Application of minimax optimization for solving the Dirac equation of an electron in the field of two fixed attractive Coulomb centers

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Outline

- The particularities of the variational solution of the Dirac equation
- The trial LCAO function and the matrix elements of the two center Dirac hamiltonian
- The spurious root
- Minimax procedure
- Results
- Conclusion

Dirac equation and its particularities

The Dirac equation

$$(\mathcal{H}_D - E_R)\Psi(\mathbf{r}) = 0, \tag{1}$$

$$\mathcal{H}_D = \mathcal{H}_0 + V(\mathbf{r})\mathbf{I}, \quad \mathcal{H}_0 = c\boldsymbol{\alpha}\boldsymbol{p} + m_e c^2 \beta \tag{2}$$

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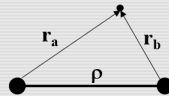
In explicit form:

$$\begin{cases} -\imath\hbar c \left[\left(\frac{\partial}{\partial x} - \imath\frac{\partial}{\partial y}\right)\psi_4 + \frac{\partial}{\partial z}\psi_3\right] + (V(\mathbf{r}) + m_e c^2 - E_R)\psi_1 = 0, \\ -\imath\hbar c \left[\left(\frac{\partial}{\partial x} + \imath\frac{\partial}{\partial y}\right)\psi_3 - \frac{\partial}{\partial z}\psi_4\right] + (V(\mathbf{r}) + m_e c^2 - E_R)\psi_2 = 0, \\ -\imath\hbar c \left[\left(\frac{\partial}{\partial x} - \imath\frac{\partial}{\partial y}\right)\psi_2 + \frac{\partial}{\partial z}\psi_1\right] + (V(\mathbf{r}) - m_e c^2 - E_R)\psi_3 = 0, \\ -\imath\hbar c \left[\left(\frac{\partial}{\partial x} + \imath\frac{\partial}{\partial y}\right)\psi_1 - \frac{\partial}{\partial z}\psi_2\right] + (V(\mathbf{r}) - m_e c^2 - E_R)\psi_4 = 0. \end{cases} \tag{3}$$

$m_e = \hbar = 1$, $c = 137.0359895$ a.u.

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Prolate spheroidal Coordonates

$$\lambda = \frac{r_a + r_b}{\rho}, \quad \mu = \frac{r_a - r_b}{\rho}, \quad \varphi$$

$$\left[\frac{d}{d\mu}\left\{(1-\mu^2)\frac{d}{d\mu}\right\} - \left\{A + \frac{k^2\rho^2\mu^2}{4} + \frac{m^2}{(1-\mu^2)} - (z_a - z_b)\rho\mu\right\}\right]S_l^m(\mu) = 0$$

$$\left[\frac{d}{d\lambda}\left\{(\lambda^2-1)\frac{d}{d\lambda}\right\} + \left\{A + \frac{k^2\rho^2\lambda^2}{4} - \frac{m^2}{(\lambda^2-1)} + (z_a + z_b)\rho\lambda\right\}\right]T_l^m(\lambda) = 0$$

$$A = -\ell^2 - \frac{\rho^2}{4}\left(\Delta - \frac{\partial^2}{\partial z^2}\right) - \rho(Z_a cos\theta_a - Z_b cos\theta_b)$$

Figure 1:

Figure 2:

-1 Dirac equation satisfies the Lorenz invariance principle

-2 Spin of the electron is included in the wave function

-3 For Dirac, the negative energy states are full.

-Vacuum consists of infinite density of negative energy electrons

- Emptying of one or more negative states can be observed
- It manifest itself as a positively charged particle with positive masse and kinetic energy. THE POSITRON .
- If an electron with positive energy emits a photon and fills an existing hole (positron), we can observe an annihilation process.

