\ +\infty, & |z| \geq L/2. \end{cases}$$

At a fixed value of the magnetic quantum number m_z the wave functions $\psi_{m_z}(z,\rho) \equiv \psi_{m_z i}(z,\rho) \in W_2^1(\Omega)$ [10] of the discrete spectrum satisfy the normalization condition

$$\langle\psi_{m_z i}(z,\rho)|\psi_{m_z j}(z,\rho)\rangle_{\Omega_{\bar{z}}} \tag{2}$$
$$= \int_0^{+\infty}\int_{-\infty}^{+\infty}\psi_{m_z i}(z,\rho)\psi_{m_z j}(z,\rho)\rho d\rho dz = \delta_{ij}.$$

Let us introduce the new independent variables $\bar{\rho} = \rho/a_0^*$, $\bar{z} = z/a_0^*$ and the notations $\bar{z}_c = z_c/a_0^*$, $2\bar{E} = E/R_0^*$, where $a_0^* = (\varepsilon_d/\beta)a_0$ and $R_0^* \equiv \text{Ry}^* = m^*e^{*4}/(2\hbar^2) = \text{Ry}\beta/(\varepsilon_d^2)$ are the reduced atomic units, $m^* = \beta m_e$ is the effective mass, $e^* = e/\sqrt{\varepsilon_d}$ is the effective charge, $a_0 = \hbar^2/(m_e e^2)$, $\omega = \gamma\hbar/(m_e\beta L^2)$, $L = a_0^*\bar{L}$, $\bar{\omega} = \gamma/\bar{L}^2$, $\omega = \hbar/(a_0^{*2}m^*)\bar{\omega}$, $\text{Ry} = m_e e^4/(2\hbar^2)$.

In the reduced atomic units the Schrödinger equation, describing the Models A and B, takes the form

$$\Big[-\frac{1}{\bar{\rho}}\frac{\partial}{\partial\bar{\rho}}\bar{\rho}\frac{\partial}{\partial\bar{\rho}} + \frac{m_z^2}{\bar{\rho}^2} - \frac{\partial^2}{\partial\bar{z}^2} + \bar{\omega}^2(\bar{z})^2 \tag{3}$$
$$- \frac{2Z}{\sqrt{(\bar{z}-\bar{z}_c)^2+\bar{\rho}^2}} - 2\bar{E}\Big]\psi_{m_z}(\bar{z},\bar{\rho}) = 0,$$
$$\Big[-\frac{1}{\bar{\rho}}\frac{\partial}{\partial\bar{\rho}}\bar{\rho}\frac{\partial}{\partial\bar{\rho}} + \frac{m_z^2}{\bar{\rho}^2} - \frac{\partial^2}{\partial\bar{z}^2} \tag{4}$$
$$- \frac{2Z}{\sqrt{(\bar{z}-\bar{z}_c)^2+\bar{\rho}^2}} - 2\bar{E}\Big]\psi_{m_z}(\bar{z},\bar{\rho}) = 0,$$

where the wave function $\psi_{m_z}(\bar{z},\bar{\rho}) \equiv \psi_{m_z i}(\bar{z},\bar{\rho};\bar{z}_c)$ at fixed m_z obeys the conditions at the boundary of the domain $\Omega_{\bar{z},\bar{\rho}} = \Omega(\bar{z},\bar{\rho})$

$$\lim_{\bar{\rho}\to 0}\bar{\rho}\frac{\partial\psi_{m_z}(\bar{z},\bar{\rho})}{\partial\bar{\rho}} = 0, \quad \text{if} \quad m = 0, \tag{5}$$
$$\text{and} \quad \psi_{m_z}(\bar{z},0) = 0, \quad \text{if} \quad m \neq 0,$$
$$\lim_{\bar{z}\to\pm\infty}\psi_{m_z}(\bar{z},\bar{\rho}) = 0 \to\leftarrow \psi_{m_z}(\bar{z}_{\min},\bar{\rho}) = 0, \tag{6}$$
$$\psi_{m_z}(\bar{z}_{\max},\bar{\rho}) = 0,$$
$$\psi_{m_z}(\bar{z}_{\min} = -\bar{L}/2,\bar{\rho}) = 0, \tag{7}$$
$$\psi_{m_z}(\bar{z}_{\max} = \bar{L}/2,\bar{\rho}) = 0.$$

The wave functions of the discrete spectrum at large $\bar{\rho} = \bar{\rho}_{\max} \gg 1$ satisfy the Dirichlet boundary condition following the asymptotic form of the solution

$$\lim_{\bar{\rho}\to+\infty} \bar{\rho}\psi_{m_z}(\bar{z},\bar{\rho}) = 0 \to \psi_{m_z}(\bar{z},\bar{\rho}_{\max}) = 0 \quad (8)$$

and the normalization condition

$$(a_0^*)^3 \int_{\bar{z}_{\min}}^{\bar{z}_{\max}} \int_0^{\bar{\rho}_{\max}} \psi_{m_z i}(\bar{z},\bar{\rho})\psi_{m_z j}(\bar{z},\bar{\rho})\bar{\rho}d\bar{\rho}d\bar{z} = \delta_{ij}. \quad (9)$$

The solution of the problem (1), (2) is sought in the form of the expansion with respect to the set of single-parameter functions $B_j(\bar{z};\bar{\rho})$:

$$\psi_{m_z i}(\bar{z},\bar{\rho}) = \sum_{j=1}^{j_{\max}} B_j(\bar{z};\bar{\rho})\chi_{ji}(\bar{\rho}). \quad (10)$$

