On calculations of two-electron atoms in spheroidal coordinates mapping on hypersphere

Sergue Vinitsky[a], A.A. Gusev[a], O. Chuluunbaatar[a], V.L. Derbov[b], and A.S. Zotkina[c]

[a]Joint Institute for Nuclear Research,141980, Dubna, Moscow Region, Russia
[b]Saratov State University, 83 Astrakhanskaya street, 410012, Saratov, Russia
[c]Saratov State Technical University, 77 Politechnicheskaya street, 410054, Saratov, Russia

ABSTRACT

3D boundary-value problem (BVP) that arises in modelling the interactions of two-electron quantum systems (atoms or ions) with laser radiation, is formulated in the internal coordinate frame with the electrons placed in the focal points of the spheroidal system of coordinates with mapping on a hypersphere.[1,2] The wave function is sought for in the form of a decomposition in the basis of surface functions of the Coulomb two-center problem having the purely discrete spectrum and parametrically depending on the hypersphere hyperradius. Surface functions are sought for in the form of an expansion in the basis of Legendre polynomials with unknown components calculated as solutions of the reduced problem. Efficiency of the approach in comparison with that of the conventional hyperspherical one[3,4] is demonstrated by the example of helium atom.

Keywords: two-electron atom, light-matter interaction, boundary-value problem, numerical modeling, Coulomb two-center problem, spheroidal coordinates

1. SETTING OF THE PROBLEM

Advanced methods of calculating two-electron atomic targets are of major importance for the appropriate descrption of their interaction with laser radiation. Efficient numerical solution of this problem is possible in the appropriately chosen coordinates system allowing for the specific symmetry of the system. Let us consider a helium atom that consists of a nucleus (mass m_n, charge number $Z = 2$) and two electrons (mass m_e, charge $-e$). The non-relativistic Hamiltonian of this system has the form

$$\hat{H} = \frac{\mathbf{p}_n^2}{2m_n} + \frac{\mathbf{p}_{e_1}^2}{2m_e} + \frac{\mathbf{p}_{e_2}^2}{2m_e} - \frac{Ze^2}{|\mathbf{r}_{e_1} - \mathbf{r}_n|} - \frac{Ze^2}{|\mathbf{r}_{e_2} - \mathbf{r}_n|} + \frac{e^2}{|\mathbf{r}_{e_1} - \mathbf{r}_{e_2}|}, \tag{1}$$

where $\mathbf{r}_n$ and $\mathbf{p}_n$ are the position and momentum of the nucleus, $\mathbf{r}_{e_i}$ and $\mathbf{p}_{e_i}$ are the position and momentum of the i-th electron, respectively. The center-of-mass motion can be separated from the internal dynamics of the atom by introducing the center-of-mass coordinate $\mathbf{R}$ and the relative coordinates $\mathbf{r}_i$, $i = 1, 2$:

$$\mathbf{R} = \frac{1}{M}(m_n\mathbf{r}_n + m_e\mathbf{r}_{e_1} + m_e\mathbf{r}_{e_2}), \quad \mathbf{r}_i = \mathbf{r}_{e_i} - \mathbf{r}_n, \quad M = m_n + 2m_e \tag{2}$$

together with their associated momenta $\mathbf{P}$ and $\mathbf{p}_i$. Using the expressions

$$\mathbf{p}_n = \frac{m_n}{M}\mathbf{P} - \mathbf{p}_1 - \mathbf{p}_2, \quad \mathbf{p}_{e_i} = \frac{m_e}{M}\mathbf{P} + \mathbf{p}_i, \tag{3}$$

the Hamiltonian describing the internal degrees of freedom can be written as

$$\hat{H} = \frac{\mathbf{P}^2}{2M} + H, \quad H = \frac{\mathbf{p}_1^2}{2\mu} + \frac{\mathbf{p}_2^2}{2\mu} + \frac{\mathbf{p}_1\mathbf{p}_2}{m_n} - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|}, \tag{4}$$

Further author information: Send correspondence to S.I.V.: E-mail: vinitsky2008@gmail.com

