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SOME METHODS FOR SOLVING THE 3-D QUANTUM MECHANICS EIGENVALUE PROBLEMS *

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The methods developed in this paper are based on two step of the Kantorovich method for solving eigenvalue problems for the Coulomb three-body systems using three-dimensional (3-D) hyperspherical map in the heliocentric coordinates. The initial 3-D problem is reduced to the solution of one-dimensional systems of the coupled second-order ordinary differential equations with variable coefficients.

All essential features and peculiarities of the problems are taken into account in the present approach in a natural and exact way. New implementations of the Kantorovich method allow us to build up a new class of 1-D orthogonal parametric angular functions. The essential feature of these functions consists of the description of the typical peculiarities of various three-body interactions on the 2-D map, depending on a set of physical parameters such as charges and masses of the particles. An exact solvable model of the 1-D parametric angular functions can be used as an analytical test for the proposed schemes.

The convergence of the Kantorovich reduction is examined numerically by calculating the energies of the ground state of some quantum mechanics system. The results are illustrated in the tables. Some distinctive features of the implementation of the Kantorovich approach are discussed

1. Introduction. Currently an ongoing work is carried out at CERN on experiments ASACUSA and ATHENA [1] studying properties of the exotic antiprotonic Coulomb systems in traps at low temperatures using new abilities of modern lasers. The experiments require various data on characteristics of the Coulomb systems, such as helium atom He and antiprotonic helium atom $\overline{\mathrm{p}}\mathrm{He}^+$ [2]. Such data can be obtained using the hyperspherical adiabatic approach [3, 4] in which the long-range dipole asymptotics of the three-body systems can be taken into account in a natural and effective way [5]. The eigensolutions obtained within this method can be further used in calculations of various processes, e.g., interactions with surrounding media like $\mathrm{He} - \overline{\mathrm{p}}\mathrm{He}^+$ interactions, etc. This approach is based on the Kantorovich method [6] of reducing a multi–dimensional boundary value problem to a system of ordinary differential equations with variable coefficients. It takes account of necessary asymptotics in a natural way, satisfies the posed boundary conditions and provides a guaranteed convergence of the

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approximated solutions to the exact ones. Recently, a new method for computation of the variable coefficients (potential matrix elements of radial coupling) of a system of ordinary second-order differential equations with a given accuracy has been proposed [7] for the helium-like systems using the heliocentric coordinates.

A goal of this paper is to show the peculiarities of a modern implementation of the Kantorovich method to numerical solution of the multi–dimensional eigenvalue problems and also to point out some prospects of its application to three-body systems based on the calculations of the low-energy spectrum of the helium atom. The quantum mechanical three-body Coulomb problem with total angular momentum $J = 0$ is formulated using an appropriate 3-D hyperspherical map in the heliocentric coordinates. A reduction of the three-dimensional eigenvalue problem to the one-dimensional one is performed using several variants of the Kantorovich method. The convergence of the resulting finite system of the ordinary second-order differential equations and the efficiency of the proposed multistep procedures are illustrated for the computation of the low-energy spectrum of helium atom including the ground state.

A significant improvement over the standard techniques of the calculation of potential matrix elements of radial and angular couplings within the multistep Kantorovich method is achieved. The results of our calculations of energy of the ground state Helium atom He and negative hydrogen ion H^- are discussed and compared with the results of other calculations.

2. 3-D eigenvalue problem for the Schrödinger equation. Time-independent Schrödinger equation for a system of three charged particles with total angular momentum $J = 0$ in the hyperspherical coordinates $(\mathcal{R}, \alpha, \theta)$ can be written [7] as an eigenvalue problem for the following 3-D elliptic equation

$$\hat{T}\Psi(\mathcal{R},\alpha,\theta) + \frac{1}{\mathcal{R}}\hat{W}(\alpha,\theta)\Psi(\mathcal{R},\alpha,\theta) = \mathcal{E}\Psi(\mathcal{R},\alpha,\theta), \tag{1}$$

where $\mathcal{E}$ is the relative energy and $\Psi(\mathcal{R}, \alpha, \theta)$ is the total wave function of the system. The differential operator of kinetic energy $\hat{T}$ and the multiplication operator of the Coulomb pair interaction $R^{-1}\hat{W}$ are defined as follows ($e = \hbar = m_e = 1$):

$$\hat{T} = -\frac{1}{\mathcal{R}^2\tau}\frac{\partial}{\partial\mathcal{R}}\frac{1}{2}\mathcal{R}^2\tau\frac{\partial}{\partial\mathcal{R}} + \hat{t}, \quad \hat{t} = -\frac{1}{\tau}\left(\frac{\partial}{\partial\alpha}\frac{1}{4}\mathcal{R}\sin^2\alpha\sin\theta\frac{\partial}{\partial\alpha} + \frac{\partial}{\partial\theta}\frac{1}{4}\mathcal{R}\sin\theta\frac{\partial}{\partial\theta}\right),$$

$$\hat{W} = \frac{Z_aZ_c}{\sin\alpha/2} + \frac{Z_bZ_c}{\cos\alpha/2} + Z_aZ_b\left[1 - \sin\alpha\cos\theta\right]^{-1/2},$$

