Minimization based approach and finite element method for solving the two-center Dirac equation

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   - Application of the FEM
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Statement of the two center Dirac problem

The Dirac equation

$$H_D \Psi(\boldsymbol{r}) = E \Psi(\boldsymbol{r}), \tag{1}$$

$$H_D = c\,\boldsymbol{\alpha}\boldsymbol{p} + c^2\beta + V(\boldsymbol{r})\boldsymbol{I}. \tag{2}$$

Here c is the speed of light, $\boldsymbol{p} = (p_x, p_y, p_z)$ is the momentum operator, and $\boldsymbol{\alpha}$, β are 4×4 Dirac matrices:

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \mathbf{I} & 0 \\ 0 & -\mathbf{I} \end{pmatrix}, \tag{3}$$

$\boldsymbol{\sigma} = (\boldsymbol{\sigma}_x, \boldsymbol{\sigma}_y, \boldsymbol{\sigma}_z)$ are the Pauli matrices, and $\boldsymbol{I}$ and $\mathbf{I}$ are 4×4 and 2×2 identity matrices.

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$\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli matrices, and $\boldsymbol{I}$ and $\mathbf{I}$ are 4×4 and 2×2 identity matrices.

The two-center attractive Coulomb potential

$$V(\boldsymbol{r}) = -\frac{Z_1}{r_1} - \frac{Z_2}{r_2}. \tag{4}$$

where Z_1 and Z_2 are the point charge of the centers 1 and 2, $\boldsymbol{r}_1 = \boldsymbol{r} + \boldsymbol{\rho}/2$, $\boldsymbol{r}_2 = \boldsymbol{r} - \boldsymbol{\rho}/2$, $\boldsymbol{\rho} = (0, 0, \rho)$, and ρ is the internuclear distance.

Reducing the minimax formulation to minimization

The minimax variational formulation

The wave function $\Psi(\boldsymbol{r})$ is presented in the form

$$\Psi(\boldsymbol{r}) = \begin{pmatrix} \boldsymbol{g}(\boldsymbol{r}) \\ \boldsymbol{f}(\boldsymbol{r}) \end{pmatrix}, \tag{5}$$

where $\boldsymbol{g}(\boldsymbol{r})$ and $\boldsymbol{f}(\boldsymbol{r})$ are the large and small components, respectively. With this definition Eq. (1) can be written in the form

$$\Big(V(\boldsymbol{r}) + c^2 - E\Big)\,\boldsymbol{g}(\boldsymbol{r}) + c\,\boldsymbol{\sigma p}\,\boldsymbol{f}(\boldsymbol{r}) = \boldsymbol{0}, \tag{6}$$

$$c\,\boldsymbol{\sigma p}\,\boldsymbol{g}(\boldsymbol{r}) + \Big(V(\boldsymbol{r}) - c^2 - E\Big)\,\boldsymbol{f}(\boldsymbol{r}) = \boldsymbol{0}. \tag{7}$$

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$$c\, \boldsymbol{\sigma p}\, \boldsymbol{g}(\boldsymbol{r}) + \Big(V(\boldsymbol{r}) - c^2 - E\Big)\, \boldsymbol{f}(\boldsymbol{r}) = \boldsymbol{0}. \tag{7}$$

The minimax variational formulation[a] :

$$-c^2 < E = \min_{\boldsymbol{g}(\boldsymbol{r})\neq 0} \max_{\boldsymbol{f}(\boldsymbol{r})} \langle H_D \rangle < c^2, \tag{8}$$

$$\langle H_D \rangle = \Big\langle \boldsymbol{g}(\boldsymbol{r}) \big| V(\boldsymbol{r}) + c^2 \big| \boldsymbol{g}(\boldsymbol{r}) \Big\rangle + 2c\, \langle \boldsymbol{g}(\boldsymbol{r}) | \boldsymbol{\sigma p} | \boldsymbol{f}(\boldsymbol{r}) \rangle + \langle \boldsymbol{f}(\boldsymbol{r}) | V(\boldsymbol{r}) - c^2 | \boldsymbol{f}(\boldsymbol{r}) \rangle. \tag{9}$$

If $V(\boldsymbol{r}) < c^2$, it can be easily shown that in the maximization problem in Eq. (8) for a given $\boldsymbol{g}(\boldsymbol{r})$ must have a solution for $\boldsymbol{f}(\boldsymbol{r})$.

