

# Electronic structure calculations with the exact pseudopotential and interpolating wavelets

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## Abstract

The singularities of the potentials in quantum mechanical systems are often handled by using pseudopotentials. We construct the exact pseudopotential method (EPP) for the quantum mechanical computations of one dimensional systems in this article. We apply the method to a basis consisting of Deslauriers-Dubuc scaling functions on a half-infinite real interval. We demonstrate the method by computing the energies of hydrogen atom 1s, 2s, and 2p orbitals and helium atom configurations He 1s<sup>2</sup>, He 1s2s <sup>1</sup>S, and He 1s2s <sup>3</sup>S.

## 1 Introduction

When atoms and molecules are computed quantum physically the potential where the electrons move contains singularities at the nuclei. These singularities are usually handled by approximating the potential with a pseudopotential that does not have those singularities. Pseudopotentials are also used to approximate the total charge of the nuclei and core electrons so that it is sufficient to take only the valence electrons in the computations of the system.

One-dimensional interpolating wavelets have been used for atomic computations for example in [1]. There we used ordinary Deslauriers-Dubuc interpolating wavelets [2, 3, 4, 5, 6] defined on the whole real axis so that we had to include the negative real axis into the computations, too. We handled the singularity at the origin by excluding the scaling function at the origin from the basis. Arias [7] and Engeness and Arias [8] developed formalism for electronic structure calculations with interpolating wavelets so that matrix elements of the operators are computed as usual and overlap matrices are used in the matrix form of the Schrödinger equation. On the other hand, we use the interpolating dual scaling functions and wavelets for the computation of matrix elements.

One-dimensional interpolating multiresolution analysis in space  $C_u(\mathbb{R})$  consisting of uniformly continuous bounded functions in  $\mathbb{R}$  has been constructed in [4]. One-dimensional interpolating multiresolution analysis in space  $C_0(\mathbb{R})$  consisting of continuous functions in  $\mathbb{R}$  vanishing at infinity has been constructed in

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[5]. Both of these constructions are based on Deslauriers-Dubuc functions [2, 3]. Donoho [5] constructs wavelets on a finite real interval, too. The EPP method was invented by Dr. T. Rantala and it was applied to the interpolating wavelet basis by M. Sc. Tommi Höynälänmaa. We compute the energies of hydrogen atom 1s, 2s, and 2p orbitals and helium atom configurations He 1s<sup>2</sup>, He 1s2s <sup>1</sup>S, and He 1s2s <sup>3</sup>S with the EPP method. We use atomic units throughout this article ( $e = m_e = \hbar = 4\pi\epsilon_0 = 1$ ).

## 2 Exact Pseudopotential Method

Suppose that we have a system consisting of a positively charged nucleus at the origin and  $N$  electrons. First we choose some small radius  $r_0$  so that inside the ball with radius  $r_0$  the wavefunctions of the system are approximated by hydrogenic wavefunctions and the actual computations are done only for values  $r \geq r_0$ . We approximate the total charge of the core region  $r \leq r_0$  by  $Z' = Z - z$  where  $Z$  is the charge of the nucleus and  $z$  is the charge of the electrons in the core region. We have

$$z = \int_{r=0}^{r_0} \rho_{\text{hydr}}(r) dr \quad (1)$$

where  $\rho_{\text{hydr}}$  is the hydrogenic charge density of the electrons in the system. Now the Schrödinger equation of the atom is solved in region  $r \geq r_0$  for electrons moving in potential

$$V(r) = -\frac{Z - z}{r}. \quad (2)$$

## 3 Interpolating Wavelets on Half-Infinite Interval

This derivation is based on section 3 in [5]. We construct a basis set on half-infinite interval  $\mathbb{R}_0 = \{r \geq 0 | r \in \mathbb{R}\}$ . We define  $\varphi$  to be a Deslauriers-Dubuc scaling function of some order  $D$  and  $\varphi_{j,k}(x) := \varphi(2^j x - k)$  for  $j, k \in \mathbb{Z}$ . We define a wavelet expansion of a compactly supported function  $f$  on  $\mathbb{R}_0$  by

$$\tilde{f} := \sum_{k=0}^D \beta_{j,k} \varphi_{j,k}^{\#} + \sum_{k=D+1}^{W-1} \beta_{j,k} \varphi_{j,k} \quad (3)$$

where  $W$  is the size of the basis. We must have  $W > 2D$  so that functions  $\varphi_{j,k}^{\#}(x)$ ,  $0 \leq k \leq D$ , vanish for  $x \geq 2^{-j}W$ .

Suppose that we are given samples  $\beta_{j,k} = f(2^{-j}k)$  for  $k \in \mathbb{N}$  and  $f$  is some function from  $[0, \infty[$  into  $\mathbb{R}$ . We define  $\pi_j^{\#}$  to be the polynomial of degree  $D$  for which  $\pi_j^{\#}(2^{-j}k) = f(2^{-j}k)$  for all  $k = 0, \dots, D$ . We use a different normalization as [5] and define

$$\beta_{j,k} := f(2^{-j}k) \quad (4)$$

and

$$\tilde{\beta}_{j,k} := \pi_j^{\#}(2^{-j}k) \quad (5)$$

Now  $f$  can be extrapolated onto the whole real line by

$$\tilde{f} = \sum_{k=-\infty}^{\infty} \tilde{\beta}_{j,k} \varphi_{j,k}. \quad (6)$$