-4 Interpretation of hyperfine structure

Figure 3:

The two-center Coulomb potential

The potential

$$V(\mathbf{r}) = -\frac{Z}{r_a} - \frac{Z}{r_b}, \tag{4}$$

$$\mathbf{r}_a = \mathbf{r} + \boldsymbol{\rho}/2, \quad \mathbf{r}_b = \mathbf{r} - \boldsymbol{\rho}/2, \quad \boldsymbol{\rho} = (0, 0, \rho), \tag{5}$$

ρ is the internuclear distance

The basis functions: the Slater type basis functions

$$\Psi(\mathbf{r}) = \begin{pmatrix} \imath f(\mathbf{r}) \\ g(\mathbf{r}) \end{pmatrix}, \tag{6}$$

$$f(\mathbf{r}) = \sum_{n=1}^{N_{\max}} \sum_{\kappa=-n,\,\kappa\neq0}^{n-1} [P_{n\kappa}(r_a)\Omega_{+\kappa m}(\theta_a, \phi_a) + \sigma_{n\kappa} P_{n\kappa}(r_b)\Omega_{+\kappa m}(\theta_b, \phi_b)], \tag{7}$$

$$g(\mathbf{r}) = \sum_{n=1}^{N_{\max}} \sum_{\kappa=-n,\,\kappa\neq0}^{n-1} [Q_{n\kappa}(r_a)\Omega_{-\kappa m}(\theta_a, \phi_a) + \sigma_{n\kappa} Q_{n\kappa}(r_b)\Omega_{-\kappa m}(\theta_b, \phi_b)], \tag{8}$$

$$\sigma_{n\kappa} = (-1)^{l_{n\kappa}} \tag{9}$$

The one centre wave function

The partial solutions

$$\Psi(\mathbf{r}) = \begin{cases} \imath P_{n\kappa}(r)\Omega_{+\kappa m}(\theta, \phi) \\ Q_{n\kappa}(r)\Omega_{-\kappa m}(\theta, \phi) \end{cases} \tag{10}$$

$P_{n\kappa}(r)$ is a large component, and $Q_{n\kappa}(r)$ is a small component

The spin spherical harmonics

$$\Omega_{\kappa m}(\theta, \phi) = \sqrt{\frac{1}{2l+1}} \begin{cases} \begin{cases} \sqrt{l+m+1/2}\, Y_{lm-1/2}(\theta, \phi) \\ \sqrt{l-m+1/2}\, Y_{lm+1/2}(\theta, \phi) \end{cases}, & \kappa = -l-1 < 0 \\ \begin{cases} -\sqrt{l-m+1/2}\, Y_{lm-1/2}(\theta, \phi) \\ \sqrt{l+m+1/2}\, Y_{lm+1/2}(\theta, \phi) \end{cases}, & \kappa = l > 0 \end{cases} \tag{11}$$

The one-center Coulomb potential

$$P_{n\kappa}(r) = \sum_{n_p=1}^{n_{p\,\max}} c_{n_p\kappa} p_{n_p\kappa}(r), \tag{12}$$

$$Q_{n\kappa}(r) = \sum_{n_q=1}^{n_{q\,\max}} d_{n_q\kappa} q_{n_q\kappa}(r), \tag{13}$$

$$p_{n_p\kappa}(r) = r^{\gamma_\kappa + n_p - 2} \exp(-\lambda_{p\kappa} r), \tag{14}$$

$$q_{n_q\kappa}(r) = r^{\gamma_\kappa + n_q - 2} \exp(-\lambda_{q\kappa} r), \tag{15}$$

$\lambda_{p\kappa}, \lambda_{q\kappa}$ are independent.

$$\gamma_\kappa = \sqrt{\kappa^2 - \frac{Z^2}{c^2}}, \quad n_{q\,\max} = \begin{cases} n_{p\,\max}, & \kappa < 0, \\ n_{p\,\max} + 1, & \kappa > 0. \end{cases} \tag{16}$$

Results

Table 1: Total numbers of NISTO depending on the maximal principal quantum number $N_{\max}$. $n_{p\,\max} = n - |\kappa| + 1 \geq 1$.

