

PAPER • OPEN ACCESS

Parametric bases for elliptic boundary value problem

To cite this article: A.A. Gusev *et al* 2018 *J. Phys.: Conf. Ser.* **965** 012016

View the [article online](#) for updates and enhancements.

Related content

- [ELLIPTIC BOUNDARY VALUE PROBLEMS FOR PSEUDODIFFERENTIAL OPERATORS ON MANIFOLDS WITH CONICAL POINTS](#)
A I Kome
- [THE STRONG ZERO THEOREM FOR AN ELLIPTIC BOUNDARY VALUE PROBLEM IN AN ANGLE](#)
V A Kozlov
- [MULTIPLE COMPLETENESS IN THE SENSE OF M. V. KELDYSHOV ROOT FUNCTIONS OF ELLIPTIC BOUNDARY VALUE PROBLEMS WITH A POLYNOMIAL SPECTRAL PARAMETER](#)
S Ya Yakubov

Parametric bases for elliptic boundary value problem

A.A. Gusev¹, S.I. Vinitsky^{1,2}, O. Chuluunbaatar^{1,3}, V.L. Derbov⁴,
A. Gózdź⁵, P. M. Krassovitskiy⁶

¹Joint Institute for Nuclear Research, Dubna, Russia

²RUDN University, Moscow, Russia, 6 Miklukho-Maklaya st, Moscow, 117198

³Institute of Mathematics, National University of Mongolia, Ulaanbaatar, Mongolia

⁴N.G. Chernyshevsky Saratov National Research State University, Saratov, Russia

⁵Institute of Physics, Maria Curie Skłodowska University, Lublin, Poland

⁶Institute of Nuclear Physics, Almaty, Kazakhstan

E-mail: gooseff@jinr.ru

Abstract. We consider the calculation schemes in the framework of Kantorovich method that consist in the reduction of a 3D elliptic boundary-value problem (BVP) to a set of second-order ordinary differential equations (ODEs) using the parametric basis functions. These functions are solution of the 2D parametric BVP. The coefficients in the ODEs are the parametric eigenvalues and the potential matrix elements expressed by the integrals of the eigenfunctions multiplied by their first derivatives with respect to the parameter. We calculate the parametric basis functions numerically in the general case using the high-accuracy finite element method. The efficiency of the proposed calculation schemes and algorithms is demonstrated by the example of the BVP describing the bound states of helium atom.

1. Introduction

The adiabatic representation is widely applied for solving multichannel scattering and bound-state problems for systems of a few quantum particles in molecular, atomic and nuclear physics [1]. Such problems are described by elliptic boundary value problems (BVPs) in a multidimensional domain of the configuration space, solved using the Kantorovich method[2], i.e., the reduction to a set of self-adjoint ordinary differential equations (ODEs) using the basis of surface functions of an auxiliary BVP depending on the independent variable of the ODEs parametrically.

We propose new calculation schemes and algorithms for solving the parametric self-adjoint elliptic BVP with the Dirichlet and/or Neumann type boundary conditions in a 2D finite domain, using high-accuracy finite element method (FEM) with triangular Lagrange elements [3]. The corresponding algorithm and programs calculate with given accuracy the parametric eigenvalues, the surface eigenfunctions with their parametric derivatives, and the potential matrix elements, expressed as integrals of the products of surface eigenfunctions and/or their first derivatives with respect to the parameter, which is a key problem in the adiabatic representation. These parametric eigenvalues (potential curves) and the potential matrix elements can be used for reducing the 3D BVP to bound-state and multi-channel scattering problems for sets of coupled second-order ODEs with the appropriate asymptotic boundary conditions [4].

In the present paper we demonstrate the efficiency of the proposed approach by benchmark calculations of helium atom bound states.