As each coefficient  $\tilde{\beta}_{j,k}$  is a linear functional of coefficients  $\beta_{j,k'}$  we may define extrapolation weights  $e_{k,k'}^{\#}$  so that

$$\tilde{\beta}_{j,k} = \sum_{k'=0}^D e_{k,k'}^{\#} \beta_{j,k'} \quad (7)$$

for  $k < 0$ . When  $f := \varphi_{j,l}$  we have

$$\tilde{\beta}_{j,k} = e_{k,l}^{\#} \quad (8)$$

where  $l \in \{0, \dots, D\}$ . Consequently the quantities  $e_{k,l}^{\#}$  can be computed by polynomial interpolation of functions  $\varphi_{j,l}$ . As

$$\text{supp } \varphi_{j,k} \subset 2^{-j}[k - D, k + D] \quad (9)$$

we need only values  $k \in \{-D, \dots, -1\}$ . We define

$$\varphi_{j,k}^{\#} := \varphi_{j,k} + \sum_{l < 0} e_{l,k}^{\#} \varphi_{j,l} \quad (10)$$

for  $k = 0, \dots, D$ . Note that

$$\langle \tilde{\varphi}_{j,k}, \varphi_{j,l}^{\#} \rangle = \delta_{k,l} \quad (11)$$

for  $k \geq 0$  and  $0 \leq l \leq D$ . Let  $A$  be a linear operator from  $C_0(\mathbb{R})$  to  $C_0(\mathbb{R})$ . The matrix elements  $A_{k,l}$ ,  $l = 0, \dots, D$  are given by

$$\langle \tilde{\varphi}_{j,k}, A\varphi_{j,l}^{\#} \rangle = \langle \tilde{\varphi}_{j,k}, A\varphi_{j,l} \rangle + \sum_{\alpha < 0} e_{\alpha,l}^{\#} \langle \tilde{\varphi}_{j,k}, A\varphi_{j,\alpha} \rangle. \quad (12)$$

Let  $v(f)$  denote the coefficient vector  $(\beta_{j,k})_{k=0}^{W-1}$  defined by equation (3) and define

$$M(f) := (f(2^{-j}k)\delta_{k,k'})_{k,k'=0}^{W-1, W-1} \quad (13)$$

for some function  $f : \mathbb{R} \rightarrow \mathbb{R}$ .

## 4 Schrödinger Equations of Hydrogen-like Atoms and Helium Atom in Our Basis

See [9, 10, 11, 12] for the Schrödinger equation of the hydrogen atom and Hartree-Fock equations of atoms. See also [1] for the representation of the Hartree-Fock equations in an interpolating wavelet basis. By doing a change of variables  $s := r - r_0$  the Schrödinger equation of a hydrogen-like atom in interval  $r \geq r_0$  takes the form

$$\left( -\frac{1}{2} \frac{d^2}{ds^2} - \frac{Z}{s+r_0} + \frac{l(l+1)}{2(s+r_0)^2} \right) \bar{P}(s) = \bar{E}\bar{P}(s), \quad s \geq 0 \quad (14)$$

where  $l$  is the angular momentum quantum number.

We define the second derivative filter by

$$a_k := \langle \tilde{\varphi}, D^2 \varphi(\cdot - k) \rangle \quad (15)$$

Matrix elements of the Laplacian operator  $L$  are computed by

$$L_{k,l} := \langle \tilde{\varphi}_{j,k}, L \varphi_{j,l}^\# \rangle = 2^{2j} \left( a_{l-k} + \sum_{\alpha=-D}^{-1} e_{\alpha,l}^\# a_{\alpha-k} \right) \quad (16)$$

for  $0 \leq l \leq D$  and

$$L_{k,l} := \langle \tilde{\varphi}_{j,k}, L \varphi_{j,l} \rangle = 2^{2j} a_{l-k} \quad (17)$$

for  $D < l < W$ . Note that matrix  $L$  is generally not hermitian. The potential energy operator is computed as a diagonal matrix

$$\hat{V}_{k,k} = V(2^{-j}k) \quad (18)$$

where

$$V(y) = -\frac{Z}{y+a} \quad (19)$$

for  $y \geq 0$ . The centrifugal potential is computed in the same way.

Define the Slater integrals

$$y_{ab}^0(r) = \int_{r'=0}^{\infty} P_a(r') \gamma(r, r') P_b(r') dr' \quad (20)$$

where  $a$  and  $b$  denote some atomic orbitals and

$$\gamma(r, r') = \frac{1}{\max\{r, r'\}}. \quad (21)$$

We use symbol  $y$  instead of  $Y$  to avoid confusion with spherical harmonics. By doing a similar change of variables  $s := r - r_0$  the Hartree-Fock equation of the ground state of the helium atom in interval  $r \geq r_0$  takes the form

$$\left( -\frac{1}{2} \frac{d^2}{ds^2} - \frac{Z}{s+r_0} + y_{1s1s}^0(s+r_0) \right) \bar{P}_{1s}(s) = \varepsilon_{1s} \bar{P}_{1s}(s), \quad s \geq 0. \quad (22)$$

The Hartree-Fock equations for the helium  $1s2s$   $^1S$  configuration are

$$\left( -\frac{1}{2} \frac{d^2}{ds^2} - \frac{2}{s+r_0} + y_{2s2s}^0(s+r_0) \right) \bar{P}_{1s}(s) = \varepsilon_{1s} \bar{P}_{1s}(s) \quad (23)$$

$$\left( -\frac{1}{2} \frac{d^2}{ds^2} - \frac{2}{s+r_0} + y_{1s1s}^0(s+r_0) \right) \bar{P}_{2s}(s) = \varepsilon_{2s} \bar{P}_{2s}(s) \quad (24)$$

and for helium  $1s2s$   $^3S$  configuration

$$\left( -\frac{1}{2} \frac{d^2}{ds^2} - \frac{2}{s+r_0} + y_{2s2s}^0(s+r_0) \right) \bar{P}_{1s}(s) = \varepsilon_{1s} \bar{P}_{1s}(s) + y_{1s2s}^0(s+r_0) \bar{P}_{2s}(s) \quad (25)$$

$$\left( -\frac{1}{2} \frac{d^2}{ds^2} - \frac{2}{s+r_0} + y_{1s1s}^0(s+r_0) \right) \bar{P}_{2s}(s) = \varepsilon_{2s} \bar{P}_{2s}(s) + \quad (26)$$