[a] J.D. Talman. Phys. Rev. Lett. 57, 1091, 1986.

Reducing the minimax formulation to minimization

Minimization variational formulation

$$\boldsymbol{f}(\boldsymbol{r}) = \frac{c}{c^2 + E - V(\boldsymbol{r})}\, \boldsymbol{\sigma p}\, \boldsymbol{g}(\boldsymbol{r}), \tag{10}$$

Reducing the minimax formulation to minimization

Minimization variational formulation

$$\boldsymbol{f}(\boldsymbol{r}) = \frac{c}{c^2 + E - V(\boldsymbol{r})}\,\boldsymbol{\sigma p}\,\boldsymbol{g}(\boldsymbol{r}), \tag{10}$$

$$\hat{H}_D\,\boldsymbol{g}(\boldsymbol{r}) = E\,\boldsymbol{g}(\boldsymbol{r}), \tag{11}$$

$$\hat{H}_D = \boldsymbol{\sigma p}\,\frac{c^2}{c^2 + E - V(\boldsymbol{r})}\,\boldsymbol{\sigma p} + \left(V(\boldsymbol{r}) + c^2\right)\mathbf{I}.$$

If $V(\boldsymbol{r}) < 0$ and $V(\boldsymbol{r}) \not< -2c^2$, the operator $\hat{H}_D$ [a] is bounded above and the bound-state spectrum will be

$$-c^2 < E = \min_{\boldsymbol{g}(\boldsymbol{r})\neq 0} \left\langle \boldsymbol{g}(\boldsymbol{r}) \left| \hat{H}_D \right| \boldsymbol{g}(\boldsymbol{r}) \right\rangle < c^2 \tag{12}$$

with the normalization condition

$$\langle \boldsymbol{g}(\boldsymbol{r}) | \boldsymbol{g}(\boldsymbol{r}) \rangle + \left\langle \boldsymbol{\sigma p}\,\boldsymbol{g}(\boldsymbol{r}) \left| \frac{c^2}{(c^2 + E - V(\boldsymbol{r}))^2} \right| \boldsymbol{\sigma p}\,\boldsymbol{g}(\boldsymbol{r}) \right\rangle = 1. \tag{13}$$

From here $c^2 + E - V(\boldsymbol{r}) > 0$.

[a] A. Kolakowska, et al., Phys. Rev. A. **53**, 168 (1996).

Application to the two-center problem

The two-center attractive Coulomb potential

$$V(\boldsymbol{r}) = -\frac{Z_1}{r_1} - \frac{Z_2}{r_2}. \tag{14}$$

where Z_1 and Z_2 are the point charge of the centers 1 and 2, $\boldsymbol{r}_1 = \boldsymbol{r} + \boldsymbol{\rho}/2$, $\boldsymbol{r}_2 = \boldsymbol{r} - \boldsymbol{\rho}/2$, $\boldsymbol{\rho} = (0, 0, \rho)$, and ρ is the internuclear distance.

Prolate spheroidal coordinates (ξ, η, φ):

$$1 \le \xi = \frac{r_1 + r_2}{\rho} < \infty, \quad -1 \le \eta = \frac{r_1 - r_2}{\rho} \le 1, \quad 0 \le \varphi < 2\pi. \tag{15}$$

We choose large component $\boldsymbol{g}(\boldsymbol{r})$ in the form

$$\boldsymbol{g}(\boldsymbol{r}) = \begin{pmatrix} g_1(\xi, \eta)\, \mathrm{e}^{\imath(j_z - 1/2)\varphi} \\ g_2(\xi, \eta)\, \mathrm{e}^{\imath(j_z + 1/2)\varphi} \end{pmatrix}, \tag{16}$$

where $j_z = \pm 1/2, \pm 3/2, \ldots$ are eigenvalues of the angular momentum J_z.