Here the vector functions $\chi_{ji}(\bar{\rho})$ are to be found, while the basis functions $B_j(\bar{z};\bar{\rho})$ are defined as the solutions of the boundary-value problem

$$\left[-\frac{\partial^2}{\partial\bar{z}^2} + \bar{\omega}^2\bar{z}^2 - \frac{2Z}{\sqrt{(\bar{z}-\bar{z}_c)^2+\bar{\rho}^2}}\right] \times B_j(\bar{z};\bar{\rho}) = \bar{E}_j(\bar{\rho})B_j(\bar{z};\bar{\rho}), \quad (11)$$

$$\left[-\frac{\partial^2}{\partial\bar{z}^2} - \frac{2Z}{\sqrt{(\bar{z}-\bar{z}_c)^2+\bar{\rho}^2}}\right] B_j(\bar{z};\bar{\rho}) = \bar{E}_j(\bar{\rho})B_j(\bar{z};\bar{\rho}). \quad (12)$$

The eigenfunctions $B_j(\bar{z};\bar{\rho})$ at each fixed value of the parameter $\bar{\rho} \in \mathbf{R}^1_+$, obey the Dirichlet boundary conditions with respect to the variable $\bar{z}$:

$$B_j(\bar{z};\bar{\rho})|_{\bar{z}=\bar{z}_{\min}} = 0, \quad B_j(\bar{z};\bar{\rho})|_{\bar{z}=\bar{z}_{\max}} = 0, \quad (13)$$

and satisfy the orthogonality and normalization conditions in the interval $\Omega_{\bar{z}} = [\bar{z}_{\min}, \bar{z}_{\max}]$:

$$\langle B_i(\bar{z};\bar{\rho})|B_j(\bar{z};\bar{\rho})\rangle_\Omega = a_0^* \int_{\bar{z}_{\min}}^{\bar{z}_{\max}} B_i(\bar{z};\bar{\rho})B_j(\bar{z};\bar{\rho})d\bar{z} = \delta_{ij}. \quad (14)$$

Note, that due to the singular behavior of the one-dimensional Coulomb potential in the vicinity of $\bar{z} = \bar{z}_c$ the eigenfunctions $B_j(\bar{z};\bar{\rho}) \in F_{\bar{\rho}} \sim L_2[\bar{z}_{\min}, \bar{z}_{\max}]$ of the problem (11)–(14) at $\bar{\rho} = 0$ have only generalized partial derivatives of the first order, i.e., belong to Sobolev space $B_j(\bar{z};\bar{\rho}) \in \overset{0}{W}{}^1_2[\bar{z}_{\min}, \bar{z}_{\max}]$ [10, 11]. The Model A is considered in configuration space $\mathbf{R}^3$ with an additional oscillator potential providing a confinement along z-axis and is known in literature as *parabolic quantum well* [1], while the Model B is considered explicitly in quasi-2D space $\mathbf{R}^2 \otimes [-\bar{L}/2, \bar{L}/2]$, and is known in literature as *quantum well* [2, 9]. As one can see, potential surface of the Model A can be considered as some approximation of potential surface of the Model B by means of appropriate variation of parameters $\bar{\omega}$ and $\bar{L}$, and $\bar{z}_c \in (-\bar{L}/2, \bar{L}/2)$ (see Fig. 1). In limits $\bar{\omega} \to \infty$ and $\bar{L} \to 0$ both models transfer to exact solvable model of planar hydrogen-like atom with known eigenfunction and eigenenergies $E_n/R_0^* = -Z^2/(n+1/2)^2, n = 0, 1, 2, \ldots$ [12].

At $\bar{\rho} \to +\infty$ the eigenfunctions $B_j(\bar{z};\bar{\rho})$ in the domain $\Omega_{\text{as}} : \dfrac{\bar{z}^2}{\bar{\rho}^2} \ll 1$ for Model B are expressed via the eigenfunctions of a one-dimensional oscillator $B_j^{(0)}(\bar{z};\bar{\rho}\to\infty) \equiv B_j^{(0)}(\bar{z})$ depending on the scaled variable ξ: $\bar{z} = a_{\bar{\omega}}\xi$, where $a_{\bar{\omega}} = (\bar{\omega})^{-1/2}$, normalized by the condition (14):

$$B_j^{(0)}(\bar{z}) = \frac{1}{(a_0^*)^{1/2}(a_{\bar{\omega}})^{1/2}\pi^{1/4}(2^n n!)^{1/2}} \times \exp\left(-\frac{1}{2}\left(\frac{\bar{z}}{a_{\bar{\omega}}}\right)^2\right) H_n\left(\frac{\bar{z}}{a_{\bar{\omega}}}\right), \quad (15)$$

where H_n are the Hermite polynomials, and the eigenvalues $\bar{E}_j(\bar{\rho}\to\infty) = \bar{E}_j^{\text{th}}$ are expressed via the corresponding eigenvalues of the energy of one-dimensional harmonic oscillator $\bar{E}_j^{\text{th}} = \bar{\omega}(2j-1) = \bar{\omega}(2n+1)$, $j = n+1 = 1, 2, \ldots, j_{\max}$ $(n = j-1 = 0, 1, \ldots, j_{\max}-1)$. This follows from the fact that at $\bar{\rho} \to \infty$ the correction $\Delta\bar{E}_j(\bar{\rho}\to\infty)$ to the eigenvalues $\bar{E}_j^{\text{th}}$, calculated using the asymptotic basis functions, has the order of smallness

$$\Delta\bar{E}_j(\bar{\rho}\to\infty) = -\frac{2Z}{\bar{\rho}} \int_{\bar{z}_{\min}}^{\bar{z}_{\max}} B_j^{(0)}(\bar{z};\bar{\rho}\to\infty) \times \frac{1}{\sqrt{1+\frac{(\bar{z}-\bar{z}_c)^2}{\bar{\rho}^2}}} B_j^{(0)}(\bar{z};\bar{\rho}\to\infty)d\bar{z} = -\frac{2Z}{\bar{\rho}} + O(\bar{\rho}^{-3}).$$