$$\tau = \frac{1}{8}\mathcal{R}^3\sin^2\alpha\sin\theta.$$

In the above, $Z_a = Z_b = -1$ and $Z_c = Z$ are the charges of particles a, b, and c with masses $M_a = 1$, $M_b = 1$, and $M_c = \infty$, respectively. Note that $Z = 1$ for the H^- negative hydrogen ion and $Z = 2$ for the He atom. Hyperradius $\mathcal{R} \in [0, \infty)$, hyperspherical angles $(\alpha, \theta) \in \Omega = \{0 \le \alpha \le \pi,\ 0 \le \theta \le \pi\}$, i.e. total set of variables $(\mathcal{R}, \alpha, \theta) \in \Omega_1 = \Omega \times [0, \infty)$.

Total wave function $\Psi(\mathcal{R}, \alpha, \theta)$ satisfies the following boundary conditions:

$$\lim_{\alpha\to 0,\pi}\sin^2\alpha\frac{\partial\Psi}{\partial\alpha} = 0, \qquad \lim_{\theta\to 0,\pi}\sin\theta\frac{\partial\Psi}{\partial\theta} = 0, \tag{2}$$

$$\lim_{\mathcal{R}\to 0} \mathcal{R}^5 \frac{\partial \Psi}{\partial \mathcal{R}} = 0, \qquad \lim_{\mathcal{R}\to \infty} \mathcal{R}^5 \Psi = 0, \tag{3}$$

and is normalized by condition

$$\int\int\int \mathcal{R}^2 \tau \Psi^2 d\alpha d\theta d\mathcal{R} = 1.$$

3. Reduction of the 3-D problem by the Kantorovich method. Consider a formal expansion of the solution of Eqs. (1)–(3) using the finite set of two-dimensional basis functions $\{\Phi_i(\alpha, \theta; \mathcal{R})\}_{i=1}^{n_{\max}}$:

$$\Psi(\mathcal{R}, \alpha, \theta) = \sum_{i=1}^{n_{\max}} \chi_i(\mathcal{R}) \Phi_i(\alpha, \theta; \mathcal{R}). \tag{4}$$

In Eq. (4), functions $\chi(\mathcal{R})^T = (\chi_1(\mathcal{R}), \chi_2(\mathcal{R}), \ldots, \chi_{n_{\max}}(\mathcal{R}))$ are unknown, and surface functions $\mathbf{\Phi}(\alpha, \theta; \mathcal{R})^T = (\Phi_1(\alpha, \theta; \mathcal{R}), \Phi_2(\alpha, \theta; \mathcal{R}), \ldots, \Phi_{n_{\max}}(\alpha, \theta; \mathcal{R}))$ form an orthonormal basis for each value of hyperradius $\mathcal{R}$ which is treated here as a slowly varying parameter.

In the Kantorovich approach [6], functions $\Phi_i(\alpha, \theta; \mathcal{R})$ are determined as solutions of the following two-dimensional parametric eigenvalue problem:

$$\left(\hat{t} + \frac{1}{\mathcal{R}}\hat{W} + \frac{2}{\mathcal{R}^2}\right) \Phi(\alpha, \theta; \mathcal{R}) = E(\mathcal{R}) \Phi(\alpha, \theta; \mathcal{R}) \tag{5}$$

with the boundary conditions derived from Eq. (2)

$$\lim_{\alpha\to 0,\pi} \sin^2\alpha \frac{\partial \Phi}{\partial \alpha} = 0, \qquad \lim_{\theta\to 0,\pi} \sin\theta \frac{\partial \Phi}{\partial \theta} = 0. \tag{6}$$

Since the operator in the left side of Eq. (5) is self-adjoint, its eigenfunctions are orthonormal:

$$\int\int \tau \Phi_i \Phi_j d\alpha d\theta = \delta_{ij}.$$

In the equation above, δ_{ij} is Kroneker's δ-symbol. Problem (5)–(6) is solved for each value of $\mathcal{R}_k \in \omega_{\mathcal{R}}$ where $\omega_{\mathcal{R}} = (\mathcal{R}_1, \mathcal{R}_2, \ldots, \mathcal{R}_k, \ldots, \mathcal{R}_{\max})$ is a given set of values of hyperradius $\mathcal{R}$.