$$y_{2s1s}^0(s+r_0) \bar{P}_{1s}(s) \quad (27)$$

We define  $P_a(r)$  to be the exact Hartree-Fock wavefunction of the orbital  $a$  of the atom. We define the operators  $\hat{U}_0$  and  $\hat{U}_\infty$  [1] by

$$(\hat{U}_0 f)(s) = \int_0^s f(s') ds' \quad (28)$$

and

$$(\hat{U}_\infty f)(s) = \int_s^\infty f(s') ds' \quad (29)$$

Define  $P_{1s,\text{hydr}}(r')$  and  $P_{2s,\text{hydr}}(r')$  to be the hydrogenic orbitals of the helium atom. We have

$$\langle \tilde{\varphi}_{j,k} \hat{U}_0 \varphi_{j,l} \rangle = 2^{-j} (\Phi(|k| - l) - \Phi - l) \quad (30)$$

and

$$\langle \tilde{\varphi}_{j,k} \hat{U}_\infty \varphi_{j,l} \rangle = 2^{-j} (1 - \Phi(|k| - l)) \quad (31)$$

where

$$\Phi(x) = \int_{-\infty}^x \varphi(y) dy. \quad (32)$$

The Slater integrals in the shifted variables are obtained from

$$\begin{aligned} \bar{y}_{ab}^0(s) &= \frac{Q_{ab}}{s + r_0} + \frac{1}{s + r_0} \int_0^s \bar{P}_a(s') \bar{P}_b(s') ds' \\ &+ \int_s^\infty \frac{1}{s' + r_0} \bar{P}_a(s') \bar{P}_b(s') ds' \end{aligned} \quad (33)$$

where  $s \geq 0$  and

$$Q_{ab} := \int_0^{r_0} P_{a,\text{hydr}}(r') P_{b,\text{hydr}}(r') dr'. \quad (34)$$

Let  $f \star g$  denote the pointwise product of functions  $f$  and  $g$ . Define

$$q(s) := \frac{1}{s + r_0} \quad (35)$$

and

$$S_0 := M(q)U_0 + U_\infty M(q). \quad (36)$$

Now

$$v(\bar{y}_{1s1s}^0) = Qv(q) + S_0 (v(\bar{P}_{1s} \star \bar{P}_{1s})) \quad (37)$$

where  $U_0$  and  $U_\infty$  are the matrices of operators  $\hat{U}_0$  and  $\hat{U}_\infty$  in the basis set constructed in section 3. We define  $\mathbf{v}_a = v(\bar{P}_a)$  and  $\mathbf{v}_b = v(\bar{P}_b)$ . The matrix of the exchange integral operator

$$(\hat{K}_a \bar{P}_a)(s) := \bar{y}_{ab}^0(s) \bar{P}_b(s) \quad (38)$$

is computed by

$$K_a := W_a + M(\mathbf{v}_b)S_0M(\mathbf{v}_a) \quad (39)$$

The term  $W_a \mathbf{v}_a$  approximates the first term in equation (33) as a linear function of  $\mathbf{v}_a$ . In order to do this we approximate the wavefunction  $P_a(r)$  in region

$r \in [0, r_0]$  by a linear function that is zero at the origin and  $\bar{P}_a(0)$  at  $r_0$ . We have

$$\frac{Q_{ab}}{s+r_0} \bar{P}_b(s) \approx \frac{1}{s+r_0} \bar{P}_a(0) \left( \int_{s'=-r_0}^0 \left( 1 + \frac{s'}{r_0} \right) P_{b,\text{hydr}}(s'+r_0) ds' \right) \bar{P}_b(s) \quad (40)$$

The wavefunction  $\bar{P}_b(s)$  is taken from the previous step of the Hartree-Fock iteration. By approximating the wavefunctions by hydrogenic ones we get the hydrogenic Slater integrals

$$y_{1s1s,\text{hydr}}^0(r) = \frac{1}{r} - e^{-2Zr} \left( \frac{1}{r} + Z \right) \quad (41)$$

$$y_{2s2s,\text{hydr}}^0(r) = \frac{1}{r} + e^{-Zr} \left( -\frac{Z^3}{8} r^2 - \frac{1}{4} Z^2 r - \frac{3Z}{4} - \frac{1}{r} \right) \quad (42)$$

$$y_{1s2s,\text{hydr}}^0(r) = \frac{1}{27\sqrt{2}} (12Z^2 r + 8Z) e^{-3Zr/2} \quad (43)$$

for  $r \geq 0$ . The scalar products involving the Slater integrals are approximated as

$$\begin{aligned} \langle P_a | y_{ab}^0 | P_b \rangle &\approx \int_{r'=0}^{r_0} P_{a,\text{hydr}}(r') y_{ab,\text{hydr}}^0(r') P_{b,\text{hydr}}(r') dr' \\ &+ \int_{s=0}^{\infty} \bar{P}_a(s) \bar{y}_{ab}^0(s) \bar{P}_b(s) ds. \end{aligned} \quad (44)$$

The energy of the hydrogen atom orbital  $a$  is

$$E_a = \bar{E}_a + E_{a,\text{hydr}} Q_a \quad (45)$$

where the second term is the contribution of the core to the total energy. We have  $E_{a,\text{hydr}} = Z^2/(2n^2)$  where  $n$  is the principal quantum number of the orbital  $a$ . The total energy of the ground state of the helium atom is

$$E(\text{He } 1s^2) = 2(\varepsilon_{1s} + E_{1s,\text{hydr}} Q_{1s}) - \langle P_{1s} | y_{1s1s}^0 | P_{1s} \rangle \quad (46)$$