Application to the two-center problem

System of two-dimensional two-variables elliptic equations

$$\left[\frac{1}{g_{00}(\xi,\eta)}\begin{pmatrix}\hat{h}_D & \hat{q}\\ -\hat{q} & \hat{h}_D\end{pmatrix}+\begin{pmatrix}V_{11}(\xi,\eta) & V_{12}(\xi,\eta)\\ V_{12}(\xi,\eta) & V_{22}(\xi,\eta)\end{pmatrix}-E\,I\right]\begin{pmatrix}g_1(\xi,\eta)\\ g_2(\xi,\eta)\end{pmatrix}=0. \tag{17}$$

$$\begin{aligned}\hat{h}_D &= -\frac{\partial}{\partial\xi}g_{11}(\xi,\eta)\frac{\partial}{\partial\xi}-\frac{\partial}{\partial\eta}g_{22}(\xi,\eta)\frac{\partial}{\partial\eta},\\ \hat{q} &= Q^{(1)}(\xi,\eta)\frac{\partial}{\partial\xi}+\frac{\partial}{\partial\xi}Q^{(1)}(\xi,\eta)+Q^{(2)}(\xi,\eta)\frac{\partial}{\partial\eta}+\frac{\partial}{\partial\eta}Q^{(2)}(\xi,\eta)\end{aligned} \tag{18}$$

Application to the two-center problem

Potential functions

$$g_{00}(\xi,\eta)=\rho^2(\xi^2-\eta^2),\quad g_{11}(\xi,\eta)=4c^2\frac{\xi^2-1}{U(\xi,\eta)},\quad g_{22}(\xi,\eta)=4c^2\frac{1-\eta^2}{U(\xi,\eta)},$$

$$Q^{(1)}(\xi,\eta)=-2c^2\frac{W(\xi,\eta)}{U^2(\xi,\eta)}\frac{\partial}{\partial\eta}V(\xi,\eta),\quad Q^{(2)}(\xi,\eta)=2c^2\frac{W(\xi,\eta)}{U^2(\xi,\eta)}\frac{\partial}{\partial\xi}V(\xi,\eta),$$

$$V_{11}(\xi,\eta)=\frac{4c^2M\left(\xi\frac{\partial}{\partial\xi}-\eta\frac{\partial}{\partial\eta}\right)V(\xi,\eta)}{\rho^2(\xi^2-\eta^2)U^2(\xi,\eta)}+\frac{4c^2M^2}{\rho^2W^2(\xi,\eta)U(\xi,\eta)}+V(\xi,\eta)+c^2, \tag{19}$$

$$V_{22}(\xi,\eta)=-\frac{4c^2(M+1)\left(\xi\frac{\partial}{\partial\xi}-\eta\frac{\partial}{\partial\eta}\right)V(\xi,\eta)}{\rho^2(\xi^2-\eta^2)U^2(\xi,\eta)}+\frac{4c^2(M+1)^2}{\rho^2W^2(\xi,\eta)U(\xi,\eta)}+V(\xi,\eta)+c^2,$$

$$V_{12}(\xi,\eta)=V_{21}(\xi,\eta)=-\frac{2c^2\,(2M+1)\left(\xi(1-\eta^2)\frac{\partial}{\partial\eta}+(\xi^2-1)\eta\frac{\partial}{\partial\xi}\right)V(\xi,\eta)}{\rho^2(\xi^2-\eta^2)W(\xi,\eta)U^2(\xi,\eta)},$$

$$U(\xi,\eta)=E+c^2-V(\xi,\eta)>0,\quad W(\xi,\eta)=\sqrt{(\xi^2-1)(1-\eta^2)},$$

$$V(\xi,\eta)\equiv V(\boldsymbol{r}),\quad M=j_z-\frac{1}{2}. \tag{20}$$

Application to the two-center problem

Singular points

$$\xi \to 1, \quad \eta \to \pm 1,$$

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$$\begin{aligned} &\xi \to 1, \quad \eta \to \pm 1, \\ &\xi + \eta \to 0, \quad \xi - \eta \to 0. \end{aligned} \tag{21}$$

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Coulomb singularity

$$\begin{aligned} &g_1(\xi,\eta) = T(\xi,\eta)\, G_1(\xi,\eta), \quad g_2(\xi,\eta) = T(\xi,\eta)\, G_2(\xi,\eta), \\ &T(\xi,\eta) = (\xi+\eta)^{a_1}(\xi-\eta)^{a_2}, \quad a_l = -1 + \gamma_{l,\kappa}, \quad l = 1,2. \end{aligned} \tag{22}$$

$$\gamma_{l,\kappa} = \sqrt{\kappa^2 - \left(\frac{Z_l}{c}\right)^2}, \quad |\kappa| = |j_z| + \frac{1}{2} = 1, 2, \ldots. \tag{23}$$