κ	States	$N_{\max} = 2$		$N_{\max} = 3$		$N_{\max} = 4$		$N_{\max} = 5$	
		$n_{p\,\max}$	$n_{q\,\max}$	$n_{p\,\max}$	$n_{q\,\max}$	$n_{p\,\max}$	$n_{q\,\max}$	$n_{p\,\max}$	$n_{q\,\max}$
- 1	$s_{1/2}$	2	2	3	3	4	4	5	5
1	$p_{1/2}$	2	3	3	4	4	5	5	6
- 2	$p_{3/2}$	1	1	2	2	3	3	4	4
2	$d_{3/2}$			2	3	3	4	4	5
- 3	$d_{5/2}$			1	1	2	2	3	3
3	$f_{5/2}$					2	3	3	4
- 4	$f_{7/2}$					1	1	2	2
4	$g_{7/2}$							2	3
- 5	$g_{9/2}$							1	1
Total number		11		24		41		62	

The total number of nonlinear parameters: $4N_{\max} - 2$.

Particularities

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

$$-c^2 \leq E_R = \min_{P_{n\kappa}(r) \neq 0} \max_{Q_{n\kappa}(r)} \langle H_D \rangle = \min_{\lambda_{p\kappa}} \max_{\lambda_{q\kappa}} \langle H_D \rangle \leq c^2, \tag{17}$$

$$\mathbf{A} \left(\begin{array}{c} \mathbf{c} \\ \mathbf{d} \end{array} \right) = E_R \mathbf{B} \left(\begin{array}{c} \mathbf{c} \\ \mathbf{d} \end{array} \right). \tag{18}$$

The spurious root

The $N + M$ eigenvalues, where N and M are total numbers of large and small components, respectively, split into N greater than $-c^2$ and M negative less than $-c^2$ eigenvalues.

A spurious root appears in the case $\kappa > 0$. This spurious root is degenerate with the lowest variational state of the same $|\kappa|$ but with a $\kappa < 0$.

Advantage of minimax

If the polynomial for small components is of higher degree than for large components, the minimax estimate will be an upper bound for the exact energy, i.e. avoid the spurious roots[a].

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[a]A. Kolakowska, J.D. Talman, K. Aashamar, Phys. Rev. A. **53**, 168–177 (1996).

TABLE I. Values of the $2p_{1/2}$ Coulomb energy for $Z = 92$ calculated with $M = N = 1$ for various values of the nonlinear parameters α and β.

β/α	30.0	31.0	32.0	33.0	34.0
115.0	−1262.04	−1265.83	−1269.22	−1272.35	−1275.37
120.0	−1262.59	−1264.32	−1265.43	−1266.09	−1266.46
125.0	−1265.93	−1265.89	−1265.04	−1263.55	−1261.57
130.0	−1271.68	−1270.13	−1267.60	−1264.25	−1260.23
135.0	−1279.49	−1276.70	−1272.74	−1267.79	−1261.99

Figure 4:

Statement of the problem

Minimax optimization

We consider the minimax optimization problem

$$\min_{\mathbf{x}\in\mathcal{X}} \max_{\mathbf{y}\in\mathcal{Y}} f(\mathbf{x}, \mathbf{y}), \qquad (19)$$

$f(\mathbf{x}, \mathbf{y})$ is twice differentiable everywhere, and $f : \mathcal{X} \times \mathcal{Y} \subset \mathbb{R}^N \times \mathbb{R}^M \to \mathbb{R}$.
We denote

$$\nabla f(\mathbf{x}, \mathbf{y}) = \mathbf{G} = \begin{pmatrix} \mathbf{G_x} \\ \mathbf{G_y} \end{pmatrix}, \quad \nabla^2 f(\mathbf{x}, \mathbf{y}) = \mathbf{H} = \begin{pmatrix} \mathbf{H_{xx}} & \mathbf{H_{xy}} \\ \mathbf{H_{yx}} & \mathbf{H_{yy}} \end{pmatrix}, \qquad (20)$$

with $\mathbf{H_{yx}^T} = \mathbf{H_{xy}}$.