After substitution of expansion (4) into the Rayleigh-Ritz variational functional (see [7]) and subsequent minimization of the functional, the solution of Eqs. (1)–(3) is reduced to a solution of an eigenvalue problem for the finite set of $n_{\max}$ ordinary second-order differential equations for determining energy $\mathcal{E}$ and coefficients (radial wave functions) $\chi(\mathcal{R})$ of expansion (4):

$$-\mathbf{I}\frac{1}{\mathcal{R}^2}\frac{d}{d\mathcal{R}}\mathcal{R}^2\frac{d}{d\mathcal{R}}\chi + \mathbf{U}(\mathcal{R})\chi + \mathbf{Q}(\mathcal{R})\frac{d\chi}{d\mathcal{R}} + \frac{1}{\mathcal{R}^2}\frac{d\mathcal{R}^2\mathbf{Q}(\mathcal{R})\chi}{d\mathcal{R}} = 2\mathcal{E}\mathbf{I}\chi, \tag{7}$$

$$\lim_{\mathcal{R}\to 0} \mathcal{R}^2 \frac{\partial \chi}{\partial \mathcal{R}} = 0, \qquad \lim_{\mathcal{R}\to \infty} \mathcal{R}^2 \chi = 0. \tag{8}$$

Here $\mathbf{I}$, $\mathbf{U}(\mathcal{R})$, and $\mathbf{Q}(\mathcal{R})$ are finite $n_{\max} \times n_{\max}$ matrices, the elements of which are given

by the relations

$$
\begin{aligned}
U_{ij}(\mathcal{R}) &= \left(E_i(\mathcal{R}) + E_j(\mathcal{R}) - \frac{1}{4\mathcal{R}^2}\right)\delta_{ij} + H_{ij}(\mathcal{R}),\\
H_{ij}(\mathcal{R}) &= H_{ji}(\mathcal{R}) = \iint \tau \frac{\partial \Phi_i}{\partial \mathcal{R}} \frac{\partial \Phi_j}{\partial \mathcal{R}} d\alpha d\theta - \frac{9}{4\mathcal{R}^2}\delta_{ij}\\
Q_{ij}(\mathcal{R}) &= -Q_{ji}(\mathcal{R}) = -\left(\iint \tau \Phi_i \frac{\partial \Phi_j}{\partial \mathcal{R}} d\alpha d\theta - \frac{3}{2\mathcal{R}}\delta_{i,j}\right),\\
I_{ij} &= \delta_{ij}, \quad i,j = 1,2,\ldots,n_{\max}.
\end{aligned}
\tag{9}
$$

Thus, the solution of problem (1)-(3) by the Kantorovich approach is reduced to the solution of the following problems:

1. Calculation of potential curves $E_i(\mathcal{R})$ and eigenfunctions $\Phi_i(\alpha,\theta;\mathcal{R})$ of the two-dimensional problem (5)-(6) for a given set of $\mathcal{R} \in \omega_{\mathcal{R}}$.

2. Calculation of derivatives $\dfrac{\partial \Phi_j}{\partial \mathcal{R}}$ and computation of the corresponding integrals (see Eq. (9)) necessary for obtaining matrix elements of radial coupling $U_{ij}(\mathcal{R})$ and $Q_{ij}(\mathcal{R})$.

3. Calculation of energies $\mathcal{E}$ and radial wave functions $\chi(\mathcal{R})$ as eigensolutions of one-dimensional eigenvalue problem (7)-(8) and examination of the convergence of obtained eigensolutions as a function of the number of channels $n_{\max}$.

4. Reduction of the 2-D problem by the Bubnov-Galerkin method. Two-dimensional parametric eigenvalue problem (5)–(6) can be solved directly [9] using the finite element method [10, 11]. In this paper, to solve this problem we apply the conventional Bubnov-Galerkin method described in [7]. Because of the symmetry of equation coefficients with respect to $\alpha = \pi/2$, problem (5) will be considered for $\alpha \in [0, \pi/2]$.

Consider the following expansion of basis surface function $\Phi_i(\alpha,\theta;\mathcal{R})$:

$$
\Phi_i(\alpha,\theta;\mathcal{R}) = \sum_{l=0}^{l_{\max}} \varphi_l^{(i)}(\alpha;\mathcal{R}) P_l(\cos\theta),
\tag{10}
$$

where $\varphi_l^{(i)}(\alpha;\mathcal{R})$ are expansion coefficients depending parametrically on $\mathcal{R}$ and $P_l(\cos\theta)$ are the Legendre polynomials. These polynomials are the eigensolutions of the following eigenvalue problem

$$
-\frac{d}{d\theta}\sin\theta \frac{dP_l(cos\theta}{d\theta} = \lambda_l \sin\theta \; P_l(cos\theta)
$$

with $\lambda_l = l(l+1), l = 0, 1, 2, \ldots$ being the corresponding eigenvalues.

Following [7] we find that eigenfunctions $\varphi_l^{(i)}(\alpha;\mathcal{R})$ and eigenvalues $E_i(\mathcal{R})$ satisfy the

following eigenvalue problem for a finite set of $l_{\max}$ ordinary differential equations

$$L(\varphi, E) \equiv \left[\mathcal{R}\left(-\frac{d}{d\alpha}\mathbf{D}\frac{d}{d\alpha} + \mathbf{\Lambda}\right) + \mathcal{R}^2\mathbf{W} - 2E_i(\mathcal{R})\mathcal{R}^3\mathbf{D}\right]\varphi^{(i)}(\alpha, \mathcal{R}) = 0,$$

(11)

$$\lim_{\alpha\to 0,\pi/2} \sin^2\alpha \frac{\partial\varphi}{\partial\alpha} = 0, \quad (\varphi^{(i)})^T = (\varphi_1^{(i)}, \varphi_2^{(i)}, \ldots, \varphi_{l_{\max}}^{(i)}).$$

