

TOMMI HÖYNÄLÄNMAA

Wavelet Approach to Electronic Structure Calculations

TOMMI HÖYNÄLÄNMAA

Wavelet Approach to Electronic Structure Calculations

ACADEMIC DISSERTATION

To be presented, with the permission of
the Faculty of Engineering and Natural Sciences
of Tampere University,
for public discussion in the old hall
of Niuvanniemi hospital, Niuvankuja 65, Kuopio,
on 5 July 2024, at 12 o'clock.

ACADEMIC DISSERTATION

Tampere University, Faculty of Engineering and Natural Sciences
Finland

*Responsible
supervisor
and Custos*

Professor Tapio Rantala
Tampere University
Finland

Supervisor

Professor Keijo Ruotsalainen
University of Oulu
Finland

Pre-examiners

Professor Hannu Häkkinen
University of Jyväskylä
Finland

Professor Tuomas Hytönen
Aalto University
Finland

Opponent

Doctor Mikael Kuisma
Technical University of Denmark
Denmark

The originality of this thesis has been checked using the Turnitin OriginalityCheck service.

Copyright ©2024 Tommi Höynälänmaa

Cover design: Roihu Inc.

ISBN 978-952-03-3512-0 (print)

ISBN 978-952-03-3513-7 (pdf)

ISSN 2489-9860 (print)

ISSN 2490-0028 (pdf)

<http://urn.fi/URN:ISBN:978-952-03-3513-7>



Carbon dioxide emissions from printing Tampere University dissertations have been compensated.

PunaMusta Oy – Yliopistopaino
Joensuu 2024

ACKNOWLEDGEMENTS

The author wants to thank Professor Tapio T. Rantala for valuable ideas, especially the exact pseudopotential method, and proofreading. Dr. Rantala also suggested the idea of this research when the author asked him for a subject of Ph.D. thesis. The author also thanks Professor Keijo Ruotsalainen for support with the first article in this thesis. Thanks to the library of Tampere University for financial support publishing the article about exact pseudopotentials.

ABSTRACT

Standard approaches to calculate properties of atoms, molecules and models of nano-structures in quantum chemistry are Hartree–Fock (HF) and density functional theory (DFT). These methods give numerical solutions of the Schrödinger equation for the wavefunctions and energies of electrons, *i.e.*, the *electronic structure*. Majority of numerical algorithms are based on finding the wavefunctions or orbitals as series expansion of basis functions, the *basis set*. In this study we consider different *wavelets* as basis functions.

Wavelets are functions constructed as translations and dilatations of the so called mother scaling function and mother wavelet. Orthonormal wavelets are orthonormal to each other and interpolating wavelets satisfy biorthogonality relations involving dual wavelets.

In order to calculate the electronic structure of atoms the radial Schrödinger and Hartree–Fock equations are solved using a Galerkin method with a Deslauriers–Dubuc wavelet basis. Several light atoms are considered as examples.

We introduce new approach called the Exact Pseudopotential (EPP), which is one method to remove the Coulomb singularity of atomic nuclei. This is tested with hydrogen and helium atom orbitals.

A three-dimensional Deslauriers–Dubuc wavelet basis is used to compute the energetics of the hydrogen and helium atoms, hydrogen molecule ion, hydrogen molecule, and lithium hydride molecule. The internuclear equilibrium distance is determined for the molecules, too.

Wavelets are applied to the path integral formulation and this method is used to calculate one- and three-dimensional harmonic oscillator and hydrogen atom in one and three dimensions.

As a conclusion, we found the Deslauriers–Dubuc wavelets a practical basis set for solving wavefunctions of electronic systems. Furthermore, Daubechies wavelets were found appropriate with the numerical path integral approach.