2. The statement of the problem

Let us consider the BVP for the parametric self-adjoint 2D partial differential equation in the domain Ω_x , $x=(x_1, x_2)$ with the piecewise continuous boundary $S=\partial\Omega_x$,

$$(D(x; z) - \varepsilon_i(z)) \Phi_i(x; z) = 0, \quad (1)$$

$$D \equiv D(x; z) = -\frac{1}{g_0(x)} \left(\sum_{ij=1}^2 \frac{\partial}{\partial x_i} g_{ij}(x) \frac{\partial}{\partial x_j} \right) + U(x; z),$$

with the mixed Dirichlet/Neumann boundary conditions

$$(I) : \Phi(x; z)|_S = 0, \quad (II) : \frac{\partial \Phi(x; z)}{\partial n_D} \Big|_S = 0, \quad \frac{\partial \Phi(x; z)}{\partial n_D} = \sum_{ij=1}^2 (\hat{n}, \hat{e}_i) g_{ij}(x) \frac{\partial \Phi(x; z)}{\partial x_j}. \quad (2)$$

Here $\frac{\partial \Phi_m(z)}{\partial n_D}$ is the derivative along the conormal direction, \hat{n} is the outer normal to the boundary $S = \partial\Omega$ of Ω , \hat{e}_i is the unit vector of $x = \sum_{i=1}^2 \hat{e}_i x_i$, and (\hat{n}, \hat{e}_i) is the scalar product in \mathcal{R}^2 , $z \in \Omega_z = [z_{\min}, z_{\max}]$ is a parameter. We assume that the functions $g_0(x) > 0$, $g_{ij}(x) > 0$, and $\partial_{x_k} g_{ij}(x)$, $U(x; z)$, $\partial_z U(x; z)$ and $\partial_z \Phi_i(x; z)$ are continuous and bounded for $x \in \Omega_x$; $g_{12}(x) = g_{21}(x)$, $g_{11}(x)g_{22}(x) - g_{12}^2(x) > 0$. We also assume that the elliptic BVP (1)–(2) has only the discrete spectrum, so that $\varepsilon(z) : \varepsilon_1(z) < \dots < \varepsilon_{j_{\max}}(z) < \dots$ is the desired set of real eigenvalues. The eigenfunctions satisfy the orthonormality conditions

$$\langle \Phi_i | \Phi_j \rangle = \int_{\Omega} g_0(x) \Phi_i(x; z) \Phi_j(x; z) dx = \delta_{ij}, \quad dx = dx_1 dx_2. \quad (3)$$

The FEM solution of the BVP (1)–(3) is reduced to the determination of stationary points of the variational functional [3, 5]

$$\Xi(\Phi_m, \varepsilon_m(z)) \equiv \int_{\Omega} dx g_0(x) \Phi_m(x; z) (D - \varepsilon_m(z)) \Phi(x; z) = \Pi(\Phi_m, \varepsilon_m(z)), \quad (4)$$

where $\Pi \equiv \Pi(\Phi_m, \varepsilon_m(z))$, $\Phi_m \equiv \Phi_m(x; z)$ is the symmetric quadratic functional

$$\Pi = \int_{\Omega} dx \left[\sum_{ij=1}^2 g_{ij}(x) \frac{\partial \Phi_m}{\partial x_i} \frac{\partial \Phi_m}{\partial x_j} + g_0(x) \Phi_m (U(x; z) - \varepsilon_m(z)) \Phi_m \right].$$

In the FEM, the function $\Phi(x; z) \in \mathcal{F}_z^h \sim \mathcal{H}^1(\Omega_x)$ is approximated by the finite sum [3]

$$\Phi^h(x; z) = \sum_{l=1}^N \Phi_l^h(z) N_l^p(x), \quad (5)$$

where the piecewise polynomial functions $N_l^p(x)$ in the domain Ω are constructed by joining the shape functions $\varphi_l^p(x)$ in the triangular subdomains Δ_q :

$$N_l^p(x) = \{\varphi_l^p(x), A_l \in \Delta_q; 0, A_l \notin \Delta_q\}$$

and possess the following properties: i) the functions $N_l^p(x)$ are continuous in the domain Ω ; ii) the functions $N_l^p(x)$ equal 1 at one of the points A_l and zero at the rest points; iii) $N_l^p(x_{1l'}, x_{2l'}) = \delta_{ll'}$ in the entire domain Ω . Here l takes the values $l = \overline{1, N}$.