In the above, $\mathbf{D}$, $\mathbf{\Lambda}$, and $\mathbf{W}$ are finite $l_{\max} \times l_{\max}$ matrices whose elements are defined by

$$D_{ii} = \frac{1}{4}\sin^2\alpha, \quad D_{ij} = 0, \ i \neq j, \quad \Lambda_{ii} = \frac{1}{4}\left(i(i+1) + \sin^2\alpha\right), \quad \Lambda_{ij} = 0, \ i \neq j,$$

$$W_{ij} = -Z\frac{1}{4}\sin\alpha\left(\cos\frac{\alpha}{2} + \sin\frac{\alpha}{2}\right)\delta_{ij} + \frac{1}{8}\sin^2\alpha W_{ij}^{rep},$$

$$W_{ij}^{rep} = \int_{-1}^{1} \frac{P_i(t)P_j(t)}{\sqrt{1 - t\sin\alpha}}dt, \quad i, j = 0, 1, 2, \ldots \ l_{\max}.$$

Thus, the solution of the two-dimensional eigenvalue problem (5)-(6) is reduced to the solution of eigenvalue problem (11) for a system of $l_{\max}$ ordinary second-order differential equations. A convergence of this method in respect to number of equations $l_{\max}$ has been studied in [7] for Helium like systems for an infinite mass case.

5. Computation of the matrix elements of radial coupling. Calculation of potential matrices $\mathbf{U}(\mathcal{R})$ and $\mathbf{Q}(\mathcal{R})$ (see [8, 9]) with sufficiently high accuracy is a very important step of solving system of radial equations (7), since otherwise it is practically impossible to get the desired energies and wave functions of three-body Coulomb systems with required precision. This implies that derivatives $\dfrac{d\varphi}{d\mathcal{R}}$ should be computed with the highest possible accuracy, which presents a difficult problem for most of numerical methods usually used in the adiabatic representation calculations [4].

An effective method, which allows to calculate derivative $\dfrac{d\varphi}{d\mathcal{R}}$ with the same accuracy as achieved for eigenfunctions of (11) and use it to compute matrix elements defined by formulas (9), has been developed in [7]. Here we only outline it briefly for completeness. Taking a derivative of (11) with respect to $\mathcal{R}$, we get that $\dfrac{d\varphi}{d\mathcal{R}}$ can be obtained as a solution of the following boundary problem

$$L\left(\frac{d\varphi}{d\mathcal{R}}, E\right) \equiv \left[\frac{d}{d\alpha}\mathbf{D}\frac{d}{d\alpha} - \mathbf{U} - 2\mathcal{R}\mathbf{W} + 6E(\mathcal{R})\mathcal{R}^2\mathbf{D} + 2E'(\mathcal{R})\mathcal{R}^3\mathbf{D}\right]\varphi = G. \quad (12)$$

The boundary conditions for function $\dfrac{d\varphi}{d\mathcal{R}}$ are the same as for function φ. Taking into account that $E(\mathcal{R})$ is an eigenvalue of operator L, problem (12) will have a solution *if and only if the right hand side term G is orthogonal to the eigenfunction φ*. From this condition we find that

$$
\begin{aligned}
&E'(\mathcal{R}) = -\int_0^{\pi/2} \left[\frac{d\varphi}{d\alpha}^T \mathbf{D} \frac{d\varphi}{d\alpha} + \varphi^T (\mathbf{U} + 2\mathcal{R}\mathbf{W})\varphi \right] d\alpha - \frac{3}{\mathcal{R}} E(\mathcal{R}), \\
&\int_0^{\pi/2} \varphi^T \frac{1}{2} \mathbf{D} \varphi d\alpha = 1
\end{aligned} \tag{13}
$$

Now problem (12) has a solution, but it is not unique. From the normalization condition we obtain the required additional condition

$$
\int_0^{\pi/2} \varphi^T \frac{1}{2} \mathbf{D} \frac{d\varphi}{d\mathcal{R}} d\alpha = -\frac{3}{2\mathcal{R}}. \tag{14}
$$

Thus, problem (12) with additional conditions (13)–(14) has now a unique solution.

6. Matrix representations of the eigenvalue problems. For numerical solution of one-dimensional eigenvalue problems (7), (11) and boundary value problem (12)–(14) subject to the corresponding boundary conditions, the high-order approximations of the finite element method [10, 11] elaborated in our previous papers [12, 13] have been used. One-dimensional finite elements of order $p = 1, 2, \ldots, 10$ have been implemented. Using the standard finite element procedures [11], problems (7) and (11) are approximated by the generalized algebraic eigenvalue problem

$$
\mathbf{A}\mathbf{F}^h = E^h \mathbf{B}\mathbf{F}^h. \tag{15}
$$

The boundary value problem (12)–(14) is approximated by the system of linear algebraic equations

$$
\hat{\mathbf{A}}\mathbf{u}^h = \mathbf{b}. \tag{16}
$$

In Eqs. (15), (16), $\mathbf{A}$ and $\mathbf{B}$ are the finite element matrices, corresponding to problems (7) or (11) (see [12, 13]), matrix $\hat{\mathbf{A}}$ and right-hand side vector $\mathbf{b}$ are obtained respectively from matrix $\mathbf{A}$ and condition (14) using the algorithm of [7], E^h is the corresponding eigenvalue, $\mathbf{F}^h$ is the vector approximating solutions of (7) or (11) on the finite-element grid, and $\mathbf{u}^h$ is the finite element approximation for $\dfrac{d\varphi}{d\mathcal{R}}$.