The total energy of the  $1s2s \ ^1S$  configuration of the helium atom is

$$\begin{aligned} E(\text{He } 1s2s \ ^1S) &= \varepsilon_{1s} + E_{1s,\text{hydr}} Q_{1s} + \varepsilon_{2s} + E_{2s,\text{hydr}} Q_{2s} \\ &- \frac{1}{2} \langle P_{1s} | y_{2s2s}^0 | P_{1s} \rangle - \frac{1}{2} \langle P_{2s} | y_{1s1s}^0 | P_{2s} \rangle \end{aligned} \quad (47)$$

and for the  $1s2s \ ^3S$  configuration

$$\begin{aligned} E(\text{He } 1s2s \ ^3S) &= \varepsilon_{1s} + E_{1s,\text{hydr}} Q_{1s} + \varepsilon_{2s} + E_{1s,\text{hydr}} Q_{2s} \\ &- \frac{1}{2} \langle P_{1s} | y_{2s2s}^0 | P_{1s} \rangle - \frac{1}{2} \langle P_{2s} | y_{1s1s}^0 | P_{2s} \rangle \\ &+ \langle P_{1s} | y_{1s2s}^0 | P_{2s} \rangle. \end{aligned} \quad (48)$$

## 5 Computations

We demonstrate the EPP method by doing computations where the EPP radius  $r_0$  and the basis size  $W$  are varied. The relative errors of the quantities are computed by

$$\varepsilon = \left| \frac{x_{\text{computed}} - x_{\text{exact}}}{x_{\text{exact}}} \right|. \quad (49)$$

Table 1: The best energies of the computed systems.

System	Energy / Ha
H 1s	-0.499999
H 2s	-0.125000
H 2p	-0.125000
He 1s <sup>2</sup>	-2.854199
He 1s2s <sup>1</sup> S	-2.153056
He 1s2s <sup>3</sup> S	-2.174211

The amount of discontinuity of a computed wavefunction at point  $r = r_0$  is measured by computing the relative error of the computed wavefunction value  $\bar{P}(0)$  compared to the hydrogenic wavefunction value  $P_{\text{hydr}}(r_0)$ . The results for the ground state of the hydrogen atom are presented in figures 1 and 2, for the 2s state in figures 3 and 4, and for the 2p state in figures 5 and 6. The results of the ground state of the helium atom are presented in figures 7 and 8. The results for He 1s2s <sup>1</sup>S are given in figures 9, 10, and 11. The results for He 1s2s <sup>3</sup>S are given in figures 12, 13, and 14. The best energies (largest basis and smallest  $r_0$ ) of the computed systems are presented in table 1.

The Hartree-Fock energy of the ground state of the helium atom is  $-2.8616800$  Ha [13]. Reference [14] gives Hartree-Fock energies  $-2.147$  Ha and  $-2.171$  Ha for the He 1s2s <sup>1</sup>S and He 1s2s <sup>3</sup>S configurations, respectively. Reference [15] gives quantities  $E(\text{He 1s2s } ^1\text{S}) - E(\text{He 1s}^2) = 0.758$  Ha and  $E(\text{He 1s2s } ^3\text{S}) - E(\text{He 1s}^2) = 0.728$  Ha.

The computations using the diagonalization of the Hamiltonian operator yielded some unphysical results. The physical admissibility of the wavefunctions  $P_{nl}(r)$  was characterized by condition

$$\lim_{r \rightarrow 0} P_{nl}(r) = 0. \quad (50)$$

We checked this condition by extrapolating solutions  $P_{nl}(r)$  polynomially at  $r = 0$ . Note that Fischer and Defranceschi [16] also get unphysical computations with wavelet computations of hydrogen-like atoms. It can be seen that the orbitals of the hydrogen atom and the 1s orbitals of He 1s2s configurations are approximately continuous at  $r_0$  whereas the 1s orbital of the helium 1s<sup>2</sup> configuration and the 2s orbitals the He 1s2s configurations are not.

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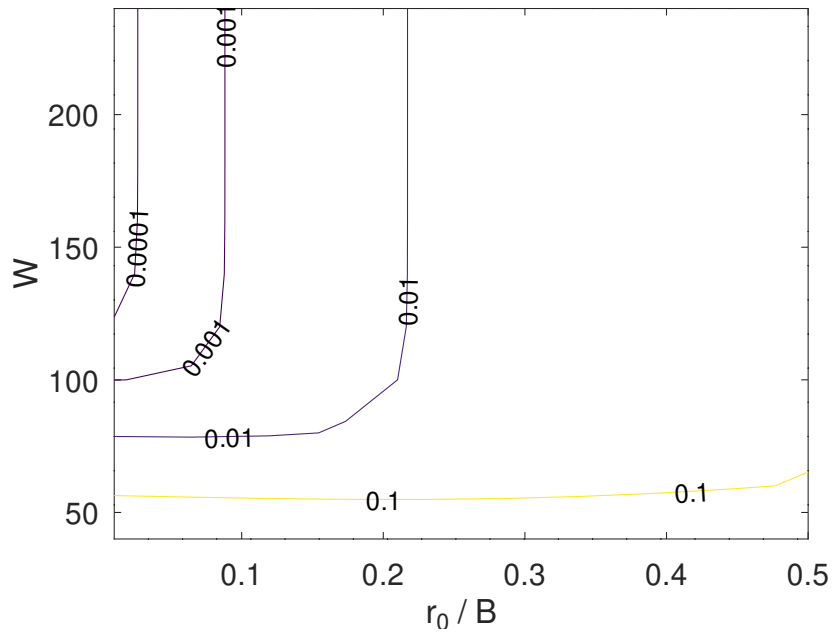


Figure 1: Hydrogen 1s orbital eigenenergy relative error.