The functions $N_l^p(x)$ form a basis in the space of polynomials of the p -th order. The vector function $\Phi^h = \{\Phi_l^h(z)\}_{l=1}^N$ has a generalized first-order partial derivative and belongs to the Sobolev space $\mathcal{H}^1(\Omega_x)$ [6]. After substituting the expansion (5) into the variational functional and minimizing it [5, 6], we arrive at the generalized eigenvalue problem

$$\mathbf{A}^p \Phi^h = \varepsilon^h \mathbf{B}^p \Phi^h. \quad (6)$$

Here \mathbf{A}^p is the stiffness matrix; \mathbf{B}^p is the positive definite mass matrix; Φ^h is the vector approximating the solution on the finite-element grid; and $\varepsilon^h \equiv \varepsilon^h(z)$ is the corresponding eigenvalue. The matrices \mathbf{A}^p and \mathbf{B}^p have the form $\mathbf{A}^p = \{a_{ll'}^p\}_{ll'=1}^N$, $\mathbf{B}^p = \{b_{ll'}^p\}_{ll'=1}^N$, where the matrix elements $a_{ll'}^p$ and $b_{ll'}^p$ are calculated for triangular elements as

$$\begin{aligned} a_{ll'}^p &= \sum_{i,j=1}^2 \int_{\Delta_q} g_{ij} \frac{\partial \varphi_l^p(x; z)}{\partial x_i} \frac{\partial \varphi_{l'}^p(x; z)}{\partial x_j} dx + \int_{\Delta_q} g_0(x) \varphi_l^p(x; z) \varphi_{l'}^p(x; z) U(x; z) dx, \\ b_{ll'}^p &= \int_{\Delta_q} g_0(x) \varphi_l^p(x; z) \varphi_{l'}^p(x; z) dx. \end{aligned} \quad (7)$$

3. The Algorithm for Calculating the Parametric Derivatives of Eigenfunctions

Differentiating Eqs. (1)–(3) with respect to the parameter z , we find that $\partial_z \Phi_i(x; z)$ is a solution of the following boundary-value problem with the mixed boundary conditions

$$\begin{aligned} (D(x; z) - \varepsilon_i(z)) \frac{\partial \Phi_i(x; z)}{\partial z} &= - \left[\frac{\partial}{\partial z} (U(x; z) - \varepsilon_i(z)) \right] \Phi_i(x; z), \\ \frac{\partial \Phi(x; z)}{\partial z} \Big|_S &= 0 \quad \text{or} \quad \frac{\partial^2 \Phi(x; z)}{\partial n_D \partial z} \Big|_S = 0. \end{aligned} \quad (8)$$

The parametric BVP (8) has a unique solution, if and only if it satisfies the conditions

$$\frac{\partial \varepsilon_i(z)}{\partial z} = \int_{\Omega} dx g_0(x) \Phi_i(x; z) \frac{\partial U(x; z)}{\partial z} \Phi_i(x; z), \quad \int_{\Omega} dx g_0(x) \Phi_i(x; z) \frac{\partial \Phi_i(x; z)}{\partial z} = 0. \quad (9)$$

Below we present the efficient numerical method that allows the calculation of $\partial_z \Phi_i(x; z)$ with the same accuracy as the one achieved for the eigenfunctions of the BVP (1)–(3) and the use of it for computing the effective potentials $H_{ij}(z) = H_{ji}(z)$ and $Q_{ij}(z) = -Q_{ji}(z)$ defined as

$$H_{ij}(z) = \int_{\Omega} dx g_0(x) \frac{\partial \Phi_i(x; z)}{\partial z} \frac{\partial \Phi_j(x; z)}{\partial z}, \quad Q_{ij}(z) = - \int_{\Omega} dx g_0(x) \Phi_i(x; z) \frac{\partial \Phi_j(x; z)}{\partial z}. \quad (10)$$

The boundary-value problem (8)–(9) is reduced to the linear system of inhomogeneous algebraic equations with respect to the unknown $\partial \Phi^h / \partial z$:

$$\mathbf{L} \frac{\partial \Phi^h}{\partial z} \equiv (\mathbf{A}^p - \varepsilon^h \mathbf{B}^p) \frac{\partial \Phi^h}{\partial z} = b, \quad b = - \left(\frac{\partial \mathbf{A}^p}{\partial z} - \frac{\partial \varepsilon^h}{\partial z} \mathbf{B}^p \right) \Phi^h. \quad (11)$$