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Singular coordinate transformations: [O. Kullie, et al., J. Phys. B 36, 4361 (2003).]

$$\xi = 1 + \sum_{i=1}^{\nu/2} c_i \sinh^{\nu+2(i-1)}\left(\frac{s}{2}\right), \quad \eta = 1 + \sum_{i=1}^{\nu/2} (-1)^i c_i \sin^{\nu+2(i-1)}\left(\frac{t}{2}\right), \tag{24}$$

where $0 \le s < \infty$, $0 \le t \le \pi$, and $\nu = 2, 4, 6, 8, 10, \ldots$.

Application to the two-center problem

Boundary conditions on domain $\Delta = [0, s_{\max}] \otimes [0, \pi]$

$$
\begin{aligned}
&\lim_{s\to 0} g_{11}(s,t)\frac{\partial G_1(s,t)}{\partial s} = 0 \quad \text{if} \quad M = 0; \quad G_1(0,t) = 0 \quad \text{if} \quad M \neq 0; \quad G_1(s_{\max},t) = 0;\\
&\lim_{t\to 0,\pi} g_{22}(s,t)\frac{\partial G_1(s,t)}{\partial t} = 0 \quad \text{if} \quad M = 0; \quad G_1(s,0) = G_1(s,\pi) = 0 \quad \text{if} \quad M \neq 0;\\
&\lim_{s\to 0} g_{11}(s,t)\frac{\partial G_2(s,t)}{\partial s} = 0 \quad \text{if} \quad M = -1; \quad G_2(0,t) = 0 \quad \text{if} \quad M \neq -1; \quad G_2(s_{\max},t) = 0;\\
&\lim_{t\to 0,\pi} g_{22}(s,t)\frac{\partial G_2(s,t)}{\partial t} = 0 \quad \text{if} \quad M = -1; \quad G_2(s,0) = G_1(s,\pi) = 0 \quad \text{if} \quad M \neq -1.
\end{aligned}
\tag{25}
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\end{aligned}
\tag{25}
$$

Boundary conditions for the homonuclear case ($Z_1 = Z_2$)

$$
\lim_{t\to \pi/2} \frac{\partial G_1(s,t)}{\partial t} = 0, \quad G_2\left(s, \frac{\pi}{2}\right) = 0 \quad \text{or} \quad G_1\left(s, \frac{\pi}{2}\right) = 0, \quad \lim_{t\to \pi/2} \frac{\partial G_2(s,t)}{\partial t} = 0. \tag{26}
$$

Application of the FEM

FEM to solve this BVP in the domain $\Delta = [0, s_{\max}] \otimes [0, \pi]$ or $\Delta = [0, s_{\max}] \otimes [\pi/2, \pi]$

Finite-element mesh:

$$\Delta = \bigcup_{q_1=1}^{N_s} \bigcup_{q_2=1}^{N_t} \Delta_{q_1 q_2}(s,t), \quad \Delta_{q_1 q_2}(s,t) = [s_{q_1}, s_{q_1+1}] \otimes [t_{q_2}, t_{q_2+1}]. \tag{27}$$

Shape functions in subdomain $\Delta_{q_1 q_2}$:

$$\varphi_{r_1 q_1 r_2 q_2}(s,t) = \varphi_{r_1 q_1}(s)\varphi_{r_2 q_2}(t), \tag{28}$$

$\varphi_{rq}(x)$ is the LIP of the order p ($p = 10$). Approximated solutions:

$$G_i(s,t) = \sum_{l=1}^{L} \Phi_l N_l(s,t), \quad N_l(s,t) = \bigcup_{q_1 q_2} \{\varphi_{r_1 q_1 r_2 q_2}(s,t),\ (s,t) \in \Delta_{q_1 q_2}(s,t)\}, \tag{29}$$

where

$$2(pN_s - 1)(pN_t - 1) \le L \le 2(pN_s + 1)(pN_t + 1) \tag{30}$$

depends on boundary conditions, $l \equiv l(i, r_1, q_1, r_2, q_2)$ is determined by the number i of solution component, the numbers r_1, r_2 of the shape function, and the numbers q_1, q_2 of the subdomain.