For Model B at $\bar{\rho} \to +\infty$ the eigenfunctions $B_j(\bar{z};\bar{\rho})$ in the domain $\Omega_{\text{as}} : \dfrac{\bar{z}^2}{\bar{\rho}^2} \ll 1$ are expressed via the eigenfunctions of the one-dimensional rectangular potential well $B_j^{(0)}(\bar{z};\bar{\rho}\to\infty) \equiv B_j^{(0)}(\bar{z})$, normalized by the condition (14):

$$B_j^{(0)}(\bar{z}) = \frac{1}{(a_0^*)^{1/2}}\sqrt{\frac{2}{\bar{L}}} \begin{cases} \sin\dfrac{\pi j}{L}\bar{z}, & \text{even} \quad j \geq 2, \\ \cos\dfrac{\pi j}{L}\bar{z}, & \text{odd} \quad j \geq 1, \end{cases}$$

while the eigenvalues $\bar{E}_j(\bar{\rho}\to\infty)=\bar{E}_j^{\rm th}$ are expressed via the corresponding eigenvalues of the energy of a particle in a one-dimensional rectangular potential well $\bar{E}_j^{\rm th}=\pi^2 j^2/\bar{L}^2$, $j=1,2,\ldots,j_{\max}$.

Under the variable change $\bar{z}'=\bar{z}-\bar{z}_c$ the eigenvalue problem (11)–(14) takes the form

$$\left[-\frac{\partial^2}{\partial\bar{z}'^2}+\bar{\omega}^2(\bar{z}'+\bar{z}_c)^2-\frac{2Z}{\sqrt{\bar{z}'^2+\bar{\rho}^2}}\right]\times\Phi_j(\bar{z}';\bar{\rho})=\bar{E}_j(\bar{\rho})\Phi_j(\bar{z}';\bar{\rho}), \tag{16}$$

$$\left[-\frac{\partial^2}{\partial\bar{z}'^2}-\frac{2Z}{\sqrt{\bar{z}'^2+\bar{\rho}^2}}\right]\Phi_j(\bar{z}';\bar{\rho})=\bar{E}_j(\bar{\rho})\Phi_j(\bar{z}';\bar{\rho}). \tag{17}$$

The eigenfunctions

$$\Phi_j(\bar{z}';\bar{\rho})=\exp(-i\bar{z}_c\bar{p}_{\bar{z}})B_j(\bar{z};\bar{\rho})=\exp\left(\bar{z}_c\frac{d}{d\bar{z}}\right)B_j(\bar{z};\bar{\rho})$$

form a complete orthogonal basis, obey the symmetry conditions

$$B_j(\bar{z};\bar{\rho},\bar{z}_c)=\exp(i\pi\nu_{m_z q})B_j(-\bar{z};\bar{\rho},-\bar{z}_c)$$

and

$$\bar{E}_j(\bar{\rho},\bar{z}_c)=\bar{E}_j(\bar{\rho},-\bar{z}_c),$$

where $\nu_{m_z q}$ is the real phase, q is the number of zeros in $\bar{z}\in\mathbf{R}$ for Model A and $\bar{z}\in[\bar{z}_{\min},\bar{z}_{\max}]$ for Model B, and the Dirichlet boundary conditions with respect to the variable $\bar{z}'$ at each fixed value of the parameter $\bar{\rho}\in\mathbf{R}^1_+$:

$$\Phi_j(\bar{z}'_{\min};\bar{\rho})=0,\quad \Phi_j(\bar{z}'_{\max};\bar{\rho})=0, \tag{18}$$
$$\bar{z}'_{\min}=\bar{z}_{\min}-\bar{z}_c,\quad \bar{z}'_{\max}=\bar{z}_{\max}-\bar{z}_c.$$

They also satisfy the orthonormality conditions in the interval $\Omega'_{\bar{z}}=[\bar{z}'_{\min}=\bar{z}_{\min}-\bar{z}_c,\bar{z}'_{\max}=\bar{z}_{\max}-\bar{z}_c]$:

$$\langle\Phi_i(\bar{z}';\bar{\rho})|\Phi_j(\bar{z}';\bar{\rho})\rangle_{\Omega'}=a_0^*\int\limits_{\bar{z}'_{\min}}^{\bar{z}'_{\max}}\Phi_i(\bar{z}';\bar{\rho})\Phi_j(\bar{z}';\bar{\rho})d\bar{z}'=\delta_{ij}. \tag{19}$$

By means of the variation of the corresponding Rayleigh–Ritz functional [7] using the expansion (10), Eq. (1) is reduced to the set of $j_{\max}$ ordinary differential equations of the second order with respect to the unknown functions $\chi(\bar{\rho})\equiv\chi^{(i)}(\bar{\rho})$:

$$\left(-\frac{1}{\bar{\rho}^{d-1}}\mathbf{I}\frac{d}{d\bar{\rho}}\bar{\rho}^{d-1}\frac{d}{d\bar{\rho}}+\mathbf{V}(\bar{\rho})+\mathbf{Q}(\bar{\rho})\frac{d}{d\bar{\rho}}+\frac{1}{\bar{\rho}^{d-1}}\frac{d\bar{\rho}^{d-1}\mathbf{Q}(\bar{\rho})}{d\bar{\rho}}-2\bar{E}\mathbf{I}\right)\boldsymbol{\chi}(\bar{\rho})=0. \tag{20}$$