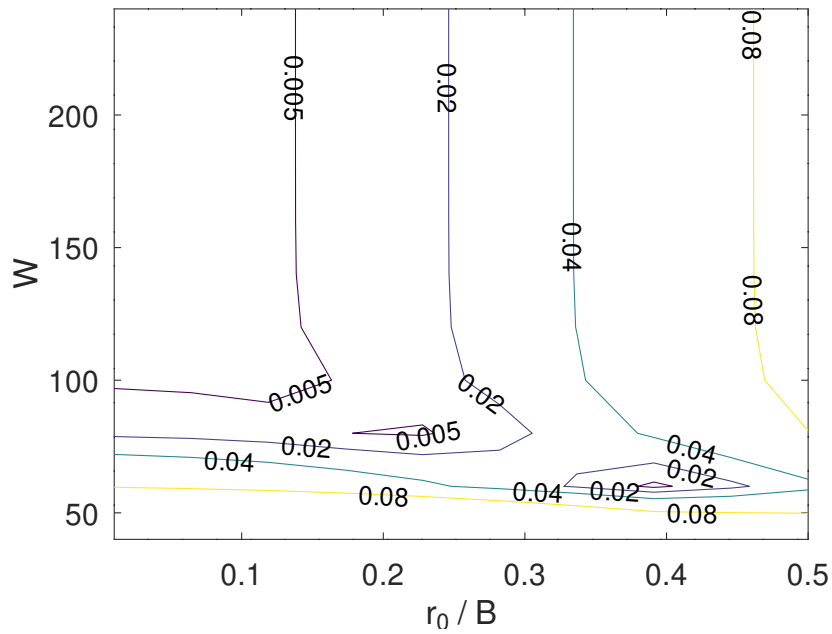


Figure 2: Relative error of the wavefunction value at the core radius for the hydrogen 1s orbital.



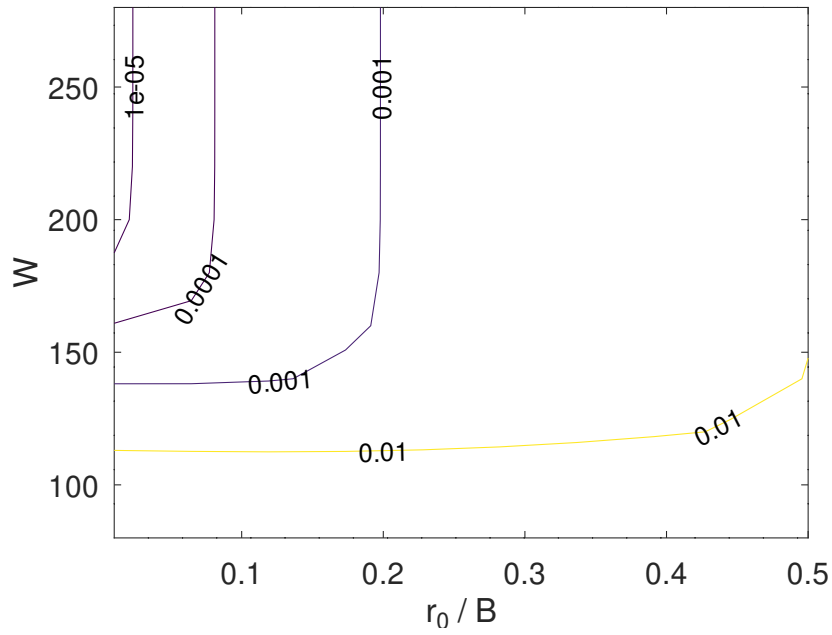


Figure 3: Hydrogen 2s orbital eigenenergy relative error.

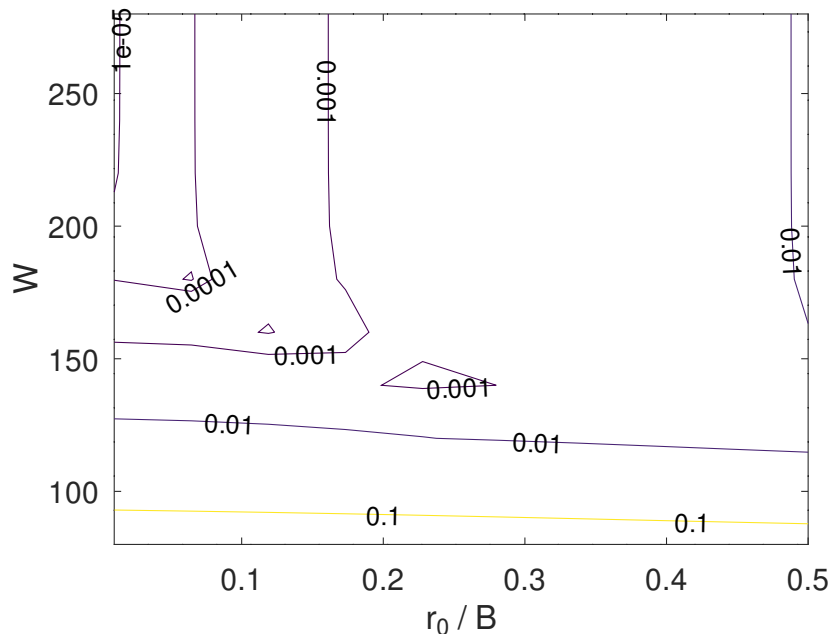


Figure 4: Relative error of the wavefunction value at the core radius for the hydrogen 2s orbital.