Let E_n, φ_n and $\dfrac{d\varphi_n}{d\mathcal{R}}$ be the exact solution of (7) or (11), (12)–(14) and $E_n^h, \mathbf{F}_n^h, \mathbf{u}_n^h$ be the numerical solution of (15) and (16). Then the following estimates are valid [10]

$$
\begin{aligned}
&|E_n - E_n^h| \le c_1(E_n) h^{2p}, \quad ||\varphi_n - \mathbf{F}_n^h||_0 \le c_2(E_n) h^{p+1}, \\
&||\frac{d\varphi_n}{d\mathcal{R}} - \mathbf{u}_n^h||_0 \le c_3 h^{p+1}, \quad c_1 > 0, \quad c_2 > 0, \quad c_3 > 0,
\end{aligned}
$$

where h is the grid step, p is the order of finite elements, n is the number of the corresponding eigensolution, and constants c_1, c_2 and c_3 do not depend on step h.

7. Test Example: Hydrogen Atom on a Three-Dimensional Sphere. Now we consider the following eigenvalue problem

$$
\begin{aligned}
&\left(-\mathcal{R}\frac{d}{d\alpha} \sin^2\alpha \frac{d}{d\alpha} - \mathcal{R}^2 \sin 2\alpha \right) \psi(\alpha; \mathcal{R}) = E(\mathcal{R}) 2\mathcal{R}^3 \sin^2\alpha \psi(\alpha; \mathcal{R}), \\
&\lim_{\alpha \to 0} \sin^2\alpha \frac{\partial\psi}{\partial\alpha} = 0, \qquad \lim_{\alpha \to \pi} \sin^2\alpha \frac{\partial\psi}{\partial\alpha} = 0.
\end{aligned} \tag{17}
$$

Problem (17) has an analytical solution

$$E_n(\mathcal{R}) = -\frac{1}{2}\left[\frac{1}{n^2} - \frac{n^2-1}{\mathcal{R}^2}\right], \quad n = 1, 2, \ldots$$

with eigenfunctions $\psi_n(\alpha; \mathcal{R})$ which are the radial functions of a hydrogen atom on a three-dimensional sphere [14, 15]

$$\psi_n(\alpha, \mathcal{R}) = C_n(\mathcal{R}) Re\{\exp[-\imath\alpha(n-1-\imath\sigma)]_2F_1(-n+1, 1+\imath\sigma, 2, 1-\exp(2\imath\alpha))\},$$

$$C_n(\mathcal{R}) = \frac{2}{\sqrt{1-\exp(-2\pi\sigma)}}\sqrt{\sigma\frac{n^2+\sigma^2}{\mathcal{R}^3}}, \quad \sigma = \frac{\mathcal{R}}{n},$$

where ${}_2F_1$ is a full hypergeometric function.

Denote the exact solutions of problem (17) by (E_n, ψ_n) and the numerical ones by (E_n^h, ψ_n^h). First, we present the results of the computation of eigenvalues and their derivatives, which were obtained using 100 finite elements of the fifth order (501 nodes). Twenty eigenvalues were calculated simultaneously at two values of hyperradius $\mathcal{R} = 1$ and 15 a.u. Some of them are presented in Tables 1 and 2 together with quantities $\epsilon = E_n^h - E_n$ and $\delta = (E_n^h)' - E_n'$ which show the actual accuracy achieved for the approximate eigenvalues and their derivatives. From the Tables, one can see an excellent agreement (10^{-10} or better) of our numerical results with the exact solutions.

Table 1. Approximate eigenvalues E_n^h of problem (20) and their derivatives $(E_n^h)'$ calculated at $\mathcal{R} = 1$ a.u. $\epsilon = E_n^h - E_n$ and $\delta = (E_n^h)' - E_n'$ where E_n and E_n' are exact solutions. The numbers in parentheses denote power of ten.

n	E_n^h	ϵ	$(E_n^h)'$	δ
1	−.4999999999(+00)	.266(−11)	−.5748734821(−11)	.575(−11)
6	.1748611111(+02)	.137(−12)	−.3500000000(+02)	−.154(−12)
10	.4949499999(+02)	.301(−13)	−.9900000000(+02)	−.144(−14)
14	.9749744897(+02)	.114(−12)	−.1949999999(+03)	−.108(−12)
20	.1994987500(+03)	.464(−12)	−.3990000000(+03)	−.107(−09)