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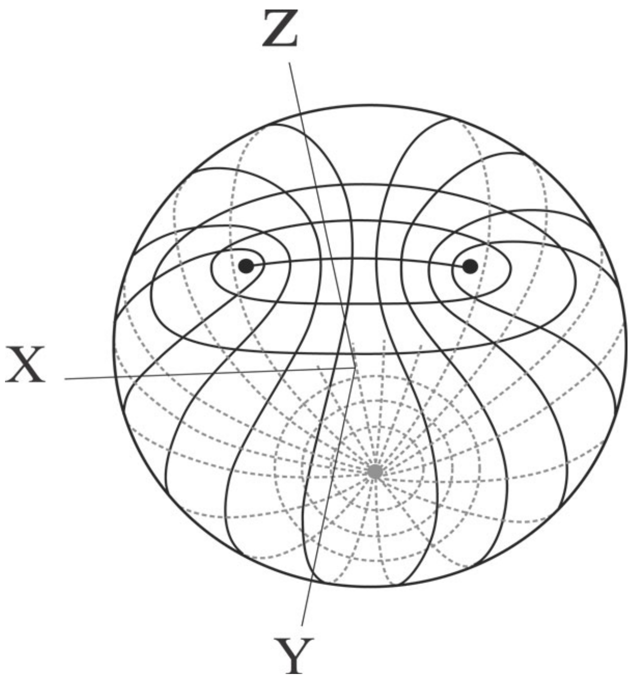

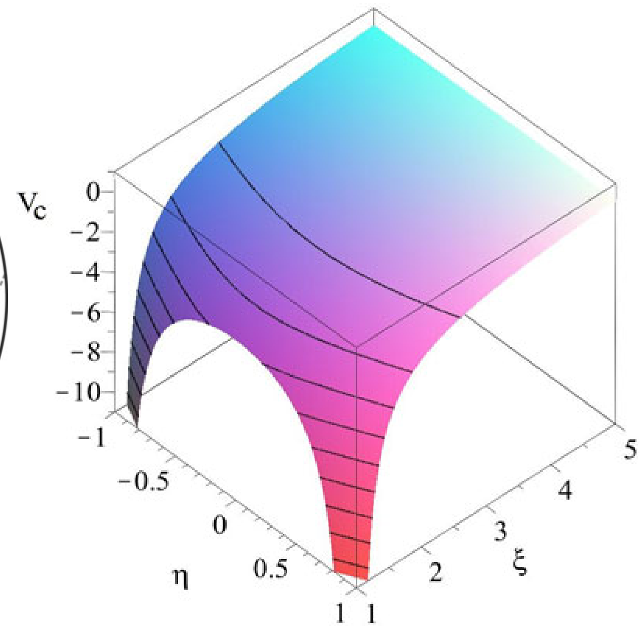

Figure 1. The coordinate system ξ, η on a sphere and Coulomb energy $V_c{=}-4/(\xi{+}\eta){-}4/(\xi{-}\eta){+}1$.

where $\mu = m_e m_n/(m_n + m_e)$ is the reduced mass, $\mathbf{p}_i = -\imath\boldsymbol{\nabla}_{\mathbf{r}_i}$, $\mathbf{r}_{12} = \mathbf{r}_2 - \mathbf{r}_1$:

$$\boldsymbol{\nabla}^2_{\mathbf{r}_1} + \boldsymbol{\nabla}^2_{\mathbf{r}_2} = \frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1} + \frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial}{\partial r_2} + 2\frac{\partial^2}{\partial r_{12}^2} + \frac{4}{r_{12}}\frac{\partial}{\partial r_{12}}$$
$$+\frac{r_1^2 + r_{12}^2 - r_2^2}{r_1 r_{12}}\frac{\partial^2}{\partial r_1 \partial r_{12}} + \frac{r_2^2 + r_{12}^2 - r_1^2}{r_2 r_{12}}\frac{\partial^2}{\partial r_2 \partial r_{12}} + \text{angular part} \tag{5}$$

with the volume element expressed as $dV = 8\pi^2 r_1 dr_1\, r_2 dr_2\, r_{12} dr_{12}$.