TIIVISTELMÄ

Standardimenetelmiä atomien, molekyylien ja nanorakenteiden laskemiseen kvanttikemiassa ovat Hartree–Fock (HF) ja tiheysfunktionaaliteoria (DFT). Nämä menetelmät antavat Schrödingerin yhtälön numeerisia ratkaisuja elektronien aaltofunktioille ja energioille, eli *elektronirakenteelle*. Useimmat numeerisista algoritmeista perustuvat aaltofunktioiden tai orbitaalien löytämiseen sarjakehitelmänä kantafunktioista, eli *kantajoukosta*. Tässä työssä tutkimme erilaisia *aallokkeita* kantafunktioina.

Aallokkeet ovat funktioita, jotka muodostetaan ns. äitiskaalausfunktion ja äitiaallokkeen translaatioina ja dilataatioina. Ortonormaalit aallokkeet ovat ortonormaalja keskenään ja interpoloivat aallokkeet toteuttavat ns. biortogonaalisuusrelaatiot, joissa käytetään duaaliaallokkeita.

Atomeille tehdään laskuja ratkaisemalla Schrödinger- ja Hartree–Fock-yhtälöt käyttäen Galerkinin menetelmää Deslauriers–Dubuc-aallokekannalla. Teoriaa sovelletaan useisiin keveisiin atomeihin.

Esittelemme uuden menetelmän nimeltä eksakti pseudopotentiaali (EPP), joka on eräs keino poistaa atomin Coulombin potentiaalin singulariteetti. Tätä testataan laskemalla vetyatomin ja heliumatomin orbitaaleja.

Vety- ja heliumatomille, vetymolekyyli-ionille, vetymolekyyllille ja litiumhydridimolekyyllille lasketaan energetiikat käyttäen kolmiulotteisista Deslauriers–Dubuc-aallokkeista koostuvaa kantaa. Molekyyleille lasketaan myös ydinten välinen tasapainoetäisyys.

Aallokkeita sovelletaan polkuintegraaliformalismiin ja tätä menetelmää käytetään yksi- ja kolmiulotteisen harmonisen oskillaattorin laskemiseen ja vetyatomin laskentaan yhdessä ja kolmessa ulottuvuudessa.

Tutkimuksen johtopäätös on, että Deslauriers–Dubucin aallokkeet ovat käytännöllinen kantafunktiojoukko elektronisysteemien aaltofunktioiden laskemiseen ja Daubechiesin aallokkeet ovat sopiva kantafunktiojoukko polkuintegraalilaskuihin.

CONTENTS

1	Introduction	1
2	Quantum Physical Calculations of Electronic Systems	3
2.1	General	3
2.2	Orbitals of Hydrogen-like Atoms.	5
2.3	Hartree–Fock Method	6
2.4	Hartree–Fock Calculations of Atoms.	8
2.5	Density Functional Theory	10
2.6	Path Integral Formulation.	11
3	Wavelets	13
3.1	General	13
3.2	Orthonormal Wavelets	13
3.3	Compactly Supported Interpolating Wavelets	14
3.3.1	Mother Scaling Function	14
3.3.2	General Definitions for Univariate MRA’s.	15
3.3.3	General Definitions for Multivariate MRA’s.	17
3.4	Compactly Supported Interpolating MRA of $C_u(\mathbb{R}^n, K)$	18
3.5	Compactly Supported Interpolating MRA of $C_0(\mathbb{R}^n, K)$	21
3.6	Polynomial Span and Regularity	24
3.7	Deslauriers–Dubuc Wavelets on a Half-Infinite Interval	24
4	Calculations of Radial Wavefunctions of Atoms Using Deslauriers–Dubuc Wavelets	27
4.1	General	27
4.2	Construction of the Basis Function Set	27
4.3	Forward and Backward Wavelet Transforms	28
4.4	Standard Operator Form and Nonstandard Operator Form	29