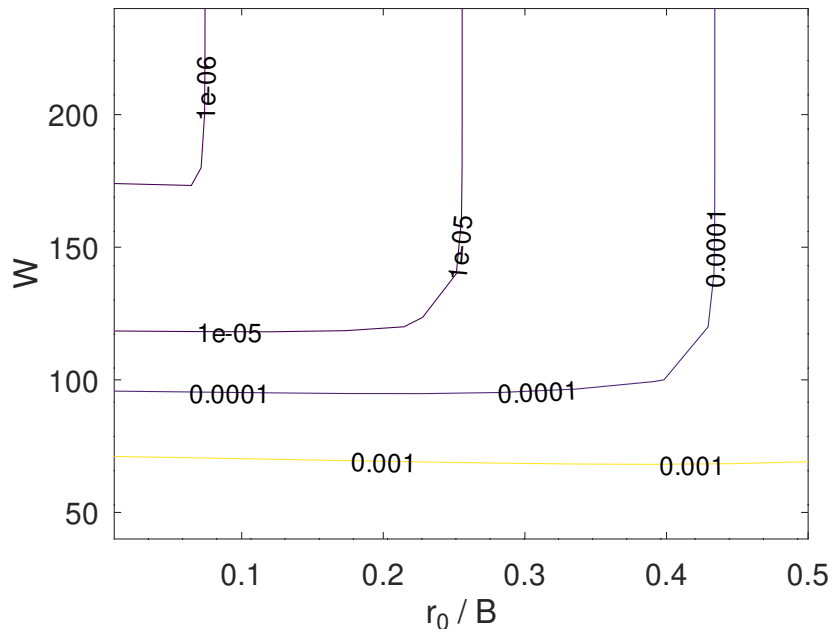


Figure 5: Hydrogen 2p orbital eigenenergy relative error.

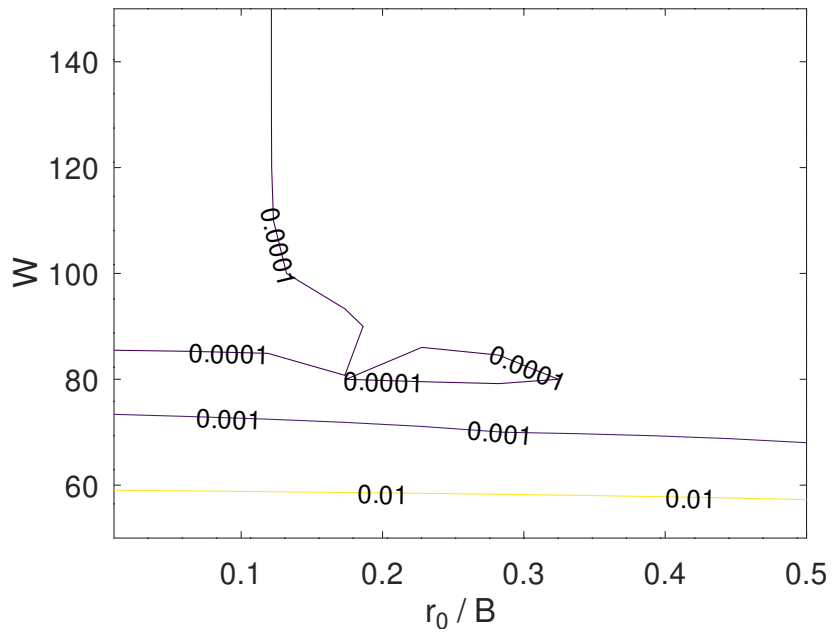


Figure 6: Relative error of the wavefunction value at the core radius for the hydrogen 2p orbital.

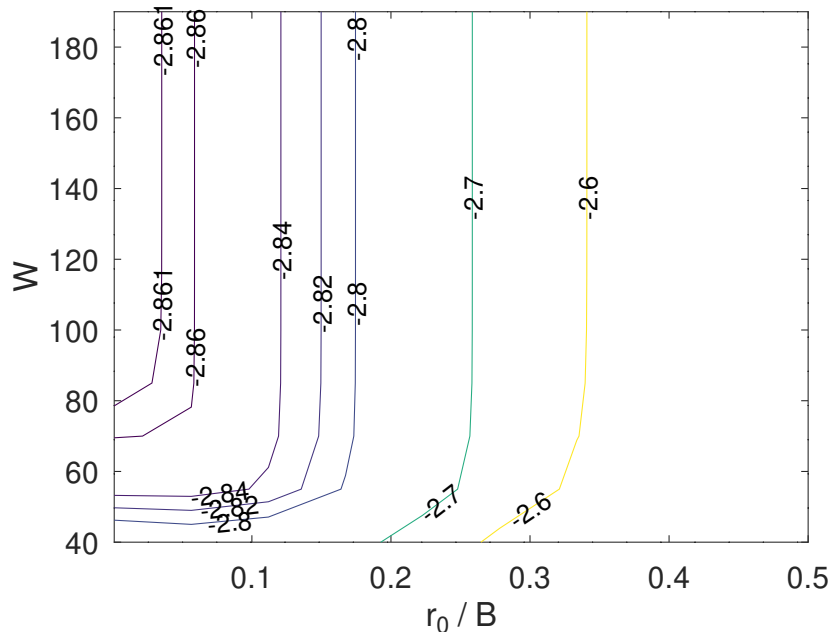


Figure 7: Energy of the ground state of the helium atom.

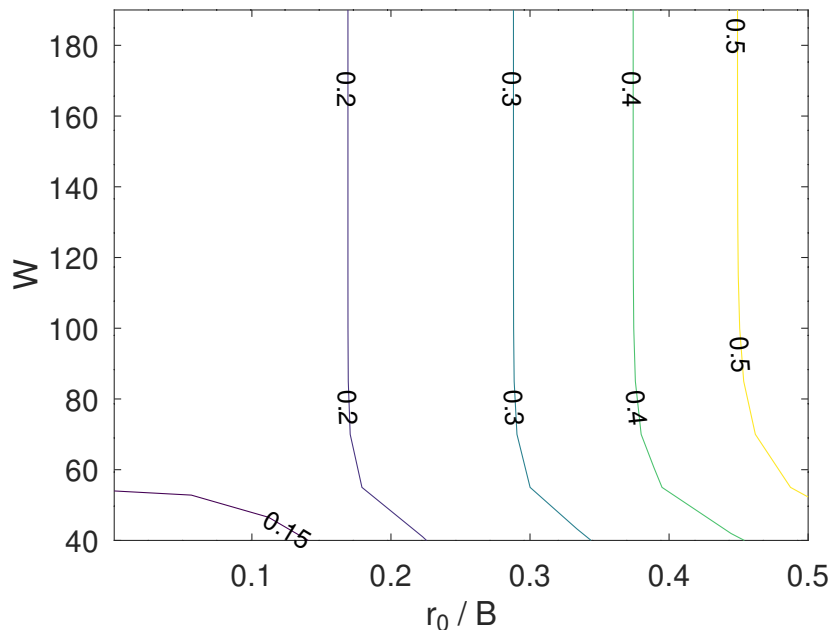


Figure 8: Relative error of the wavefunction value at the core radius for the 1s orbital of the ground state of the helium atom.