Here, $d=2$ is the dimensionality of the space, $\mathbf{I}$, $\mathbf{V}(\bar{\rho})$, and $\mathbf{Q}(\bar{\rho})$ are $j_{\max}\times j_{\max}$ matrices, the elements of which are defined by the relations

$$V_{ij}(\bar{\rho})=H_{ij}(\bar{\rho})+\frac{\bar{E}_i(\bar{\rho})+\bar{E}_j(\bar{\rho})}{2}\delta_{ij}+\frac{m_z^2}{\bar{\rho}^2}\delta_{ij},\quad I_{ij}=\delta_{ij}, \tag{21}$$

$$H_{ij}(\bar{\rho})=H_{ji}(\bar{\rho})=\left\langle\frac{\partial B_i(\bar{z}';\bar{\rho})}{\partial\bar{\rho}}\middle|\frac{\partial B_j(\bar{z}';\bar{\rho})}{\partial\bar{\rho}}\right\rangle_{\Omega_{\bar{z}'}},$$

$$Q_{ij}(\bar{\rho})=-Q_{ji}(\bar{\rho})=-\left\langle B_i(\bar{z}';\bar{\rho})\middle|\frac{\partial B_j(\bar{z}';\bar{\rho})}{\partial\bar{\rho}}\right\rangle_{\Omega_{\bar{z}'}}.$$

Due to (5)–(9) the discrete spectrum solutions obey the asymptotic boundary and orthonormality conditions

$$\lim_{\bar{\rho}\to0}\bar{\rho}^{d-1}\frac{d\boldsymbol{\chi}(\bar{\rho})}{d\bar{\rho}}=0,\quad\text{if}\quad m_z=0, \tag{22}$$
$$\text{and}\quad\boldsymbol{\chi}(0)=0,\quad\text{if}\quad m_z\neq0,$$

$$\lim_{\bar{\rho}\to\infty}\bar{\rho}^{d-1}\boldsymbol{\chi}^{(i)}(\bar{\rho})=0\to\boldsymbol{\chi}^{(i)}(\bar{\rho}_{\max})=0, \tag{23}$$

$$(a_0^*)^d\int\limits_0^{\bar{\rho}_{\max}}\bar{\rho}^{d-1}\left(\boldsymbol{\chi}^{(i)}(\bar{\rho})\right)^T\boldsymbol{\chi}^{(j)}(\bar{\rho})d\bar{\rho}=\delta_{ij}. \tag{24}$$

Since the equation (16) (or (17)) is linear and the boundary conditions (18) are homogeneous, the sign of the phase of the basis functions is arbitrary. Hence, the sign of the phase at the point $\bar{z}'_{\min}$ was fixed by imposing the condition

$$\frac{\partial}{\partial\bar{z}'}\Phi_j(\bar{z}';\bar{\rho})\Big|_{\bar{z}'=\bar{z}'_{\max}}>0,$$

which is necessary for the calculation of integrals (21), including the basis functions and their derivatives with respect to the parameter $\bar{\rho}$, i.e., the variables coefficients in Eq. (20).

3. ADIABATIC REPRESENTATION FOR THE PARABOLIC QUANTUM WELL IN SPHERICAL COORDINATES

Using the reduced atomic units the Schrödinger equation (1) in the spherical coordinates $(\bar{r},\eta=\cos\theta,\phi)$ takes the form

$$\left(-\frac{1}{\bar{r}^2}\frac{\partial}{\partial\bar{r}}\bar{r}^2\frac{\partial}{\partial\bar{r}}+\frac{1}{\bar{r}^2}\hat{A}(c)-\frac{2Z}{\bar{r}}\right)\times\psi_{m_z}(\bar{r},\eta)=2\bar{E}\psi_{m_z}(\bar{r},\eta). \tag{25}$$

Here $\hat{A}(c) \equiv \hat{A}(c,b) = \hat{A}^{(0)}(c) + c^2 + f$, $\hat{A}^{(0)}(c)$ is the operator of modified angular functions [13] that at $b = 0$ corresponds to prolate spheroidal functions [14]

$$\hat{A}^{(0)}(c) = -\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta} + \frac{m_z^2}{1-\eta^2} + c^2(\eta^2-1) - b\eta, \quad (26)$$

where $c = \bar{\omega}\bar{r}^2$, $b = -2\bar{\omega}^2\bar{z}_c\bar{r}^3$, and $f = (\bar{\omega}\bar{z}_c\bar{r})^2$ are the parameter depending on $\bar{\omega}$, z_c, and $\bar{r} \in \mathbf{R}^1_+$. The wave functions $\psi_{m_z}(\bar{r},\eta,b) \equiv \psi_{m_z i}(\bar{r},\eta,b) \equiv \psi_{m_z i}(\bar{r},\eta,\bar{z}_c)$ at fixed m_z obey the conditions at the boundary of the domain $\Omega_{\bar{r},\eta} = \Omega(\bar{r},\eta)$

$$\lim_{\eta\to\pm1}(1-\eta^2)\frac{\partial\psi_{m_z}(\bar{r},\eta)}{\partial\eta} = 0, \quad \text{if} \quad m_z = 0,$$
$$\text{and} \quad \psi_{m_z}(\bar{r},\pm1) = 0, \quad \text{if} \quad m_z \neq 0,$$
$$\lim_{\bar{r}\to0}\bar{r}^2\frac{\partial\psi_{m_z}(\bar{r},\eta)}{\partial\bar{r}} = 0.$$

At large $\bar{r} = \bar{r}_{\max} \gg 1$ the discrete-spectrum wave functions obey the Dirichlet boundary condition that follows from the asymptotic behavior of the solution

$$\lim_{\bar{r}\to+\infty}\bar{r}^2\psi_{m_z}(\bar{r},\eta) = 0$$
$$\to \psi_{m_z}(\bar{r}_{\max},\eta) = 0,$$

and also the orthonormality condition

$$(a_0^*)^3\int_0^{\bar{r}_{\max}}\int_{-1}^{1}\psi_{m_z i}(\bar{r},\eta) \times \psi_{m_z j}(\bar{r},\eta)\bar{r}^2 d\bar{r}d\eta = \delta_{ij}. \quad (27)$$