1.1 The 3D BVP in hyperspheroidal coordinates

Assuming the nuclear mass to be infinite, $m_n = \infty$, and the electron mass to be unit, $m_e = 1$, we carry out the transformation to hyperspheroidal coordinates

$$r_{12} = \frac{\sqrt{2}R}{\sqrt{\xi^2+\eta^2}}, \quad r_1 = \frac{R(\xi+\eta)}{\sqrt{2}\sqrt{\xi^2+\eta^2}}, \quad r_2 = \frac{R(\xi-\eta)}{\sqrt{2}\sqrt{\xi^2+\eta^2}} \tag{6}$$

with the volume element $dV = 8\pi^2 R^5 \frac{\xi^2-\eta^2}{(\xi^2+\eta^2)^3} dR d\xi d\eta$. In these coordinates the Laplacian (5) has the form

$$\boldsymbol{\nabla}^2_{\mathbf{r}_1} + \boldsymbol{\nabla}^2_{\mathbf{r}_2} = \frac{1}{R^5}\frac{\partial}{\partial R}R^5\frac{\partial}{\partial R} + \frac{1}{R^2}\frac{(\xi^2+\eta^2)^3}{\xi^2-\eta^2}\left(\frac{\partial}{\partial \xi}\frac{\xi^2-1}{\xi^2+\eta^2}\frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta}\frac{1-\eta^2}{\xi^2+\eta^2}\frac{\partial}{\partial \eta}\right) + \text{angular part.} \tag{7}$$

The equation for the wave functions $\Psi(R,\xi,\eta)$ for S-states reads as

$$\Bigg[-\frac{1}{R^5}\frac{\partial}{\partial R}R^5\frac{\partial}{\partial R} - \frac{1}{R^2}\frac{(\xi^2+\eta^2)^3}{\xi^2-\eta^2}\left(\frac{\partial}{\partial \xi}\frac{\xi^2-1}{\xi^2+\eta^2}\frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta}\frac{1-\eta^2}{\xi^2+\eta^2}\frac{\partial}{\partial \eta}\right)$$
$$+\sqrt{2}\frac{\sqrt{\xi^2+\eta^2}}{R}\left(1 - \frac{4}{\xi+\eta} - \frac{4}{\xi-\eta}\right) - 2E\Bigg]\Psi(R,\xi,\eta) = 0, \tag{8}$$

where E is the energy of the system. The coordinate system ξ, η on a sphere[1] and the potential energy are presented in Fig. 1. Performing the transformation of the wave functions $\Psi(R,\xi,\eta)=\sqrt{\xi^2+\eta^2}\Phi(R,\xi,\eta)$ and the volume element $dV=8\pi^2R^5\frac{\xi^2-\eta^2}{(\xi^2+\eta^2)^2}dRd\xi d\eta$, we arrive at the 3D BVP for the function $\Phi(R,\xi,\eta)$

$$\Bigg[-\frac{1}{R^5}\frac{\partial}{\partial R}R^5\frac{\partial}{\partial R}-\frac{3}{R^2}-\frac{1}{R^2}\frac{(\xi^2+\eta^2)^2}{\xi^2-\eta^2}\left(\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi}+\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}\right)$$
$$+\sqrt{2}\frac{\sqrt{\xi^2+\eta^2}}{R}\left(1-\frac{8\xi}{\xi^2-\eta^2}\right)-2E\Bigg]\Phi(R,\xi,\eta)=0. \quad (9)$$

The function $\Phi(R,\xi,\eta)$ satisfies the boundary conditions

$$\begin{aligned}
&\lim_{R\to0}R^5\frac{\partial\Phi(R,\xi,\eta)}{\partial R}=0, \quad \lim_{R\to\infty}R^5\Phi(R,\xi,\eta)=0,\\
&\lim_{\xi\to1}(\xi^2-1)\frac{\partial\Phi(R,\xi,\eta)}{\partial\xi}=0, \quad \lim_{\xi\to\infty}\Phi(R,\xi,\eta)=0,\\
&\lim_{\eta\to\pm1}(1-\eta^2)\frac{\partial\Phi(R,\xi,\eta)}{\partial\eta}=0,
\end{aligned} \quad (10)$$

and is normalized by the condition

$$8\pi^2\int_0^\infty dRR^5\int_1^\infty d\xi\int_{-1}^1 d\eta\frac{\xi^2-\eta^2}{(\xi^2+\eta^2)^2}\Phi^2(R,\xi,\eta)=1. \quad (11)$$