The normalization condition (3), the condition of orthogonality between the function and its parametric derivative and the additional conditions (9) for the solution of (11) read as

$$\left(\Phi^h \right)^T \mathbf{B}^p \Phi^h = 1, \quad \left(\frac{\partial \Phi^h}{\partial z} \right)^T \mathbf{B}^p \Phi^h = 0, \quad \frac{\partial \varepsilon^h}{\partial z} = \left(\Phi^h \right)^T \frac{\partial \mathbf{A}^p}{\partial z} \Phi^h. \quad (12)$$

Then the potential matrix elements $H_{ij}^h(z)$ and $Q_{ij}^h(z)$ (10) can be calculated using the formulas

$$H_{ij}^h(z) = \left(\frac{\partial \Phi_i^h}{\partial z} \right)^T \mathbf{B}^p \frac{\partial \Phi_j^h}{\partial z}, \quad Q_{ij}^h(z) = - \left(\Phi_i^h \right)^T \mathbf{B}^p \frac{\partial \Phi_j^h}{\partial z}. \quad (13)$$

Since ε^h is an eigenvalue of (6), the matrix \mathbf{L} in Eq. (11) is degenerate. In this case, the algorithm for solving Eq. (11) can be written in three steps as follows:

Step k1. Calculate the solutions \mathbf{v} and \mathbf{w} of the auxiliary inhomogeneous systems of algebraic equations

$$\bar{\mathbf{L}}\mathbf{v} = \bar{\mathbf{b}}, \quad \bar{\mathbf{L}}\mathbf{w} = \mathbf{d}, \quad (14)$$

with the non-degenerate matrix $\bar{\mathbf{L}}$ and the right-hand sides $\bar{\mathbf{b}}$ and \mathbf{d}

$$\bar{L}_{ss'} = \begin{cases} L_{ss'}, & (s-S)(s'-S) \neq 0, \\ \delta_{ss'}, & (s-S)(s'-S) = 0, \end{cases} \quad (15)$$

$$\bar{b}_s = \begin{cases} b_s, & s \neq S, \\ 0, & s = S, \end{cases} \quad d_s = \begin{cases} L_{sS}, & s \neq S, \\ 0, & s = S, \end{cases} \quad (16)$$

where S is the number of the element of the vector $\mathbf{B}^p \Phi^h$ having the greatest absolute value.

Step k2. Evaluate the coefficient γ

$$\gamma = -\frac{\gamma_1}{(\mathbf{D}_S - \gamma_2)}, \quad \gamma_1 = \mathbf{v}^T \mathbf{B}^p \Phi^h, \quad \gamma_2 = \mathbf{w}^T \mathbf{B}^p \Phi^h, \quad \mathbf{D}_S = (\mathbf{B}^p \Phi^h)_S. \quad (17)$$

Step k3. Evaluate the vector $\partial_z \Phi^h$

$$\frac{\partial \Phi_s^h}{\partial z} = \begin{cases} v_s - \gamma w_s, & s \neq S, \\ \gamma, & s = S. \end{cases} \quad (18)$$

From the above consideration, it is evident that the computed derivative has the same accuracy as the calculated eigenfunction itself. Let $D(x; z)$ in Eq. (1) be a continuous and bounded positive definite operator on the space \mathcal{H}^1 with the energy norm, $\varepsilon_i(z)$, $\Phi_i(x, z) \in \mathcal{H}^2$ being the exact solutions of Eqs. (1)–(3), and $\varepsilon_i^h(z)$, $\Phi_i^h(x; z) \in \mathcal{H}^1$ being the corresponding numerical solutions. Then the following estimates are valid [6]

$$\left| \varepsilon_i(z) - \varepsilon_i^h(z) \right| \leq c_1 h^{2p}, \quad \left\| \Phi_i(x; z) - \Phi_i^h(x; z) \right\|_0 \leq c_2 h^{p+1}, \quad (19)$$

$$\left\| \Phi_i(x; z) \right\|_0^2 = \int_{\Omega_x} dx g_0(x) \Phi_i(x; z) \Phi_i(x; z), \quad (20)$$

where h is the largest distance between any two points in Δ_q , p is the order of the finite elements, i is the number of the corresponding solutions, and the constants c_1 and c_2 are independent of the step h . The following theorem can be formulated.