Application of the FEM

Nonlinear generalized eigenvalue problem

$$\mathbf{A}(E^h)\mathbf{\Phi}^h = E^h\mathbf{B}\mathbf{\Phi}^h, \quad \left(\mathbf{\Phi}^h\right)^T \mathbf{B}\mathbf{\Phi}^h = 1. \tag{31}$$

This problem is solved using a continuous analogue of Newton's method with the optimal iteration parameter described in [a].

[a] T. Zhanlav, O. Chuluunbaatar, New developments of Newton-type iterations for solving nonlinear problems, Switzerland, Springer Nature, pp. 281 (2024).
E. Zemlyanaya, O. Chuluunbaatar, Nat. Sci. Rev. **3**, 200605–1–63 (2026).

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Estimations of the numerical solutions: [K.J. Bathe, Finite Element Procedures . . . (1982).]

The approximate solution E^h, $\mathbf{\Phi}^h \in \mathcal{H}_2^1(\Delta)$ from the exact one E, $\mathbf{\Phi}(s,t) \in \mathcal{H}_2^2(\Delta)$ is estimated as

$$\left|E - E^h\right| \le c_1 h^{2p}, \quad \left\|\mathbf{\Phi}(s,t) - \mathbf{\Phi}^h\right\|_0 \le c_2 h^{p+1}, \tag{32}$$

where h is the maximal size of the finite element $\Delta_{q_1 q_2}$, p is the FEM scheme order, $c_1 > 0$ and $c_2 > 0$ are coefficients independent of h, and

$$\|\mathbf{\Phi}(s,t)\|_0^2 = \int_\Delta g_{00}(s,t)\, \mathbf{\Phi}^T(s,t)\mathbf{\Phi}(s,t)\, dsdt. \tag{33}$$

Numerical results for H_2^+: $\xi_{max} = 50$

The relativistic $1s\sigma_g$ state energy E_R of H_2^+ at $\rho = 2$ and $c = 137.03599\,9084$.

All calculations were performed using the multiprecision arithmetic MPFUN2020-Fortran package with 54-digit floating point numbers.
Parameters: $p = 10$, ν, N_t, N_s.
E_{exact} is obtained at $N_s = 120$, $N_t = 60$, and $\nu = 8$.

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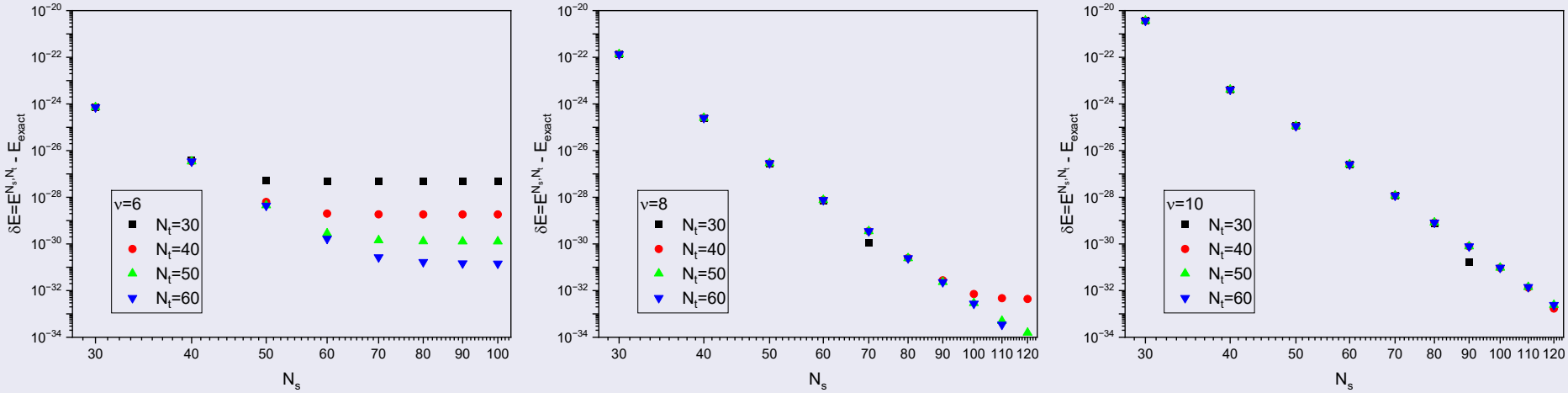