Table 2. Approximate eigenvalues E_n^h of problem (20) and their derivatives $(E_n^h)'$ calculated at $\mathcal{R} = 15$ a.u. $\epsilon = E_n^h - E_n$ and $\delta = (E_n^h)' - E_n'$ where E_n and E_n' are exact solutions.

n	E_n^h	ϵ	$(E_n^h)'$	δ
1	−.4999999999(+00)	.857(−11)	.6063205493(−12)	.606(−12)
6	.6388888888(−01)	.144(−11)	−.1037037037(−01)	−.555(−12)
10	.2150000000(+00)	.496(−12)	−.2933333333(−01)	−.459(−12)
14	.4307823129(+00)	.252(−12)	−.5777777777(−01)	−.294(−12)
20	.8854166666(+00)	.823(−12)	−.1182222222(+00)	−.782(−10)

The accuracy of calculation of the matrix **H** and **Q** is the same as the analytical ones (see [7]).

8. Numerical results for He and H^-. In this section we present our numerical results for the low-energy spectrum of Helium atom He and negative hydrogen ion H^- including the ground state. To calculate matrix elements (9) thirteen ($l_{\max} = 12$) Legendre polynomials in expansion (10) have been used. System (11) has been solved using 100 finite elements of the 7-th order for the first 28 eigensolutions. Problems (15) and (16) were solved by the subspace iteration method [11]. All eigenvalues and the corresponding matrix elements were calculated with relative accuracy of 10^{-10}. The grid in $\mathcal{R}$ has been chosen as follows, 0.02(0.02)0.1(0.05)6.1(0.1)20.0(0.2)35.0(0.25)50.0 (number in parentheses denotes the step in $\mathcal{R}$). For the results presented in Table 3 maximum values of hyperradius $\mathcal{R}_{\max} = 50.0$ a.u. have been used. System (7) has been solved using 220 finite elements of the seventh order (1541 grid points, grid step $h = 0.00051$). The cubic splines have been used to interpolate the coefficients of system (7) and to construct the radial finite element grid.

Table 3. Convergence of the ground state energy (in a.u.) for He and H^- with the number of coupled channels n.

n	He	H^-
1	−2.88791168	−0.52241442
2	−2.89137991	−0.52472087
3	−2.90287002	−0.52732522
6	−2.90300448	−0.52751473
10	−2.90363613	−0.52768020
15	−2.90370549	−0.52773607
21	−2.90372264	−0.52774928
28	−2.90372266	−0.52774970

In Table 3 energy values for the He and H^- obtained in [7] using the heliocentric coordinates are compared with the results obtained in this work by solving problem (1)–(3) for different number of radial equations in system (7). Such comparison demonstrates the convergence of the Kantorovich reduction of the 3-D problem using expansion (4) and also stability of the Bubnov-Galerkin method (10) for solving the 2-D parametric boundary problems (11) and (12).

A convergence study of the ground state energy of He and H^- with the number of radial equations is presented in Table 3. One can see that the energy eigenvalues converge monotonically from above, with the 28-channel value being $\mathcal{E}_{\rm He} = -2.90372266$ a.u. and $\mathcal{E}_{\rm H^-} = -0.52774970$ a.u. As shown these values are very close to the precision variational results: $\mathcal{E}^{\rm VAR}_{\rm He} = -2.90372437$ a.u. [16] and $\mathcal{E}^{\rm VAR}_{\rm H^-} = -0.52775102$ a.u. [17]. Since the calculation of matrix elements have accuracy approximately 10^{-8} it is shown that we have the same accuracy for eigenvalues. It is evident that our results agree very well with these high precision calculations.

9. Two new schemes of the 2-D Kantorovich reduction. In the present paper we would like to suggest a more efficient way to solve the two-dimensional problem (5)

using the Kantorovich method. Expansion (10) can be rewritten in two different forms:

$$\Phi_i(\alpha,\theta;\mathcal{R}) = \sum_{l=0}^{l_{\max}} \varphi_l^{(i)}(\alpha;\mathcal{R}) G_l(\theta;\alpha,\mathcal{R}), \tag{18}$$

$$\Phi_i(\alpha,\theta;\mathcal{R}) = \sum_{l=0}^{l_{\max}} \varphi_l^{(i)}(\theta;\mathcal{R}) F_l(\alpha;\theta,\mathcal{R}). \tag{19}$$

In the expansions above, basis functions $G_l(\theta;\alpha,\mathcal{R})$ and $F_l(\alpha;\theta,\mathcal{R})$ are the solutions of the following two one-dimensional parametric eigenvalue problems:

$$\left(-\frac{d}{d\theta}\frac{\mathcal{R}}{4}\sin\theta\frac{d}{d\theta} + \frac{\mathcal{R}^2}{8}\sin^2\alpha\sin\theta\hat{W}(\theta,\alpha) + \frac{\mathcal{R}}{4}\sin^2\alpha\sin\theta\right)G = \lambda(\alpha;\mathcal{R})\frac{\mathcal{R}^3}{8}\sin^2\alpha\sin\theta G, \tag{20}$$