Theorem Let $D(x; z)$ in Eq. (1) be a continuous and bounded positive definite operator on the space \mathcal{H}^1 with the energy norm. Also let $\partial_z U(x; z)$ be continuous and bounded for each value of the parameter z . Then for the exact values of the solutions $\partial_z \varepsilon_i(z)$, $\partial_z \Phi_i(x; z) \in \mathcal{H}^2$, $H_{ij}(z)$, $Q_{ij}(z)$ from (8)–(10) and the corresponding numerical values $\partial_z \varepsilon_i^h(z)$, $\partial_z \Phi_i^h(x; z) \in \mathcal{H}^1$, $H_{ij}^h(z)$, $Q_{ij}^h(z)$ from (11)–(13), the following estimates are valid:

$$\left| \frac{\partial \varepsilon_i(z)}{\partial z} - \frac{\partial \varepsilon_i^h(z)}{\partial z} \right| \leq c_3 h^{2p}, \quad \left\| \frac{\partial \Phi_i(x; z)}{\partial z} - \frac{\partial \Phi_i^h(x; z)}{\partial z} \right\|_0 \leq c_4 h^{p+1}, \quad (21)$$

$$\left| Q_{ij}(z) - Q_{ij}^h(z) \right| \leq c_5 h^{2p}, \quad \left| H_{ij}(z) - H_{ij}^h(z) \right| \leq c_6 h^{2p},$$

where h is the largest distance between any two points of the finite element Δ_q , p is the order of finite elements, i, j are the numbers of the corresponding solutions, and the constants c_3, c_4, c_5 , and c_6 are independent of the step h .

The proof is straightforward following the scheme in accordance with [6].

4. Benchmark calculations of helium atom bound states

In the hyperspheroidal coordinates, $0 \leq \rho < \infty$, $1 \leq \xi < \infty$, $-1 \leq \eta \leq 1$, related to the perimetrical ones r_1, r_2 and r_{12} as

$$r_{12} = \sqrt{2}\rho/\sqrt{\xi^2 + \eta^2}, \quad r_1 = \rho(\xi + \eta)/(\sqrt{2}\sqrt{\xi^2 + \eta^2}), \quad r_2 = \rho(\xi - \eta)/(\sqrt{2}\sqrt{\xi^2 + \eta^2}), \quad (22)$$

the equation for the solution $\Psi(\rho, \xi, \eta) = \sqrt{\xi^2 + \eta^2}\Phi(\rho, \xi, \eta)$ describing S-states of the Helium atom reads as [7]

$$\left[-\frac{1}{\rho^5} \frac{\partial}{\partial \rho} \rho^5 \frac{\partial}{\partial \rho} - \frac{3}{\rho^2} + \frac{1}{\rho^2} \frac{(\xi^2 + \eta^2)^2}{\xi^2 - \eta^2} h(\xi, \eta; \rho) - 2E_m \right] \Phi_m(\rho, \xi, \eta) = 0, \quad (23)$$

$$h(\xi, \eta; \rho) = -\frac{\partial}{\partial \xi} (\xi^2 - 1) \frac{\partial}{\partial \xi} - \frac{\partial}{\partial \eta} (1 - \eta^2) \frac{\partial}{\partial \eta} + \frac{\sqrt{2}\rho(\xi^2 - \eta^2 - 8\xi)}{\sqrt{\xi^2 + \eta^2}^3}. \quad (24)$$