The solution of (25)–(27) at fixed m_z is sought in the form of the expansion with respect to single-parameter functions $\Phi_j(\eta;\bar{r}) \equiv \Phi_{m_z j}(\eta;\bar{r})$:

$$\psi_{m_z i}(\bar{r},\eta) = \sum_{j=1}^{j_{\max}}\Phi_{m_z j}(\eta;\bar{r})\chi_{ji}(\bar{r}). \quad (28)$$

Here the vector functions $\chi_{ji}(\bar{r})$ are to be found, while the basis functions $\Phi_j(\eta;\bar{r}) \in F_{\bar{\rho}} \sim L_2[-1,1]$ are defined as a set of regular solutions of the eigenvalue problem:

$$\hat{A}(c)\Phi_{m_z j}(\eta;\bar{r}) = \bar{E}_j(\bar{r})\Phi_{m_z j}(\eta;\bar{r}). \quad (29)$$

The eigenfunctions $\Phi_{m_z j}(\eta;\bar{r}) \equiv \Phi_{m_z j}(\bar{r},\eta,z_c)$ at fixed m_z obey the symmetry condition $\Phi_{m_z j}(\bar{r},\eta,\bar{z}_c) = \exp(i\pi\nu_{m_z q})\Phi_{m_z j}(\bar{r},-\eta,-\bar{z}_c)$, where $\nu_{m_z q}$ is the real phase, q is the number of zeros in $\eta \in [-1,1]$, $\bar{E}_j(\bar{r},\bar{z}_c) = \bar{E}_j(\bar{r},-\bar{z}_c)$, and the boundary conditions with respect to the variable η, analogous to those imposed on the wave function $\psi_j(\eta,\bar{r})$ at each fixed value of the parameter $\bar{r} \in \mathbf{R}^1_+$

$$\lim_{\eta\to\pm1}(1-\eta^2)\frac{\partial\Phi_{m_z j}(\eta;\bar{r})}{\partial\eta} = 0, \quad \text{if} \quad m_z = 0,$$
$$\text{and} \quad \Phi_{m_z j}(\bar{r},\pm1) = 0, \quad \text{if} \quad m_z \neq 0, \quad (30)$$

as well as the orthonormality conditions in the interval $\Omega_\eta = [-1,1]$:

$$\langle\Phi_{m_z i}(\eta;\bar{r})|\Phi_{m_z j}(\eta;\bar{r})\rangle_{\Omega_\eta} = \int_{-1}^{1}\Phi_{m_z i}(\eta;\bar{r})\Phi_{m_z j}(\eta;\bar{r})d\eta = \delta_{ij}. \quad (31)$$

By means of the variation of the corresponding Rayleigh–Ritz functional [7, 8] using the expansion (28) Eq. (25) is reduced to the set of $j_{\max}$ ordinary differential equations of the second order with respect to the unknown functions $\chi(\bar{r}) \equiv \chi^{(i)}(\bar{r})$:

$$\left(-\frac{1}{\bar{r}^{d-1}}\mathbf{I}\frac{d}{d\bar{r}}\bar{r}^{d-1}\frac{d}{d\bar{r}} + \frac{\mathbf{U}(\bar{r})}{\bar{r}^2} + \mathbf{Q}(\bar{r})\frac{d}{d\bar{r}} + \frac{1}{\bar{r}^{d-1}}\frac{d\bar{r}^{d-1}\mathbf{Q}(\bar{r})}{d\bar{r}} - 2\bar{E}\mathbf{I}\right)\boldsymbol{\chi}(\bar{r}) = 0. \quad (32)$$

Here, $d = 3$ is the dimensionality of the space, $\mathbf{I}$, $\mathbf{U}(\bar{r})$, and $\mathbf{Q}(\bar{r})$ are $j_{\max}\times j_{\max}$ matrices with the elements defined by the relations similar to (21) with $\mathbf{V}(\bar{r})$ replaced with $\mathbf{U}(\bar{r})$, the Coulomb potential $-2Z\bar{r}\delta_{ij}$ added and with additional division by $\bar{r}^2$ due to the definition of $\hat{A}(c)$:

$$U_{ij}(\bar{r}) = \bar{r}^2 H_{ij}(\bar{r}) + \frac{\bar{E}_i(\bar{r}) + \bar{E}_j(\bar{r})}{2}\delta_{ij} - 2Z\bar{r}\delta_{ij}, \quad I_{ij} = \delta_{ij}, \quad (33)$$
$$H_{ij}(\bar{r}) = H_{ji}(\bar{r}) = \left\langle\frac{\partial\Phi_i(\eta;\bar{r})}{\partial\bar{r}}\middle|\frac{\partial\Phi_j(\eta;\bar{r})}{\partial\bar{r}}\right\rangle_{\Omega_\eta},$$
$$Q_{ij}(\bar{r}) = -Q_{ji}(\bar{r}) = -\left\langle\Phi_i(\eta;\bar{r})\middle|\frac{\partial\Phi_j(\eta;\bar{r})}{\partial\bar{r}}\right\rangle_{\Omega_\eta}.$$

Note, that Eq. (29) is linear and the boundary conditions (31) are homogeneous, the sign of the phase of the basis functions $\Phi_j(\eta;\bar{r})$ is arbitrary. Hence, we fix the phase sign at the point $\eta = +1$ by the condition

$$\left.\frac{\partial}{\partial\eta}\Phi_{m_z j}(\eta;\bar{r})\right|_{\eta=+1} > 0,$$

which is necessary to calculate the integrals (33) involving the basis functions and their derivatives with respect to the parameter $\bar{r}$, i.e., the variable coefficients in Eq. (32).