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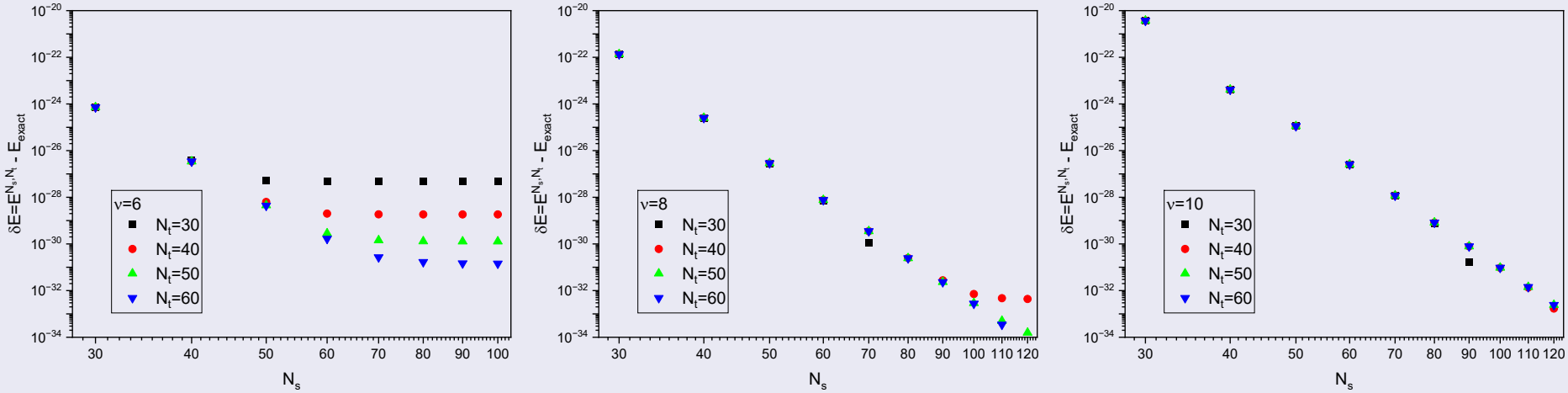

The convergence order $\hat{p}$ of the calculated energy E

$$\frac{E^{N_s,N_t} - E^{N_s+10,N_t}}{E^{N_s+10,N_t} - E^{N_s+20,N_t}} - \frac{N_s^{-2\hat{p}} - (N_s+10)^{-2\hat{p}}}{(N_s+10)^{-2\hat{p}} - (N_s+20)^{-2\hat{p}}} = 0. \qquad (34)$$

$\hat{p} = 5.55 \div 13.09$ for $\nu = 6$; $\hat{p} = 9.96 \div 10.02$ for $\nu = 8$; and $\hat{p} = 7.99 \div 10.37$ for $\nu = 10$.

Numerical results for H_2^+

The relativistic $1s\sigma_g$ state energy $E_e = E_R - c^2$ of H_2^+ at $\rho = 2$ and $c = 137.03599\,9084$.

N_s	N_t	$\nu = 8$
40	40	$-1.10264\,15810\,32577\,16411\,81247$
60	40	— " — 998
80	40	— " — 99957
100	40	— " — 99957 6490
120	40	— " — 99957 6517
60	50	$-1.10264\,15810\,32577\,16411\,81249$ 998
80	50	— " — 99957
100	50	— " — 99957 6532
120	50	— " — 99957 6560
60	60	— " — 998
80	60	— " — 99957
100	60	— " — 99957 6534
120	60	— " — 99957 6561
[a]		— " — 99957 65
[b]		$-1.10264\,15810\,32577\,16411\,811$
[c]		$-1.10264\,15810\,32577\,16411\,72569\,1$

[a] H.D. Nogueira and J.-P. Karr, Phys. Rev. A **107**, 042817 (2023).
[b] O. Kullie, Phys. Rev. A **110**, 052808 (2024).
[c] O. Kullie et al., Phys. Rev. A **105**, 052801 (2022).