The function $\Phi_m(\rho, \xi, \eta)$ satisfies the boundary conditions (BCs)

$$\lim_{\rho \rightarrow 0} \rho^5 \frac{\partial \Phi_m(\rho, \xi, \eta)}{\partial \rho} = 0, \quad \lim_{\rho \rightarrow \infty} \rho^5 \Phi_m(\rho, \xi, \eta) = 0, \quad (25)$$

$$\lim_{\xi \rightarrow 1} (\xi^2 - 1) \frac{\partial \Phi_m(\rho, \xi, \eta)}{\partial \xi} = 0, \quad \lim_{\xi \rightarrow \infty} \Phi_m(\rho, \xi, \eta) = 0, \quad \lim_{\eta \rightarrow \pm 1} (1 - \eta^2) \frac{\partial \Phi_m(\rho, \xi, \eta)}{\partial \eta} = 0, \quad (26)$$

and is normalized by the condition

$$8\pi^2 \int_0^\infty dR R^5 \int_1^\infty d\xi \int_{-1}^1 d\eta \frac{\xi^2 - \eta^2}{(\xi^2 + \eta^2)^2} \Phi_m(R, \xi, \eta) \Phi_{m'}(R, \xi, \eta) = \delta_{mm'}. \quad (27)$$

The parametric functions $\phi_i \equiv \phi_i(\xi, \eta; \rho)$ and the eigenvalues $\varepsilon_i(\rho)$ are eigensolutions of the 2D BVP having purely discrete spectrum. The functions satisfy the BCs (26) and the normalization condition

$$\left[h(\xi, \eta; \rho) - \varepsilon_i(\rho) \frac{\xi^2 - \eta^2}{(\xi^2 + \eta^2)^2} \right] \phi_i = 0, \quad \langle \phi_i | \phi_j \rangle = \int_1^\infty d\xi \int_{-1}^1 d\eta \frac{\xi^2 - \eta^2}{(\xi^2 + \eta^2)^2} \phi_i(\xi, \eta; \rho) \phi_j(\xi, \eta; \rho) = \delta_{ij}. \quad (28)$$

The 2D BVP (28) was solved in terms of scaled variable and parametric surface functions

$$\xi = \xi(\lambda) = \frac{1 + \lambda}{1 - \lambda}, \quad 0 \leq \lambda < 1, \quad \phi_i(\xi, \eta; \rho) = \frac{p_i(\xi, \eta; \rho)}{\xi + 1} \equiv \frac{p_i(\lambda, \eta; \rho)}{\xi(\lambda) + 1}. \quad (29)$$

As an example consider the calculation of the potential curves $E_j(\rho) = (\varepsilon_j(\rho) - 3)/\rho^2$ and the matrix elements

$$Q_{ij}(\rho) = - \left\langle \phi_i(\xi, \eta; \rho) \left| \frac{\partial \phi_j(\xi, \eta; \rho)}{\partial \rho} \right. \right\rangle, \quad H_{ij}(\rho) = \left\langle \frac{\partial \phi_i(\xi, \eta; \rho)}{\partial \rho} \left| \frac{\partial \phi_j(\xi, \eta; \rho)}{\partial \rho} \right. \right\rangle.$$

The calculations were implemented by means of the program POTHEA 2.0 using the server with 2x4 kernels i7k (i7-3770K 4.5 GHz, 32 GB RAM, GPU GTX680), and the Intel Fortran

compiler 17.0. The computing time per one point ρ for the considered examples with 10^{-12} accuracy with triangular Lagrange elements of 5th order on the uniform 2D grids $\lambda = \{0(L)1\}$, $\eta = \{0(L)1\}$ at $L = 10, 20, 40$ is 0.38, 5.08, and 41.21 seconds, respectively.

Let us find the solution of the BVP (23)–(27) using the Kantorovich expansion [2]

$$\Phi_m(\rho, \xi, \eta) = \sum_{j=1}^{j_{\max}} \phi_j(\xi, \eta; \rho) \chi_{jm}(\rho) \quad (30)$$

where $\phi_j(\xi, \eta; \rho)$ are eigenfunctions of the parametric 2D BVP with purely discrete spectrum $E_j(\rho) = (\varepsilon_j(\rho) - 3)/\rho^2, j = 1, 2, \dots$. Substituting the expansion (30) into the 3D BVP (23)–(26), we arrive at the 1D BVP for a finite set of j_{\max} coupled second-order ODEs for $\chi_m(\rho) = \{\chi_{1m}(\rho), \dots, \chi_{Nm}(\rho)\}^T$