Definition of the Nash equilibrium and minimax

Proposition 1: First-order necessary condition

Any local Nash and/or minimax point $(\mathbf{x}, \mathbf{y})$ satisfies

$$\nabla f(\mathbf{x}, \mathbf{y}) = 0. \tag{21}$$

Proposition 2: Second-order sufficient condition

Any stationary point $(\mathbf{x}, \mathbf{y})$ satisfying the following condition is a local Nash:

$$\mathbf{H_{yy}} \prec 0, \quad \mathbf{H_{xx}} \succ 0. \tag{22}$$

Proposition 3: Second-order sufficient condition

Any stationary point $(\mathbf{x}, \mathbf{y})$ satisfying the following condition is a local minimax:

$$\mathbf{H_{yy}} \prec 0, \quad \mathbf{H_{xx}} \underbrace{- \mathbf{H_{xy}} \mathbf{H_{yy}^{-1}} \mathbf{H_{yx}}}_{\succ 0} \succ 0. \tag{23}$$
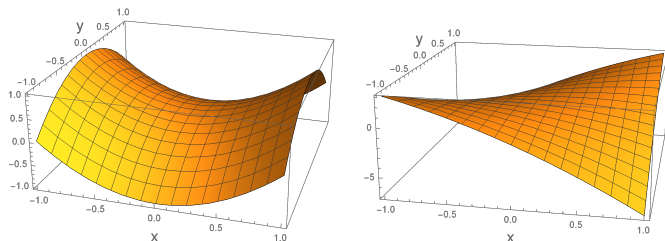
Statement of the problem

Figure 1: **Left:** $f(x, y) = x^2 - y^2$ where $(0, 0)$ is both local Nash and local minimax. **Right:** $f(x, y) = -x^2 + 5xy - y^2$ where $(0, 0)$ is not local Nash but local minimax with $h(\delta) = \delta$.

Numerical algorithm and package programs

1. There are many algorithms and methods for the Nash problem. Most of them only work for convex-concave domain.
2. There are only a few algorithms and methods for the minimax problem.
3. There are no program packages for the Nash and minimax problems.

Numerical methods

Iterative

$$(\mathbf{x}_n, \mathbf{y}_n) \to (\mathbf{x}_{n+1}, \mathbf{y}_{n+1}) \tag{24}$$

$$\delta\mathbf{x}_n = \mathbf{x}_{n+1} - \mathbf{x}_n, \quad \delta\mathbf{y}_n = \mathbf{y}_{n+1} - \mathbf{y}_n \tag{25}$$

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Convex-concave case: Newton type method

$$\mathbf{H_{yy}} \prec 0, \quad \mathbf{H_{xx}} - \mathbf{H_{xy}}\mathbf{H_{yy}}^{-1}\mathbf{H_{yx}} \succ 0; \quad \mathbf{x} = \mathbf{x}_n, \mathbf{y} = \mathbf{y}_n. \tag{26}$$

$$\begin{pmatrix} \delta\mathbf{x} \\ \delta\mathbf{y} \end{pmatrix} = -\tau \begin{pmatrix} \mathbf{H_{xx}} & \mathbf{H_{xy}} \\ \mathbf{H_{yx}} & \mathbf{H_{yy}} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{G_x} \\ \mathbf{G_y} \end{pmatrix}, \quad \tau \in (0, 2) \tag{27}$$

Numerical methods

Nonconcave case: Gradient descent method

$$\mathbf{H_{yy}} \not\prec 0 \tag{28}$$
$$\delta\mathbf{y} = \eta\mathbf{G_y} \tag{29}$$

The negative curvature direction method

$\mathbf{u}$ is the eigenvector associated with the largest positive eigenvalue of $\mathbf{H_{yy}}$:

$$\delta\mathbf{y} = \eta\mathbf{u}, \quad \mathbf{u}^T\mathbf{G_y} > 0. \tag{30}$$