Numerical results for H_2^+

The relativistic energy E_e of first eight excited states of H_2^+ at $\rho = 2$. Here $N_s = 100$, $N_t = 60$, and $\nu = 8$ for $|j_z| = 1/2$, and $\nu = 6$ for $j_z = 3/2$.

State	j_z	This work	[a]
$2p\sigma_u$	$1/2$	$-0.66755\,27719\,93113\,04580\,98309\,94632\,1$	$-0.66755\,27719\,93113\,04580\,9$
$2p\pi_u$	$-1/2$	$-0.42878\,11602\,12631\,30343\,94372\,42911\,7$	$-0.42878\,11602\,12631\,30344\,2$
$2p\pi_u$	$3/2$	$-0.42877\,44479\,92646\,21640\,43445\,15141\,4$	$-0.42877\,44479\,92646\,21640\,4$
$2s\sigma_g$	$1/2$	$-0.36087\,10705\,77597\,64090\,13308\,90179\,6$	$-0.36087\,10705\,77597\,64090\,1$
$2p\sigma_u$	$1/2$	$-0.25541\,97047\,48235\,32392\,74800\,35302\,6$	$-0.25541\,97047\,48235\,32406\,1$
$3d\sigma_g$	$1/2$	$-0.23578\,12684\,52381\,62910\,30159\,51282\,3$	$-0.23578\,12684\,52381\,62910\,3$
$3d\pi_g$	$-1/2$	$-0.22670\,30713\,40986\,07289\,27553\,70886\,1$	$-0.22670\,30713\,40986\,07289\,3$
$3d\pi_g$	$3/2$	$-0.22670\,14939\,71348\,87626\,84904\,02724\,4$	$-0.22670\,14939\,71348\,87626\,8$

[a] O. Kullie, Phys. Rev. A **110**, 052808 (2024).

Numerical results for Th_2^{179+}: $\xi_{max} = 45$

The relativistic $1s\sigma_g$ state energy E_R of Th_2^{179+} at $\rho = 2/90$.

E_{exact} is obtained at $N_s = 100$, $N_t = 60$, and $\nu = 10$.

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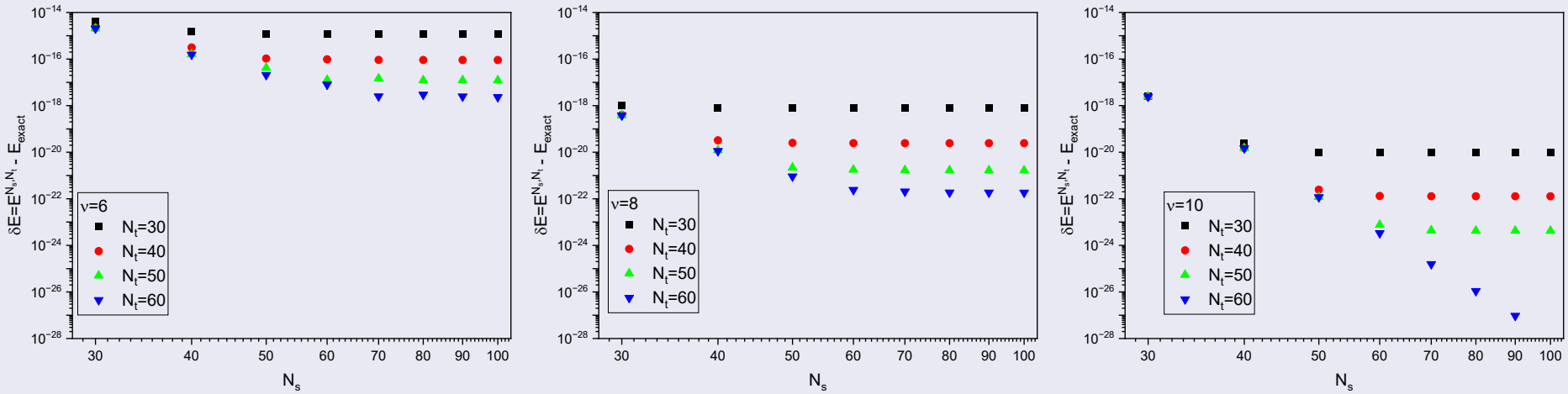

$\hat{p} = 0.85 \div 10.65$ for $\nu = 8$ and $\hat{p} = 9.72 \div 10.88$ for $\nu = 10$.