Table 1. Dependence of the calculated binding energy $E_B/R_0^* = -(2\bar{E}(\bar{z}_c) - \bar{E}_i(\infty))$ of the parabolic quantum well upon the number of the basis functions $j_{\max}$, compared with the energy obtained by means of the crude adiabatic approximation (C) and variation calculation (V) from [1]

$j_{\max}$	$\bar{z}_c = 0$	$\bar{z}_c = \pm 0.2$	$\bar{z}_c = \pm 0.3$	$\bar{z}_c = \pm 0.5$
Cylindrical coordinates				
C	1.86807	1.80379	1.72781	1.51517
1	1.53006	1.44930	1.35848	1.13252
4	1.71971	1.67525	1.60682	1.40688
8	1.77801	1.71637	1.63800	1.42465
12	1.79548	1.72927	1.64846	1.43391
16	1.80389	1.73567	1.65399	1.43763
20	1.80878	1.73948	1.65764	1.43958
24	1.81194	1.74201	1.66020	1.44081
V	1.72040	1.63506	1.54708	1.32406
Spherical coordinates				
C	2.04328	2.00216	1.94853	1.77774
1	1.75493	1.62950	1.50485	1.23289
2	1.75493	1.69037	1.61395	1.40265
4	1.82171	1.75050	1.66764	1.44490
6	1.82758	1.75567	1.67215	1.44803
8	1.82773	1.75581	1.67228	1.44813
10	1.82774	1.75582	1.67229	1.44814

The discrete-spectrum solutions obey the asymptotic boundary conditions and the orthonormality condition

$$\lim_{\bar{r}\to 0} \bar{r}^{d-1} \frac{d\boldsymbol{\chi}(\bar{r})}{d\bar{r}} = 0, \tag{34}$$

$$\lim_{\bar{r}\to\infty} \bar{r}^{d-1} \boldsymbol{\chi}^{(i)}(\bar{r}) = 0 \to \boldsymbol{\chi}^{(i)}(\rho_{\max}) = 0,$$

$$(a_0^*)^d \int_0^{\bar{r}_{\max}} \bar{r}^{d-1} \left(\boldsymbol{\chi}^{(i)}(\bar{r})\right)^T \boldsymbol{\chi}^{(j)}(\bar{r}) d\bar{r} = \delta_{ij}. \tag{35}$$

4. ANALYSIS AND DISCUSSION OF NUMERICAL RESULTS

Solving the boundary problems (20)–(24) and (32)–(35), the eigenfunctions $\chi(\bar{\rho})$ and $\chi(\bar{r})$, as well as the corresponding energy eigenvalues $2\bar{E}$ are calculated, in terms of which the total energy E in reduced Rydbergs $E/R_0^* = 2\bar{E}$, the relative energy $\bar{\varepsilon}_i = 2\bar{E} - \bar{E}_i(\infty)$ with respect to the threshold $\bar{E}_i(\infty) = \bar{E}_i^{\text{th}}$ and the binding energy $\bar{\varepsilon}_i^B = -(2\bar{E} - \bar{E}_i(\infty))$ or $E_B/R_0^* = -(2\bar{E}(\bar{z}_c) - \bar{E}_i(\infty))$ are expressed. For GaAs we use the following parameters: $a_0^* = 102$ Å, $R_0^* = 5.2$ meV, $\beta = 0.067$, $\varepsilon_d = 13.18$, $L = 102$ Å, $\gamma = 3$.

Table 2. Dependence of the calculated binding energy $E_B/R_0^* = -(2\bar{E}(\bar{z}_c) - \bar{E}_i(\infty))$ of the rectangular quantum well with infinitely high walls upon the number of the basis functions $j_{\max}$, compared with the energy obtained by means of the crude adiabatic approximation (C) and variation calculation (V) from [16]

$j_{\max}$	$\bar{z}_c = 0$	$\bar{z}_c = \pm 0.1$	$\bar{z}_c = \pm 0.2$	$\bar{z}_c = \pm 0.3$	$\bar{z}_c = \pm 0.4$
C	2.38323	2.30772	2.10042	1.81957	1.55033
1	2.13116	2.02095	1.75055	1.46353	1.28534
2	2.13117	2.16691	2.02381	1.76819	1.51999
3	2.32502	2.23095	2.02692	1.78287	1.52827
4	2.32502	2.26106	2.04603	1.78449	1.52974
8	2.35034	2.27160	2.05932	1.78818	1.53035
12	2.35281	2.27363	2.06042	1.78852	1.53038
16	2.35338	2.27409	2.06065	1.78863	1.53041
20	2.35356	2.27422	2.06074	1.78869	1.53042
24	2.35366	2.27430	2.06079	1.78871	1.53042
V	2.31025	2.21933	1.99129	1.72052	1.48128

Model A. The calculations for the parabolic quantum well were carried out with $Z = 1$, $\bar{\omega} = 3$, $m_z = 0$, and $\bar{z}_c \in [-0.5, 0.5]$ using the software package, based on the program KANTBP [7], implementing the finite-element method for solving the boundary problems (11), (13), (14) (or (16), (18), (19)) and (29)–(31) on the grids $\Omega_{\bar{z}} = \{-12(70) - 5(100) - 1(200)1(100)5(70)12\}$ and $\Omega_\eta = \{-1(800)1\}$ with the Lagrange elements of the order $p = 4$ between the nodes, respectively (the number of elements given in parentheses). For the problems (20)–(24) and (32)–(35) we used the finite-element grid $\Omega_{\bar{\rho}} = \Omega_{\bar{r}} = \{0(200)1(200)5(200)100\}$ with the Lagrange elements of the order $p = 4$ between the nodes, $\bar{\rho} = \bar{\rho}_{\max}$.