2. THE 2D BVP FOR SURFACE FUNCTIONS

The parametric wave function $\phi_i(\xi,\eta;R)$ and the corresponding potential curves $\varepsilon_i(R)$ are eigensolutions of the 2D BVP having a purely discrete spectrum

$$\left[-\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi}-\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}+\frac{\sqrt{2}R}{\sqrt{\xi^2+\eta^2}^3}\left(\xi^2-\eta^2-8\xi\right)-\varepsilon_i(R)\frac{\xi^2-\eta^2}{(\xi^2+\eta^2)^2}\right]\phi_i(\xi,\eta;R)=0 \quad (12)$$

subject to the following boundary conditions

$$\lim_{\xi\to1}(\xi^2-1)\frac{\partial\phi_i(\xi,\eta;R)}{\partial\xi}=0, \quad \lim_{\xi\to\infty}\phi_i(\xi,\eta;R)=0, \quad \lim_{\eta\to\pm1}(1-\eta^2)\frac{\partial\phi_i(\xi,\eta;R)}{\partial\eta}=0, \quad (13)$$

and the normalization condition

$$\int_1^\infty d\xi\int_{-1}^1 d\eta\frac{\xi^2-\eta^2}{(\xi^2+\eta^2)^2}\phi_i^2(\xi,\eta;R)=1. \quad (14)$$

We seek for the solution of the 2D BVP (12)–(14) in the form of expansion over Legendre polynomials $P_j(\eta)$

$$\phi_i(R,\xi,\eta)=\sum_{j=1}^{j_{\max}}P_{2j-2}(\eta)B_j^{(i)}(\xi;R), \quad (15)$$

where $\mathbf{B}^{(i)}(\xi;R)=(B_1^{(i)}(\xi;R),B_2^{(i)}(\xi;R),\ldots,B_{j_{\max}}^{(i)}(\xi;R))^T$ is eigensolution of the 1D BVP for the system of $j_{\max}$ second-order ordinary differential equations (SOODEs)

$$\left(-\mathbf{I}\frac{\partial}{\partial\xi}(\xi^2-1)\frac{\partial}{\partial\xi}+\mathbf{V}(\xi,R)-\varepsilon_i(R)\mathbf{F}(\xi)\right)\mathbf{B}^{(i)}(\xi;R)=0, \quad (16)$$

with boundary conditions

$$\lim_{\xi\to 1}(\xi^2-1)\frac{\partial \mathbf{B}^{(i)}(\xi;R)}{\partial \xi}=0,\quad \lim_{\xi\to\infty}\mathbf{B}^{(i)}(\xi;R). \tag{17}$$

Here $\mathbf{I}$, $\mathbf{V}(\xi,R)$ and $\mathbf{F}(\xi)$ are $j_{\max}\times j_{\max}$ matrices

$$\begin{aligned}
&I_{ij}=\delta_{ij},\\
&V_{ij}(\xi,R)=V_{ji}(\xi,R)=(2i-2)(2i-1)\delta_{ij}+\sqrt{2}R\int_{-1}^{1}d\eta P_{2i-2}(\eta)\frac{\xi^2-\eta^2-8\xi}{\sqrt{\xi^2+\eta^2}^3}P_{2j-2}(\eta),\\
&F_{ij}(\xi)=F_{ji}(\xi)=\int_{-1}^{1}d\eta P_{2i-2}(\eta)\frac{\xi^2-\eta^2}{(\xi^2+\eta^2)^2}P_{2j-2}(\eta).
\end{aligned} \tag{18}$$