$$\left(-\frac{d}{d\alpha}\frac{\mathcal{R}}{4}\sin^2\alpha\frac{d}{d\alpha} + \frac{\mathcal{R}^2}{8}\sin^2\alpha\sin\theta\hat{W}(\theta,\alpha) + \frac{\mathcal{R}}{4}\sin^2\alpha\sin\theta\right)F = \lambda(\theta;\mathcal{R})\frac{\mathcal{R}^3}{8}\sin^2\alpha\sin\theta F, \tag{21}$$

with the boundary and normalization conditions

$$\lim_{\theta\to 0,\pi}\sin\theta\frac{\partial G}{\partial\theta} = 0, \quad \int_0^\pi \sin\theta G^2 d\theta = 1,$$
$$\lim_{\alpha\to 0,\pi}\sin^2\alpha\frac{\partial F}{\partial\alpha} = 0, \quad \int_0^\pi \sin^2\alpha F^2 d\alpha = 1.$$

respectively. Note, that the differential operators in Eqs. (20) and (21) are self-adjoint. This circumstance guarantees that eigenfunctions G_l and F_l form full orthonormal systems.

Let $\lambda_l(\alpha;\mathcal{R})$ and $G_l(\theta;\alpha,\mathcal{R})$ be the solutions of problem (19). After substituting expansion (17) into the Rayleigh-Ritz functional for a problem (5), and its subsequent minimization we get the following system of coupled ordinary second order equations for obtaining the unknown eigenfunctions $\varphi^{(i)}(\alpha;\mathcal{R})$, $(\varphi^{(i)})^T = (\varphi_1^{(i)}, \varphi_2^{(i)}, \cdots, \varphi_{l_{\max}}^{(i)})$ and eigenvalues $E_i(\mathcal{R})$

$$-R\frac{d}{d\alpha}\mathbf{D}\frac{d}{d\alpha}\varphi + \frac{\mathcal{R}^3}{8}\mathbf{\Lambda}\varphi + \frac{\mathcal{R}}{4}\sin^2\alpha\overline{\mathbf{H}}\varphi + \frac{\mathcal{R}}{4}\sin^2\alpha\overline{\mathbf{Q}}\frac{d\varphi}{d\alpha} + \frac{\mathcal{R}}{4}\frac{d\sin^2\alpha\overline{\mathbf{Q}}\varphi}{d\alpha} = \frac{\mathcal{R}^3}{2}E(\mathcal{R})\mathbf{D}\varphi, \tag{22}$$

with boundary conditions $\lim_{\alpha\to 0,\pi}\sin^2\alpha\frac{\partial\varphi}{\partial\alpha} = 0$. Here $\mathbf{D}$, $\mathbf{\Lambda}$, $\overline{\mathbf{H}}$, and $\overline{\mathbf{Q}}$ are finite $l_{\max}\times l_{\max}$ matrices, elements of which are given by relations

$$\Lambda_{ll} = \sin^2\alpha\lambda_l(\alpha;\mathcal{R}), \quad D_{ll} = \frac{\sin^2\alpha}{4}, \quad \Lambda_{ll'} = 0, \quad D_{ll'} = 0 \quad l \neq l',$$

$$\overline{H}_{ll'} = \int_0^\pi \sin\theta\frac{\partial G_l}{\partial\alpha}\frac{\partial G_{l'}}{\partial\alpha}d\theta, \quad \overline{Q}_{ll'} = -\overline{Q}_{l'l} = -\int_0^\pi \sin\theta G_l\frac{\partial G_{l'}}{\partial\alpha}d\theta, \tag{23}$$

$$l, l' = 1, 2, \ldots, l_{\max}.$$

Let $\lambda_l(\theta;\mathcal{R})$ and $F_l(\theta;\alpha,\mathcal{R})$ be the solutions of problem (20). Following the same procedure as above we obtain the unknown eigenfunctions $\varphi^{(i)}(\theta;\mathcal{R})$, $(\varphi^{(i)})^T = (\varphi_1^{(i)}, \varphi_2^{(i)}, \cdots, \varphi_{l_{\max}}^{(i)})$ and eigenvalues $E_i(\mathcal{R})$ as the solutions of system

$$(24)\quad -R\frac{d}{d\theta}\mathbf{D}\frac{d}{d\theta}\varphi + \frac{\mathcal{R}^3}{8}\mathbf{\Lambda}\varphi + \frac{\mathcal{R}}{4}\sin\theta\overline{\mathbf{H}}\varphi + \frac{\mathcal{R}}{4}\sin\theta\overline{\mathbf{Q}}\frac{d\varphi}{d\theta} + \frac{\mathcal{R}}{4}\frac{d\sin\theta\overline{\mathbf{Q}}\varphi}{d\theta} = \frac{\mathcal{R}^3}{2}E(\mathcal{R})\overline{\mathbf{D}}\varphi,$$

with boundary conditions $\lim\limits_{\theta\to 0,\pi}\sin\theta\dfrac{\partial\varphi}{\partial\theta} = 0$. Matrices $\mathbf{D}$, $\mathbf{\Lambda}$, $\overline{\mathbf{H}}$, and $\overline{\mathbf{Q}}$ are defined as