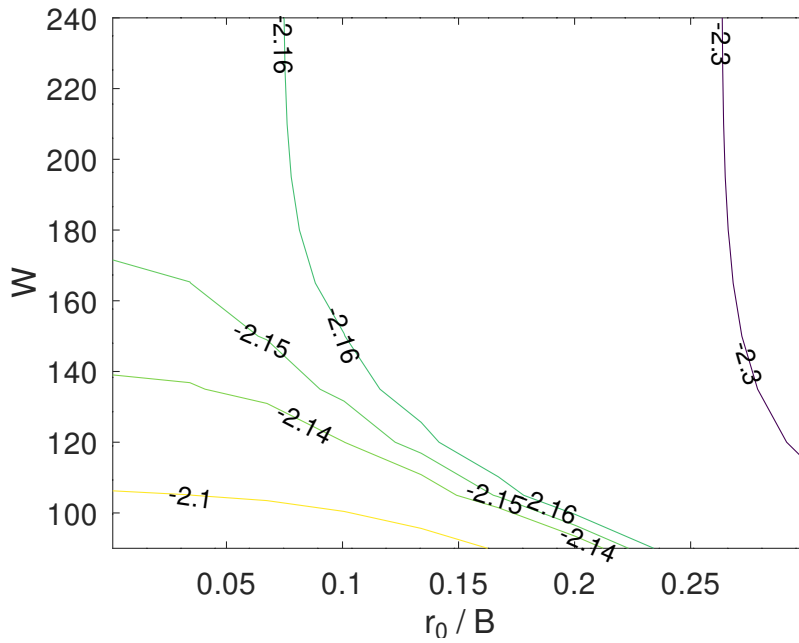


Figure 9: Helium 1s2s  $^1S$  total energy.

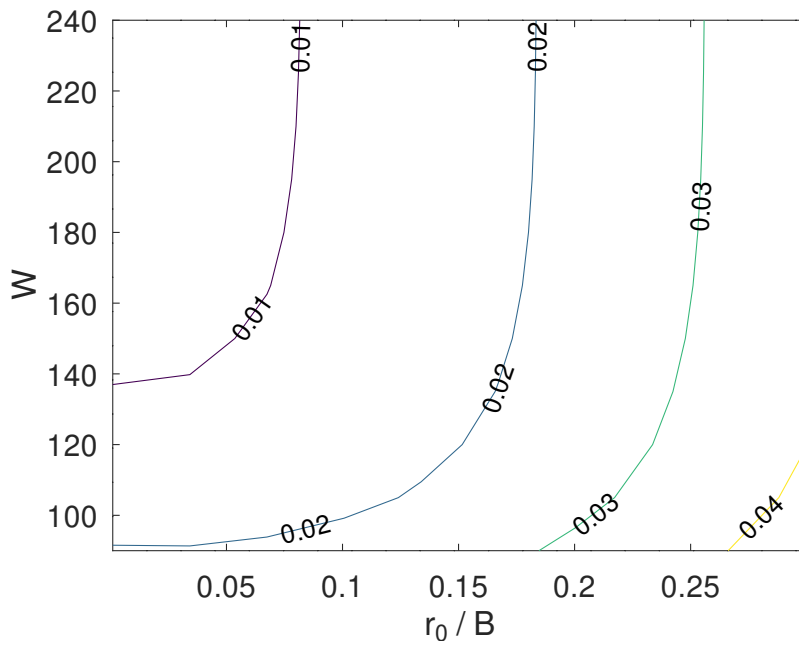


Figure 10: Relative error of the 1s wavefunction value at the core radius for the He 1s2s  $^1S$  configuration.

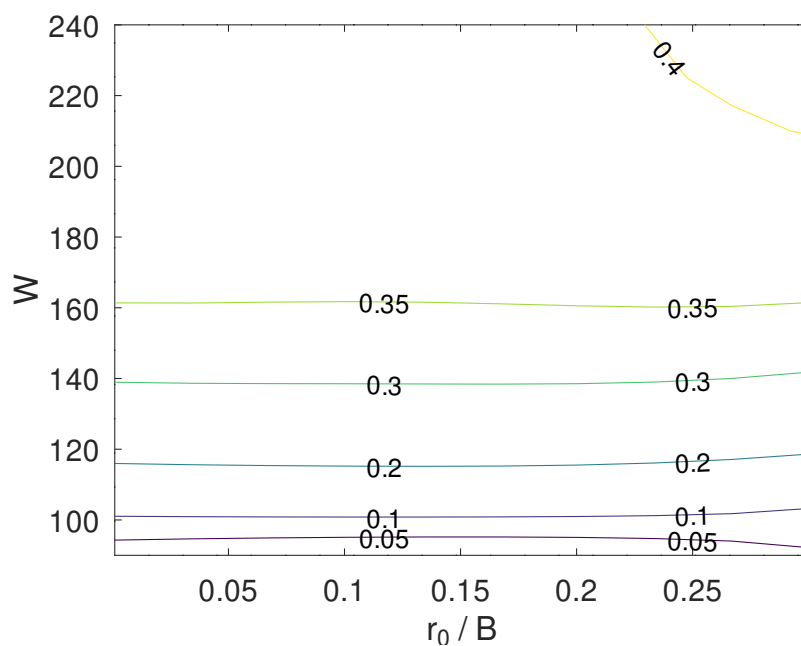


Figure 11: Relative error of the 2s wavefunction value at the core radius for the He 1s2s  $^1S$  configuration.