The asymptotic solutions at $\xi\to\infty$ and fixed R are

$$B_{l+1}^{(i)}(\xi;R)=\int_{-1}^{1}d\eta\phi_i(\xi,\eta;R)P_{2l}(\eta)\sim\frac{1}{(\xi+1)^{2l+1}}+\left(\frac{\sqrt{2}R}{(4l+2)}+2l+1\right)\frac{1}{(\xi+1)^{2l+2}}+\ldots, \tag{19}$$

$$B_{1}^{(i)}(\xi;R)=\int_{-1}^{1}d\eta\phi_i(\xi,\eta;R)P_{0}(\eta)\sim\frac{1}{(\xi+1)}+\left(\frac{\sqrt{2}R}{2}+1\right)\frac{1}{(\xi+1)^{2}}+\left(\frac{R^2}{6}-\frac{\sqrt{2}R}{3}-\frac{\varepsilon_i(R)}{6}+\frac{4}{3}\right)\frac{1}{(\xi+1)^{3}}+\ldots \tag{20}$$

2.1 2D BVP for the surface functions in terms of scaled variable

In terms of scaled variable and parametric surface functions

$$\xi=\frac{1+\lambda}{1-\lambda},\quad 0\le\lambda<1,\quad \phi_i(\xi,\eta;R)=\frac{p_i(\xi,\eta;R)}{\xi+1}\equiv\frac{p_i(\lambda,\eta;R)}{\xi+1}, \tag{21}$$

we rewrite the 2D BVP (12)–(14) in the form

$$\begin{aligned}
&\left[-\frac{\partial}{\partial\lambda}\lambda(1-\lambda)^2\frac{\partial}{\partial\lambda}+1-\lambda-\frac{\partial}{\partial\eta}(1-\eta^2)\frac{\partial}{\partial\eta}\right.\\
&\left.+\sqrt{2}R(1-\lambda)\frac{(1+\lambda)^2-(1-\lambda)^2\eta^2-8(1-\lambda^2)}{\sqrt{(1+\lambda)^2+(1-\lambda)^2\eta^2}^3}-\varepsilon_i(R)(1-\lambda)^2\frac{(1+\lambda)^2-(1-\lambda)^2\eta^2}{((1+\lambda)^2+(1-\lambda)^2\eta^2)^2}\right]p_i(\lambda,\eta;R)=0.
\end{aligned} \tag{22}$$

The surface functions $p_i(\lambda,\eta;R)$ satisfy the following boundary and normalization conditions

$$\lim_{\lambda\to 0,1}\lambda(1-\lambda)\frac{\partial p_i(\lambda,\eta;R)}{\partial\lambda}=0,\quad \lim_{\eta\to\pm1}(1-\eta^2)\frac{\partial p_i(\lambda,\eta;R)}{\partial\eta}=0, \tag{23}$$

$$\frac{1}{2}\int_0^1 d\lambda\int_{-1}^{1}d\eta(1-\lambda)^2\frac{(1+\lambda)^2-(1-\lambda)^2\eta^2}{((1+\lambda)^2+(1-\lambda)^2\eta^2)^2}p_i^2(\lambda,\eta;R)=1. \tag{24}$$

The asymptotic solutions at $\xi\to\infty$ (or $\lambda\to 1$) and fixed R are

$$\int_{-1}^{1}d\eta p_i(\lambda,\eta;R)P_{2l}(\eta)\sim\left(\frac{1-\lambda}{2}\right)^{2l}+\left(\frac{\sqrt{2}R}{(4l+2)}+2l+1\right)\left(\frac{1-\lambda}{2}\right)^{2l+1}+\ldots, \tag{25}$$

$$\int_{-1}^{1}d\eta p_i(\lambda,\eta;R)P_{0}(\eta)\sim 1+\left(\frac{\sqrt{2}R}{2}+1\right)\left(\frac{1-\lambda}{2}\right)+\left(\frac{R^2}{6}-\frac{\sqrt{2}R}{3}-\frac{\varepsilon_j(R)}{6}+\frac{4}{3}\right)\left(\frac{1-\lambda}{2}\right)^{2}\ldots \tag{26}$$

Table 1. Convergence of the ground state energy (in a.u.) for a helium atom versus the number N of basis functions and the number $j_{\max}$ of Legengre polynomials. The mesh points are $\lambda = \{0(200)1\}$ and $R = \{0(50)5(75)20\}$.