$$\left(-\frac{1}{\rho^5} \mathbf{I} \frac{d}{d\rho} \rho^5 \frac{d}{d\rho} + \mathbf{V}(\rho) + \mathbf{Q}(\rho) \frac{d}{d\rho} + \frac{1}{\rho^5} \frac{d\rho^5 \mathbf{Q}(\rho)}{d\rho} - 2E_m \mathbf{I} \right) \chi_m(\rho) = 0, \quad (31)$$

with the boundary and normalization conditions for the discrete spectrum of E : $E_1 < E_2 < \dots < E_m < \dots$

$$\lim_{\rho \rightarrow 0} \rho^5 \left(\frac{d\chi_m(\rho)}{d\rho} - \mathbf{Q}(\rho) \chi_m(\rho) \right) = 0, \quad \lim_{\rho \rightarrow \infty} \rho^5 \chi_m(\rho) = 0, \quad 8\pi^2 \int_0^\infty d\rho \rho^5 (\chi_m(\rho))^T \chi_{m'}(\rho) = \delta_{mm'}. \quad (32)$$

The solution of this BVP with the help of KANTBP program [8] using Lagrange elements of the 5th order on the non-uniform grids $\rho = \{0(50)5(75)20\}$ using calculated $E_j(\rho)$, $V_{ij}(\rho) = H_{ij}(\rho) + E_j(\rho)\delta_{ij}$, $Q_{ij}(\rho)$, $i, j = 1, \dots, 12$ yields the upper estimate of the helium atom energy in the ground and the first excited state $E_1 = -2.903\,724\,30$ a.u. and $E_2 = -2.145\,973\,22$ a.u. with 8 significant digits similar to the results of POTHEA[9].

5. Conclusion

The proposed calculation schemes, algorithms and software implementing the high-accuracy FEM for solving the elliptic boundary value problems can be applied to the analysis of few-body scattering dynamics and quantum tunneling and diffraction models[10, 11, 12, 13]. Detailed description of the implementation of the FEM algorithm and program will be given elsewhere.

The authors thank Prof. F.M. Penkov for collaboration. The work was supported partially by grant MES RK 0333/GF4 and grant of Plenipotentiary Representative of the Government of the Republic of Kazakhstan in the framework of collaboration program JINR-RK N 337, 2017. The work was partially funded by the RFBR (grants Nos. 16-01-00080 and 17-51-44003 Mong), the Bogoliubov-Infeld program and the RUDN University Program 5-100.

References

- [1] Greene C H, Giannakeas P and Pérez-Ríos J 2017 *Rev. Mod. Phys.* **89** 035006
- [2] Kantorovich L V and Krylov V I 1964 *Approximate methods of higher analysis* (New York, Wiley)
- [3] Ciarlet P 1978 *The Finite Element Method for Elliptic Problems* (Amsterdam, North-Holland Publ.)
- [4] Kadomtsev M B, Vinitzky S I and Yukajlovic F R 1987 *Phys.Rev. A* **36** 4652
- [5] Bathe K J 1982 *Finite Element Procedures in Engineering Analysis*, (New York, Englewood Cliffs, Prentice Hall)
- [6] Strang G. and Fix G J 1973 *An Analysis of the Finite Element Method* (New York, Englewood Cliffs, Prentice Hall)
- [7] Vinitzky S I, Gusev A A, Chuluunbaatar O et al 2016 *Proc. SPIE* **9917** 99172Z
- [8] Chuluunbaatar O, Gusev A A, Vinitzky S I and Abrashkevich A G 2008 *Comput. Phys. Commun.* **179** 685
- [9] Gusev A A, Chuluunbaatar O, Vinitzky S I and Abrashkevich A G 2014 *Comput. Phys. Commun.* **185** 2636
- [10] Gusev A A, Vinitzky S I, Chuluunbaatar O et al 2014 *Phys. Atom. Nucl.* **77** 389
- [11] Krassovitskiy P M and Penkov F M 2014 *J. Phys. B* **47** 225210
- [12] Krassovitskiy P M and Penkov F M 2017 *Bull. Russian Acad. Sci.: Phys.* **81** 730
- [13] Gusev A A, Vinitzky S I, Chuluunbaatar O et al 2017 *Acta Phys. Polonica B Proc. Sup.* **10** 269