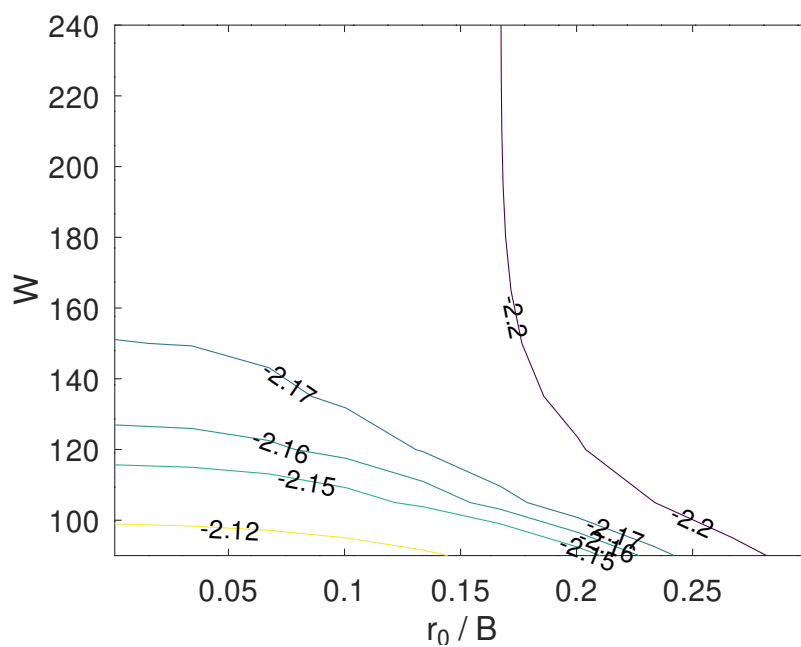


Figure 12: Helium 1s2s  $^3S$  total energy.

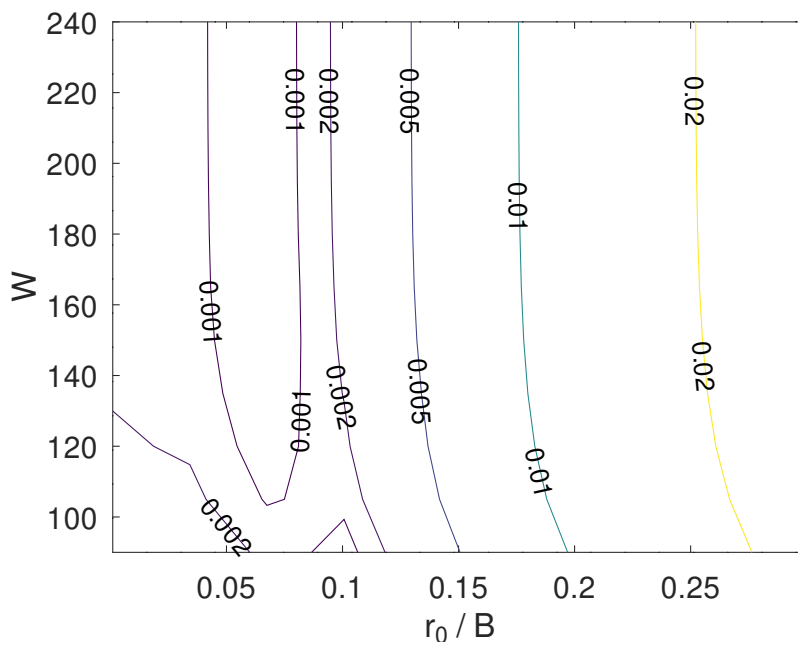


Figure 13: Relative error of the 1s wavefunction value at the core radius for the He 1s2s  $^3S$  configuration.

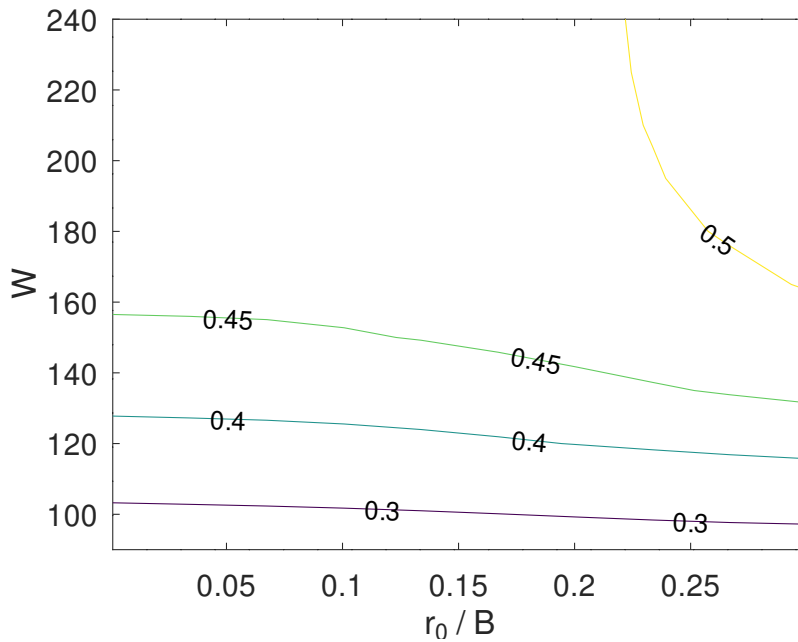


Figure 14: Relative error of the 2s wavefunction value at the core radius for the He 1s2s  $^3S$  configuration.

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