N	$j_{\max} = 8$	$j_{\max} = 10$	$j_{\max} = 12$ ref.[4]	$j_{\max} = 12$
1	-2.895 553 913	-2.895 553 913	-2.895 539 19	-2.895 553 913
2	-2.898 645 854	-2.898 645 854	-2.898 631 57	-2.898 645 854
6	-2.903 658 663	-2.903 658 663	-2.903 644 06	-2.903 658 663
10	-2.903 717 499	-2.903 717 499	-2.903 702 86	-2.903 717 499
15	-2.903 723 210	-2.903 723 308	-2.903 708 67	-2.903 723 308
21	-2.903 724 105	-2.903 724 130		-2.903 724 130
28	-2.903 724 174	-2.903 724 132		-2.903 724 132
35	-2.903 724 299	-2.903 724 304		-2.903 724 304

Table 2. Convergence of the ground state energy (in a.u.) for a helium atom versus the number N of basis functions and the number $j_{\max}$ of Legengre polynomials. The mesh points are $\lambda = \{0(200)1\}$ and $R = \{0(50)5(75)20\}$. Continuation of Table 1.

N	$j_{\max} = 21$ ref.[4]	$j_{\max} = 21$	$j_{\max} = 28$ ref.[4]	$j_{\max} = 28$
1	-2.895 551 19	-2.895 553 913	-2.895 552 76	-2.895 553 913
2	-2.898 643 21	-2.898 645 854	-2.898 644 74	-2.898 645 854
6	-2.903 655 96	-2.903 658 663	-2.903 657 52	-2.903 658 663
10	-2.903 714 79	-2.903 717 499	-2.903 716 36	-2.903 717 499
15	-2.903 720 60	-2.903 723 308	-2.903 722 16	-2.903 723 308
21		-2.903 724 130	-2.903 722 99	-2.903 724 130
28		-2.903 724 132		-2.903 724 132
35		-2.903 724 303		-2.903 724 303

3. 1D BVP WITH RESPECT TO THE HYPERRADIAL VARIABLE

We seek for the solution of the 3D BVP (9)–(11) in the form of Kantorovich expansion

$$\Phi(R,\xi,\eta) = \sum_{j=1}^{N} \phi_j(\xi,\eta;R)\chi_j(R) \tag{27}$$

over the eigenfunctions $\phi_j(\xi,\eta;R)$ of the parametric 2D BVP having a purely discrete spectrum $\varepsilon_j(R) = E_j(R)R^2, j = 1, 2, ...$

Substituting the expansion (27) into the 3D BVP Eq. (9)– (11) and averaging over the surface functions (12)–(14), in terms of the scaled variable and parametric surface functions (21), we get the 1D BVP for a finite set of N coupled SOODEs for $\boldsymbol{\chi}(R) = \{\chi_1(R), ..., \chi_N(R)\}^T$

$$\left(-\frac{1}{R^5}\mathbf{I}\frac{d}{dR}R^5\frac{d}{dR} + \mathbf{U}(R) + \mathbf{Q}(R)\frac{d}{dR} + \frac{1}{R^5}\frac{dR^5\mathbf{Q}(R)}{dR} - 2E\,\mathbf{I}\right)\boldsymbol{\chi}(R) = 0, \tag{28}$$

with the boundary and normalization conditions

$$\lim_{R\to 0} R^5\frac{d\boldsymbol{\chi}(R)}{dR} = 0, \quad \lim_{R\to\infty} R^5\boldsymbol{\chi}(R) = 0, \quad 8\pi^2\int_0^\infty dRR^5(\boldsymbol{\chi}(R))^T\boldsymbol{\chi}(R) = 1. \tag{29}$$

Table 3. Convergence of the ground state energy (in a.u.) for a Helium atom versus the number N of basis functions and the number $j_{\max}$ of Legengre polynomials. The mesh points are $\lambda = \{0(100)0.2(80)0.4(60)0.6(40)0.8(20)1\}$ and $R = \{0(100)5(150)20\}$.