$$\Lambda_{ll} = \sin\theta\lambda_l(\theta;\mathcal{R}), \quad D_{ll} = \frac{\sin\theta}{4}, \quad \Lambda_{ll'} = 0, \quad D_{ll'} = 0, \quad l \neq l',$$

$$(25)\qquad \overline{H}_{ll'} = \int_0^\pi \sin^2\alpha\frac{\partial F_l}{\partial\theta}\frac{\partial F_{l'}}{\partial\theta}d\alpha, \quad \overline{Q}_{ll'} = -\overline{Q}_{l'l} = -\int_0^\pi \sin^2\alpha F_l\frac{\partial F_{l'}}{\partial\theta}d\alpha,$$

$$l, l' = 1, 2, \ldots, l_{\max}.$$

10. Summary. In this paper we have shown that the proposed implementation of the Kantorovich method is an effective computational tool for solving multi-dimensional eigenvalue problems for the three-body Coulomb problem. All essential features and peculiarities of the problem are taken into account in the present approach in a natural and exact way. New implementations of the Kantorovich method proposed in section 8 allow us to build up a new class of the 1-D orthogonal parametric angular functions. The essential feature of these functions consists of the description of the typical peculiarities of various three-body interactions on the 2-D map, depending on a set of physical parameters such as charges and masses of the particles. An exact solvable model of the 1-D parametric angular functions can be used as an analytical test for the proposed schemes.

In the present work we have suggested the following implementation of the multistep Kantorovich method:

1. Solve Eqs. (19) or (20) for eigensolutions λ_l and F_l or G_l, respectively.
2. Solve the one-dimensional angular systems (21) or (23) to find potential curves $E(\mathcal{R})$ and 1-D angular basis functions $\varphi_l^{(i)}$.
3. Calculate matrix elements $\overline{\mathbf{H}}$ and $\overline{\mathbf{Q}}$.
4. Calculate energies $\mathcal{E}$ and radial wave functions $\chi(\mathcal{R})$ as eigensolutions of one-dimensional eigenvalue problem (7)-(8).

The present study of the multistep Kantorovich reduction opens new possibilities for using optimal approximations to solutions of 2-D and 3-D eigenvalue problems.

Here we show in Table 4 the results of solving the Eq.19 and system (21) for $\mathcal{R} = 80$ a.u. This is convenient because the asymptotic values of the terms are known. One can see that three eigenvalues and eigenfunctions of Eq.(19) are enough to obtain the accuracy 10^{-6} while the Bubnov-Galerkin methods used the 13 Legendre polynomials (see [7]). In this table l denotes the number of equations in system (22).

Using modern computer architectures such as vector and parallel facilities combined with such techniques as the Gauss quadrature grids for the one-dimensional problems,

Table 4. Comparison of the numerical potential curves $E_i(\mathcal{R})$ of Eq. (20), (22) with the dipole asymptotics, $E_i^{\rm as}(\mathcal{R})$, for the $^1S^e$ state of He calculated at $\mathcal{R} = 80$, a.u.

i	$l=1$	$l=2$	$l=3$	$l=6$	$E_i^{\rm as}(\mathcal{R})$
1	-2.01253	-2.01253	-2.01254	-2.01254	-2.01254
2	-0.51266	-0.51280	-0.51280	-0.51280	-0.51280
3	-0.23503	-0.51228	-0.51228	-0.51228	-0.51228
4	-0.13798	-0.23557	-0.23563	-0.23563	-0.23560
5	-0.09435	-0.23438	-0.23468	-0.23468	-0.23465
6	-0.07231	-0.13918	-0.23403	-0.23403	-0.23403

etc. can significantly reduce the cost of the solution of multi-dimensional problems with overall improvement in performance, effectiveness and accuracy required in modern computational physics.

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НЯКОИ МЕТОДИ ЗА РЕШАВАНЕ НА ТРИМЕРНИ КВАНТОВО–МЕХАНИЧНИ ЗАДАЧИ ЗА СОБСТВЕНИ СТОЙНОСТИ

М. С. Касчиев

Методите, разработени в тази работа, се базират на двустъпковия метод на Канторович за решаване на задачи за собствени стойности за Кулонови тричастични системи с използване на тримерна хиперсферична мрежа в хелиоцентрични координати. Тази задача се редуцира до решението на едномерни системи обикновени диференциални уравнения от втори ред с променливи коефициенти.

Всички съществени особености на проблемите се взевмат предвид по естествен и точен начин. Това приложение на метода на Канторович позволява да бъде построен нов клас едномерни параметрични ъглови функции. Особеността на тези функции съдържа описанието на типичните свойста на различни тричастични взаимодействия в двумерна мрежа, зависиша от физичните параметри, такива като зарядите и масите на частиците. Точно решаем модел от едномерни параметрични ъглови функции е използван като тест за предложените схеми.

Сходимостта на редукцията на Канторович се изследва числено при пресмятането на енергията на основното състояние на някои квантово-механични системи. Резултатите са илюстрирани в таблици. Обсъждат се отличителните черти при приложението на метода на Канторович.