Numerical methods

Nonconcave case: Gradient descent method

$$\mathbf{H_{yy}} \nprec 0 \tag{28}$$
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Nonconvex-concave case: Gradient descent method

$$\mathbf{H_{yy}} \prec 0, \quad \mathbf{H_{xx}} - \mathbf{H_{xy}}\mathbf{H_{yy}^{-1}}\mathbf{H_{yx}} \nsucc 0. \tag{31}$$
$$\delta\mathbf{x} = -\eta\mathbf{G_x} \tag{32}$$

The negative curvature direction method

$\mathbf{u}$ is the eigenvector associated with the smallest negative eigenvalue of $\mathbf{H_{xx}}$:

$$\delta\mathbf{x} = \eta\mathbf{u}, \quad \mathbf{u}^T\mathbf{G_x} < 0. \tag{33}$$

Numerical test

Example

$$f(x, y) = 2x^2 + y^2 + 4xy + \frac{4}{3}y^3 - \frac{1}{4}y^4, \tag{34}$$

$$\mathbf{z}_1 = (0, 0), \quad \mathbf{z}_2 = (-2 - \sqrt{2}, 2 + \sqrt{2}), \quad \mathbf{z}_3 = (-2 + \sqrt{2}, 2 - \sqrt{2}), \tag{35}$$

$$\mathbf{H}(\mathbf{z}_1) = \begin{pmatrix} 4 & 4 \\ 4 & 2 \end{pmatrix}, \ \mathbf{H}(\mathbf{z}_2) = \begin{pmatrix} 4 & 4 \\ 4 & -4\sqrt{2} \end{pmatrix}, \ \mathbf{H}(\mathbf{z}_3) = \begin{pmatrix} 4 & 4 \\ 4 & 4\sqrt{2} \end{pmatrix}. \tag{36}$$
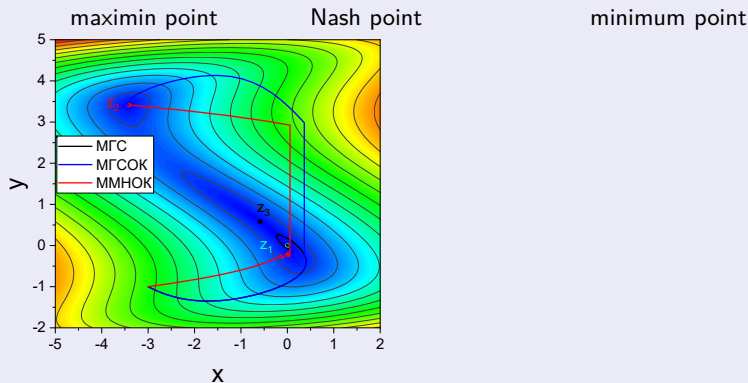
maximin point   Nash point   minimum point

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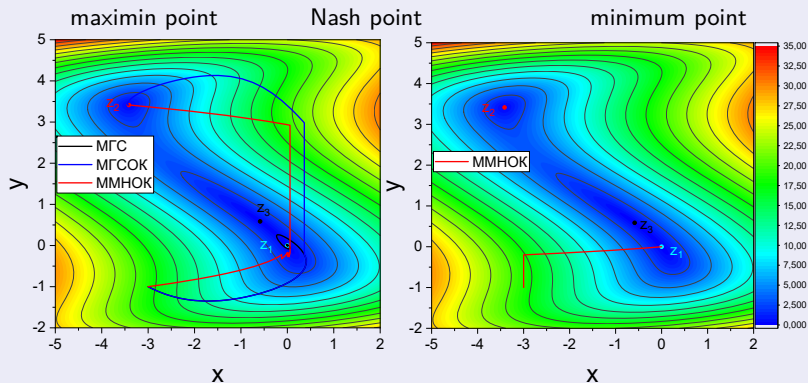