N	$j_{\max} = 6$	$j_{\max} = 8$	$j_{\max} = 10$	$j_{\max} = 12$
1	-2.895 553 913	-2.895 553 913	-2.895 553 913	-2.895 553 913
2	-2.898 645 854	-2.898 645 854	-2.898 645 854	-2.898 645 854
6	-2.903 658 663	-2.903 658 663	-2.903 658 663	-2.903 658 663
10	-2.903 717 578	-2.903 717 499	-2.903 717 499	-2.903 717 499
15	-2.903 723 327	-2.903 723 321	-2.903 723 308	-2.903 723 308
21	-2.903 723 995	-2.903 724 103	-2.903 724 130	-2.903 724 130
28	-2.903 724 182	-2.903 724 174	-2.903 724 134	-2.903 724 132
35	-2.903 724 323	-2.903 724 299	-2.903 724 304	-2.903 724 304
ref.[5]				-2.903 724 37

Here $\mathbf{I}$, $\mathbf{U}(R)$ and $\mathbf{Q}(R)$ are $N \times N$ matrices

$$I_{ij} = \delta_{ij}, U_{ij}(R) = U_{ji}(R) = 2\frac{\varepsilon_i(R) + \varepsilon_j(R)}{R^2}\delta_{ij} + H_{ij}(R) \tag{30}$$

$$H_{ij}(R) = H_{ji}(R) = \int_1^\infty d\xi \int_{-1}^1 d\eta \frac{\xi^2 - \eta^2}{(\xi^2 + \eta^2)^2} \frac{\partial \phi_i(\xi, \eta; R)}{\partial R} \frac{\partial \phi_j(\xi, \eta; R)}{\partial R},$$

$$Q_{ij}(R) = -Q_{ji}(R) = -\int_1^\infty d\xi \int_{-1}^1 d\eta \frac{\xi^2 - \eta^2}{(\xi^2 + \eta^2)^2} \phi_i(\xi, \eta; R) \frac{\partial \phi_j(\xi, \eta; R)}{\partial R}$$

In the vicinity of $R = 0$ the numbers N and $j_{\max}$ satisfy the condition $N \leq j_{\max}(j_{\max} + 2)/4$ at fixed $j_{\max}$.

4. CONCLUSION

The calculation of eigenenergies of a helium atom in the hyperspheroidal coordinates reduces number $j_{\max}$ of the required Legendre polynomials in the expansion (15) of the surface functions (21) and provides the economy of computer resources as compared to the conventional hyperspherical coordinates used earlier.[3,4] For the ground state energy the use of the hyperspheroidal coordinates provides an upper estimate with the accuracy $\sim 10^{-7}$ at $N = 35$ and $j_{\max} = 12$ with respect to the variational calculation[5] (see Table 3), while the conventional ones provide only $\sim 10^{-6}$ at $N = 35$ and $j_{\max} = 28$ (see Tables 1 and 2). The work was supported by the Russian Foundation for Basic Research (RFBR) grant No. 14-01-00420.

REFERENCES

[1] Bolsinov A.V. and Fomenko A.T., *Integrable Hamilton Systems V. 2,* Udmurt State University Press, Izhevsk, 105 (1999).

[2] Abramov D.I., J. Phys. B,"Hyperspherical Coulomb spheroidal representation in the Coulomb three-body problem," 41 (17), 175201 (2008).

[3] Vinitsky S., Gusev A., Chuluunbaatar O., Derbov V., Klombotskaya A., and Gozdz A., "Models of two-electron composite quantum systems," Proc. SPIE 9031, 90311E (2014).

[4] Gusev A.A., Chuluunbaatar O., Vinitsky S.I., and Abrashkevich A.G., , "POTHEA: a program for computing eigenvalues and eigenfunctions and their first derivatives with respect to the parameter of the parametric self-adjoined 2D elliptic partial differential equation," Comput. Phys. Commun. 185 (10), 2636–2654 (2014).

[5] Chuluunbaatar O., Puzynin I.V., Vinitsky S.I., "Uncoupled correlated calculations of helium isoelectronic bound states," J. Phys. B 34 (14), L425–L432 (2001).