As follows from the theorem [15], for the ground state the adiabatic approximation ($j_{\max} = 1$) gives the upper bound for the energy, while in the so-called crude adiabatic approximation, when the diagonal adiabatic positive correction $H_{jj}(\bar{\rho}) = 0$ is neglected, one gets the lower bound for the energy. The corresponding inverse estimators for the binding energy E_B/R_0^* in cylindrical and spherical coordinates are presented in Table 1. From this table it fol-

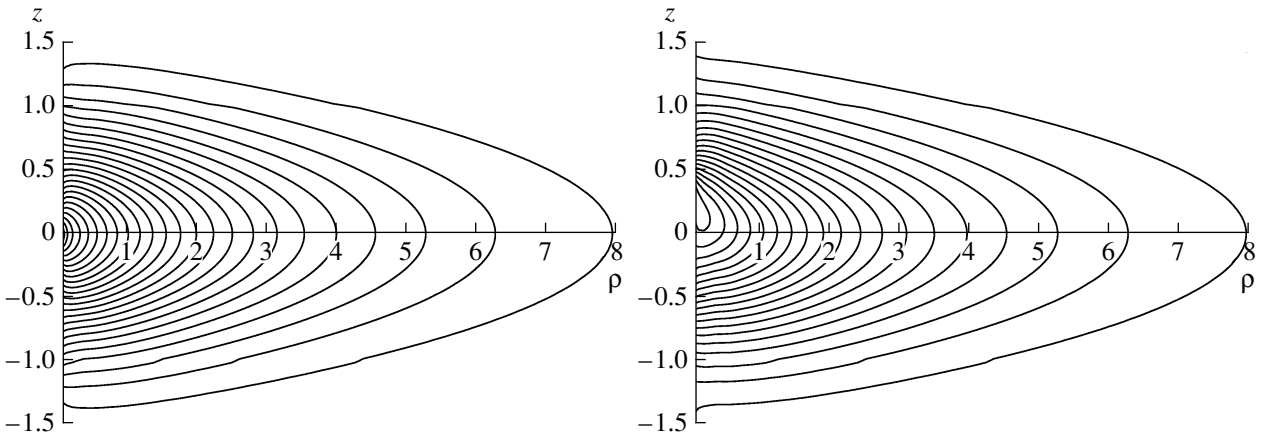

Fig. 2. Isolines of ground-state wave function of Model A for values of parameters $m_z = 0$, $Z = 1$, and $\bar{\omega} = 3$. Left panel: $\bar{z}_c = 0$, right panel: $\bar{z}_c = 0.4$.

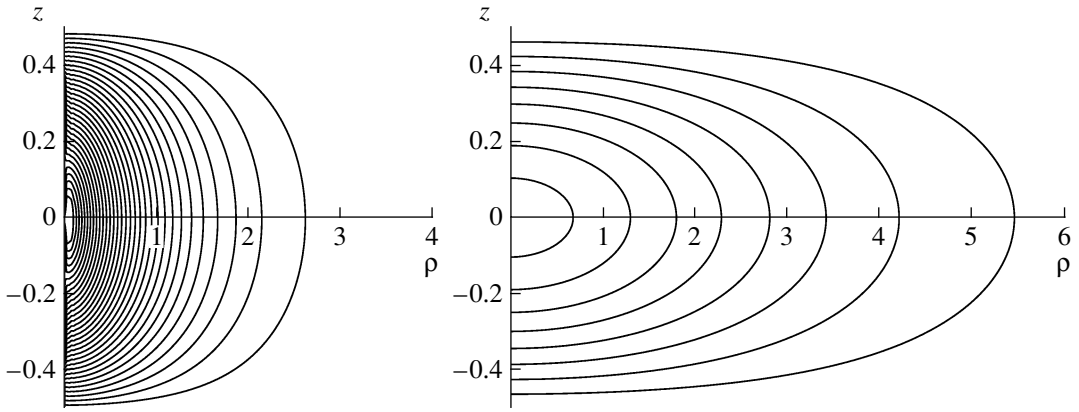

Fig. 3. Isolines of ground-state wave function of Model B for values of parameters $m_z = 0$, $Z = 1$, and $\bar{L} = 1$. Left panel: $\bar{z}_c = 0$, right panel: $\bar{z}_c = 0.4$.

lows that these values are upper and lower estimates of the binding energy from the variational calculation [1]. The corresponding inverse lower estimators of the binding energy for increasing number of single-parameter basis functions $j_{\max}$ allow one to analyze the convergence rate of the method used for the solution of the boundary problem in the two-dimensional domain (for example, see Fig. 2). As seen from table 1, the lower estimate of the binding energy, calculated in the cylindrical coordinates at $j_{\max} = 4$, is closest to the variational calculation. This is because in the variational calculation at all values of $\bar{\rho} \in \mathbf{R}_1{}^+$ the function $B_1^{(0)}$ of the ground state of the oscillator with the threshold energy $\bar{E}_1^{\text{th}} = \bar{\omega}$, corresponding to the single-parameter basis function $B_1(\bar{z}; \bar{\rho} \to \infty)$ at $\bar{\rho} \to \infty$, was used. From Table 1 it is seen that the rate of convergence with respect to the basis functions' number in the spherical parameterization (29) is considerably higher than that in the cylindrical one (11), (16). This is due to the singular behavior of the Coulomb potential, which for the choice of the basis in the cylindrical parameterization leads to the solution of the problem in the class of generalized functions belonging to the Sobolev space W_2^1.