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$$\mathbf{H}(\boldsymbol{z}_1) = \left(\begin{array}{cc} 4 & 4 \\ 4 & 2 \end{array} \right), \; \mathbf{H}(\boldsymbol{z}_2) = \left(\begin{array}{cc} 4 & 4 \\ 4 & -4\sqrt{2} \end{array} \right), \; \mathbf{H}(\boldsymbol{z}_3) = \left(\begin{array}{cc} 4 & 4 \\ 4 & 4\sqrt{2} \end{array} \right). \tag{36}$$
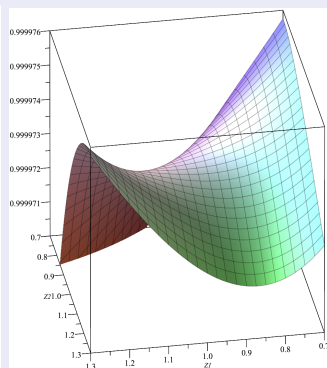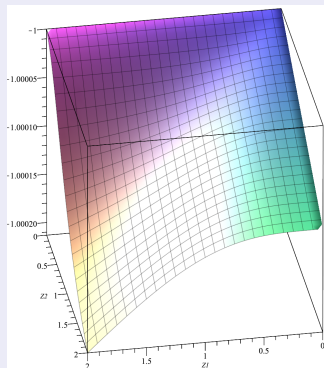
The one-center Coulomb potential

$Z = 1$, Minimax BF

$$P_{1-1}(r) = e^{-Z_1 r} r^{\gamma - 1}, \quad Q_{1-1}(r) = e^{-Z_2 r} r^{\gamma - 1}, \qquad (37)$$

$Z_1 = Z_2 = 1$ is the Nash and minimax point

$c^{-2} E_{1-1}$

Results

Table 2: Total numbers of NISTO depending on the maximal principal quantum number N_{max}. $n_{p\,max} = n - |\kappa| + 1 \geq 1$.

κ	States	$N_{max} = 2$		$N_{max} = 3$		$N_{max} = 4$		$N_{max} = 5$	
		$n_{p\,max}$	$n_{q\,max}$	$n_{p\,max}$	$n_{q\,max}$	$n_{p\,max}$	$n_{q\,max}$	$n_{p\,max}$	$n_{q\,max}$
- 1	$s_{1/2}$	2	2	3	3	4	4	5	5
1	$p_{1/2}$	2	3	3	4	4	5	5	6
- 2	$p_{3/2}$	1	1	2	2	3	3	4	4
2	$d_{3/2}$			2	3	3	4	4	5
- 3	$d_{5/2}$			1	1	2	2	3	3
3	$f_{5/2}$					2	3	3	4
- 4	$f_{7/2}$					1	1	2	2
4	$g_{7/2}$							2	3
- 5	$g_{9/2}$							1	1
Total number		11		24		41		62	

The total number of nonlinear parameters: $4N_{max} - 2$.

Results

Table 3: The relativistic $1\sigma_g$ state energy $E_e = E_R - c^2$ at $\rho = 2/Z$.

Z	Ion	N_{max}	Energy	Energy (Tupitsyn)
1	H_2^+	2	-1.102 248 990	
		3	-1.102 624 606	
		4	-1.102 640 853	
		5	-1.102 641 574	-1.102 641 581
20	Ca_2^{39+}	2	-442.073 489 140	
		3	-442.231 839 925	
		4	-442.239 683 071	
		5	-442.239 984 905	-442.239 997 265
100	Fm_2^{199+}	2	-11942.178 005 611	
		3	-11951.832 987 584	
		4	-11952.939 381 324	
		5	-11952.941 727 610	-11952.941 940 110
118	Og_2^{235+}	2	-17461.232 762 069	
		3	-17477.122 912 713	
		4	-17479.073 413 320	
		5	-17479.125 249 624	

I.I. Tupitsyn, et al, Optics and Spectroscopy **117**, 351–357 (2014)., 570–598 Gaussian BF