Numerical results for Th_2^{179+}

The relativistic $1s\sigma_g$ state energy $E_e = E_R - c^2$ of Th_2^{179+} at $\rho = 2/90$.

N_s	N_t	$\nu = 10$
40	40	−9504.75664 84340 09500 76067
60	40	— ″ — 076
80	40	— ″ — 0799 12
100	40	— ″ — 0799 23
60	50	— ″ — 200
80	50	— ″ — 2040 39
100	50	— ″ — 2040 50
60	60	— ″ — 204
80	60	— ″ — 2082 69
100	60	— ″ — 2082 80
[a]		−9504.75664 84340 09500 732
[b]		−9504.75664 84340 09500 723

[a] H.D. Nogueira and J.-P. Karr, Phys. Rev. A **107**, 042817 (2023).
[b] O. Kullie, Phys. Rev. A **110**, 052808 (2024).

Numerical results for Th_2^{179+}

The relativistic energy E_e of first eight excited states of Th_2^{179+} at $\rho = 2/90$. Here $N_s = 100$, $N_t = 60$, and $\nu = 10$ for $|j_z| = 1/2$, and $\nu = 8$ for $j_z = 3/2$.

State	j_z	This work	[a]†
$2p\sigma_u$	$1/2$	−6815.51298 78479 80388 34196 43730 83	−6815.51321 79
$2p\pi_u$	$-1/2$	−4127.89083 61977 64790 37761 03056 69	
$2p\pi_u$	$3/2$	−3653.56792 61946 91492 85963 74152 38	
$2s\sigma_g$	$1/2$	−3374.51993 11919 18575 52852 46732 37	−3374.52000 72
$2p\sigma_u$	$1/2$	−2564.18065 18146 66937 89842 40376 68	−2564.18073 00
$3d\sigma_g$	$1/2$	−2455.95612 46833 24544 25485 51641 61	−2455.95625 91
$3d\pi_g$	$-1/2$	−2010.66348 16546 12483 17798 39615 30	−2010.66350 13
$3d\pi_u$	$-1/2$	−1917.12388 24217 05141 34542 84978 15	−1917.12393 18

† $c = 137.03598\,95$.

[a] O. Kullie et al., J. Phys. B **36**, 4361 (2003).

Conclusion

- We presented the transformation of the Dirac equation into nonlinear system of the self-adjoint two coupled elliptic equations with respect to relativistic energy.
- We investigated the behavior of the electron in its $1s\sigma_g$ and first eight excited levels of the two homonuclear molecular ions H_2^+ and Th_2^{179+} at the internuclear distance of $\rho = 2/Z$.
- High-precision (35 digits for H_2^+ and 30 digits for Th_2^{179+}) in energy values is obtained, which contribute to the state of the art in comparison to relatively recent confirmed results obtained by different procedures.
- We developed and tested our computational schemes for solving 2D BVPs of a system of self-adjoint multidimensional elliptic equations (35) on hyperparallelepid domain using FEM.

$$\left(\mathbf{I}T(x) + \mathbf{Q}(x)\frac{\partial}{\partial x} + \frac{\partial}{\partial x}\mathbf{Q}(x) + \mathbf{V}(x) - E\mathbf{I}\right)\mathbf{\Phi}(x) = 0, \quad x = (x_1, \ldots, x_d) \tag{35}$$

$$T(x) = -\frac{1}{g_0(x)}\sum_{i,j=1}^{d}\frac{\partial}{\partial x_i}g_{ij}(x)\frac{\partial}{\partial x_j}, \quad g_{ij}(x) = g_{ji}(x),$$

$$\mathbf{Q}(x)\frac{\partial}{\partial x} + \frac{\partial}{\partial x}\mathbf{Q}(x) = \sum_{i=1}^{d}\frac{1}{g_0(x)}\mathbf{Q}^{(i)}(x)\frac{\partial}{\partial x_i} + \sum_{i=1}^{d}\frac{1}{g_0(x)}\frac{\partial}{\partial x_i}\mathbf{Q}^{(i)}(x).$$

Thank you for your attentions!