Model B. The calculations for the rectangular quantum well with infinitely high walls were carried out with $Z = 1$, $\bar{L} = 1$, $m_z = 0$ and $\bar{z}_c \in (-0.5, 0.5)$ using the above-mentioned software package implementing the finite-element method for solving the boundary problems (12), (13), (14) (or (17), (18), (19)) on the grid $\Omega_{\bar{z}} = \{-0.5(200)0.25(200)0.25(200)0.5\}$ with the Lagrange elements of the order $p = 4$ between the nodes (the number of elements given in parentheses). For the problem (20)–(24) we used the finite-element grid $\Omega_{\bar{\rho}} = \Omega_{\bar{r}} = \{0(50)1(50)5(50)100\}$ with the Lagrange elements of the order $p = 4$ between the nodes. $\bar{\rho} = \bar{\rho}_{\max}$.

The corresponding inverse estimators of the binding energy E_B/R_0^*, calculated in the cylindrical co-

ordinates, are presented in Table 2. From this table it follows that these values are upper and lower estimates of the binding energy from the variational calculations, carried out in [2]. The corresponding inverse lower estimates of the binding energy for increasing number $j_{\max}$ of single-parameter basis functions alow one to analyze numerically the rate of convergence of the method of solving the boundary problem in the two-dimensional domain (for example, see Fig. 3). As seen from Table 2, the lower estimate of the binding energy, calculated in the cylindrical coordinates at $j_{\max} = 4$ is closest to the variational calculation. This is because in the variational calculation at all values of $\bar{\rho} \in \mathbf{R}_1{}^+$ the function $B_1^{(0)}$ of the ground state of the rectangular well with the threshold energy $\bar{E}_1^{\text{th}} = \pi^2/L^2$, corresponding to the single-parameter basis function $B_1(\bar{z}; \bar{\rho} \to \infty)$ at $\bar{\rho} \to \infty$ was used.

5. CONCLUSION

We presented the scheme of the solution of the boundary problem with discrete spectrum for a parabolic quantum well and a rectangular quantum well with infinitely high walls in the adiabatic representation. The upper and lower bounds for the energy of the ground state of the systems are obtained under the conditions of the shift of the Coulomb center in a given range of the parameter with respect to earlier variational estimates. It is shown that the rate of convergence depends significantly on the appropriate choice of the adiabatic basis parameterization taking the specific features of the considered problem into account. The presented results allow one to estimate the efficiency of the method and the software package developed for the investigation of the semiconductor nanostructure models. Further development of the method and the software package is planned in relation with solving the quasi-2D and quasi-1D boundary problems with both discrete and continuous spectrum, which are necessary for calculating the optical transition rates and transport characteristics in the models like quantum wells and quantum wires.

The work was carried out in the framework of the Collaboration Protocol JINR-YeSU 3720 of May 26, 2006 and the National Program of the Republic of Armenia "Semiconductor micro- and nanoelectronics" and supported partially by RFBR (grants nos. 07-01-00660 and 08-01-00604) and CRDF–NFSAT (grant no. UC-06/07).

REFERENCES

1. E. M. Kazaryan, A. A. Kostanyan, and H. A. Sarkisyan, Physica E **28**, 423 (2005).
2. M. S. Atoyan, E. M. Kazaryan, and H. A. Sarkisyan, Physica E **22**, 860 (2004); A. M. Kazaryan and E. M. Kazaryan, Fiz. Tekh. Poluprovodnikov **7**, 1983 (1977) [Sov. Phys. Semicond. **7**, 1322 (1977)]; G. Bastard, Phys. Rev. B **24**, 4714 (1981).
3. A. N. Vasilyev, S. I. Vinitsky, and D. A. Tarkhov, in *Computer Modeling* (Polytechn. Univ., Saint-Petersburg, 2007), p. 90 [in Russian].
4. H. Voss, Comput. Phys. Commun. **174**, 441 (2006).
5. W. Wang, T.-M. Hwang, and J.-C. Jang, Comput. Phys. Commun. **174**, 371 (2006).
6. L. V. Kantorovich and V. I. Krylov, *Approximate Methods of Higher Analysis* (Interscience, New York, 1964).
7. O. Chuluunbaatar et al., Comput. Phys. Commun. **177**, 649 (2007).
8. O. Chuluunbaatar et al., Comput. Phys. Commun. **178**, 301 (2008).
9. A. I. Gusev, and A. A. Rempel, *Nanocrystalline Materials* (Cambridge Int. Sci., Cambridge, 2004); A. I. Gusev, *Nanomateries, Nanostructures, Nanotechnologies* (Fizmatlit, Moscow, 2007) [in Russian].
10. A. N. Tikhonov and A. A. Samarskii, *Equations of Mathematical Physics* (Dover, New York, 1990), p. 777.
11. R. Loudon, Am. J. Phys. **27**, 649 (1959); S. I. Vinitsky, G. S. Pogosyan, A. N. Sissakian, and V. M. Ter-Antonyan, Preprint no. P2-86-571, JINR (Dubna, 1986); L. D. Landau and E. M. Lifshitz, *Quantum Mechanics*, 3rd ed. (Pergamon, Oxford, 1977).
12. L. G. Mardoyan, G. S. Pogosyan, A. N. Sissakian, and V. M. Ter-Antonyan, *Quantum Systems with Hidden Symmetry. Interbasis Expansions* (Fizmatlit, Moscow, 2006) [in Russian].
13. S. Yu. Slavyanov and W. Lay, *Special Functions* (Oxford Univ., Oxford, 2000).
14. M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1972).
15. F. D. Bratsev, Dokl. Akad. Nauk SSSR **160**, 570 (1965) [Sov. Phys. Dokl. **10**, 44 (1965)].
16. A. A. Kostanyan, PhD Thesis (Russ.-Armen. (Slavonic) Univ., Yerevan, 2007).