Matrix elements

Two center integrals

$$F_{l_1 l_2}^{m_1 m_2}(a_1, \nu_1, a_2, \nu_2, \rho) = \int d\vec{r}\, r_1^{\nu_1-1} e^{-a_1 r_1} Y_{l_1 m_1}^*(\vec{r}_1) r_2^{\nu_2-1} e^{-a_2 r_2} Y_{l_2 m_2}(\vec{r}_2), \quad (38)$$

$$= 8 \sum_{l=|l_1-l_2|,2}^{l_1+l_2} (-1)^{\frac{3l+l_1-l_2}{2}} Y_{l0}(\vec{\rho}) \, \Upsilon_{l l_1 l_2}^{0 m_1 m_2}$$

$$\times \int_0^\infty dp\, p^2 j_l(\rho p) g_{l_1}(a_1, \nu_1, p) g_{l_2}(a_2, \nu_2, p), \quad (39)$$

where

$$\Upsilon_{l l_1 l_2}^{m m_1 m_2} = \int d\Omega_p Y_{lm}(\vec{p}) Y_{l_1 m_1}^*(\vec{p}) Y_{l_2 m_2}(\vec{p}), \quad (40)$$

$$g_l(a, \nu, p) = \int_0^\infty dr\, r^{\nu+1} \exp(-ar) j_l(pr), \quad \nu+1+l > -1. \quad (41)$$

Here a_1, a_2 are positive numbers; ν_1, ν_2 are non-integer numbers; $\max(\nu_1, \nu_2) > 0$, $\min(\nu_1, \nu_2) > -1$.

Computational time

$N_{\max} = 5$, dimension of matrices is 62×62 and 18 nonlinear parameters

Condition number of matrices: $\sim 10^8$
Accuracy: 10^{-20}

For energy: required to calculate 8808 one-dimensional integrals.
For gradient: required to calculate 33672 one-dimensional integrals.
For hessian: required to calculate 556368 one-dimensional integrals.
Total: 598848

Computational time of one iteration on the supercomputer Govorun is ~ 60 min.
After using special algorithm (including Adelson-Velsky and Landis tree ...) – only 12 min.

Research paper

Accurate calculations for the Dirac electron in the field of two-center Coulomb field: Application to heavy ions

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A B S T R A C T

The relativistic Dirac equation for a bound electron in the field of two fixed positive charges is revisited. In contrast to the one center case this three dimensional equation is separable only partially around the azimuthal angle φ, because of the commutation of the Dirac Hamiltonian only with the z component of the total angular momentum J_z. In this work we determine the variational exact solution of this two center problem using a basis constructed by linear combinations of relativistic Slater type spinor wave functions with non integer powers of the radii r_1 and r_2 on the two centers. We present in some detail the determination of the two center integrations involved. The solutions are obtained by a minimax procedure, that we have developed with a new iterative scheme. We use independent large and small components of the Dirac spinor. This permits us to take control of the spurious solutions, and gives us the possibility to avoid them by the appropriate choice of the wave function parameters. We investigate the behavior of the electron in its $1s s_g$ level of the diatomic homo-nuclear systems $A_2^{(2Z-1)+}$, where A represents the heavy element and Z its atomic number. In the case of heavy ions we study the dependance of the electron energy on the internuclear distance, this gives us an indication for the conditions of atomic collapse, which can induce electron-positron pair production. Our approach has the advantage of needing small basis sets for a relative error of the of $10^{-7} - 10^{-8}$. It can also be extended easily to the excited level such as the $1s s_u$ level.

Conclusion

- We developed a new iterative scheme based on the Newton-type and gradient descent methods combined with negative curvature methods for solving the min-max problem and applied it to obtain a robust relativistic solution.
- We have found the way to avoid spurious solutions resulting from the presence of the negative energies.
- We realized by original approches the calculations of two center integrals with non-integer powers of r.
- We investigated the electronic energy of the fundamental $1s\sigma_g$ level for different nuclear charges.
- Our method can produce the solutions of $1s\sigma_u$ and higher levels needed in the case of large internuclear distances.

Thank you for your attentions!