4.5	Evaluation of Matrix Elements	32
4.6	Solving the Hartree–Fock Equations	33
4.7	Results	35
5	Exact Pseudopotential	37
5.1	General	37
5.2	Hydrogen-like Atoms	37
5.3	Hartree–Fock Equations for Helium Atom	38
5.4	EPP of Helium Atom	39
5.5	Total Energy of Helium Atom	42
5.6	Combination of EPP with Finite Difference Method	42
5.7	Results	44
6	Calculations of Atoms and Molecules using Three-dimensional Deslaurliers– Dubuc Wavelets	47
6.1	Interpolating Wavelet Basis Set	47
6.2	Interpolating Wavelet Transforms.	49
6.3	Constant and Interpolated Pseudopotentials	51
6.4	HGH Pseudopotential	52
6.5	Atomic and Molecular Orbitals	53
7	Fourier Transform and Wavelet Approaches to the Path Integral Formu- lation	61
7.1	Stationary State Energies and Wavefunctions	61
7.2	Quantum Harmonic Oscillator and Hydrogen-like Atom	63
7.3	Wavelet Bases	65
7.3.1	Interpolating Wavelets	65
7.3.2	Orthonormal Wavelets	66
7.4	Application to the Harmonic Oscillator and Hydrogen Atom.	67
8	Conclusions	71
	References	73
	Publication I	79
	Publication II	95

Publication III	133
Publication IV	151
Publication V	165

List of Figures

3.1	The 8th order Deslauriers–Dubuc fundamental function	15
6.1	Pseudopotentials V_{interp} with $D = 7$. Parameter c is the cutoff value, see section 6.3.	52
6.2	Energy of H_2 as a function of internuclear distance calculated with Hartree–Fock method and HGH pseudopotential. The solid line is our computation with interpolating wavelets and grid spacing $g = 0.25$ B and the dashed line is computed with BigDFT and (fine) grid spacing $g = 0.225$ B.	58
6.3	Total energy of the lithium hydride molecule as a function of the internuclear distance calculated with the Hartree–Fock method and HGH pseudopotential. The solid line has been computed with interpolating wavelets and grid spacing $g = 0.25$ B and the dashed line with BigDFT and (fine) grid spacing $g = 0.225$ B.	59
7.1	Probability density function $ \psi(x) ^2$ of the one-dimensional harmonic oscillator computed with the exact kernel.	67
7.2	Radial probability density function $ P_{1s}(r) ^2$ of the hydrogen atom computed with the midpoint kernel in one dimension.	68
7.3	Energy spectrum of the three-dimensional harmonic oscillator calculated with the midpoint kernel.	69

List of Tables

4.1	Results from Hartree–Fock calculations for helium, beryllium, neon, magnesium, and argon. Deviation from the accurate value [23] is given in parentheses so that negative deviation means that the computed value is less than the accurate value.	36
4.2	Results from Hartree–Fock calculations for lithium and sodium. Deviation from the accurate value [23] is given in parentheses so that negative deviation means that the computed value is less than the accurate value.	36
5.1	Hartree–Fock total energies of H and He occupation configurations. E_{ref} are chosen reference values. E_{EPP} is the energy given by the EPP–Galerkin-method, h_{EPP} is the grid spacing in the EPP–Galerkin method, E_{OIW} is the energy given by the OIW–Galerkin method, and E_{FDM} is the energy given by the Finite Difference Method. For EPP, the most accurate results are given. For OIW approach, the number of basis functions is 201 and the finest grid spacing is 0.00625 a.u.. The number of FDM computation points is 2001 for the second and third systems and 1001 for the other ones.	45
6.1	Total energy of the hydrogen atom. Quantity g is the distance between grid points in the highest resolution level. “TH” means this work. . . .	55
6.2	Hydrogen atom orbital energies with the HGH pseudopotential. We labelled the resulting 2p orbitals with a, b, and c. All the orbitals presented are approximately orthogonal.. . . .	55
6.3	Energetics of the helium atom. All our and BigDFT computations use HGH pseudopotential. “TH” means this work.. . . .	56
6.4	Hydrogen molecule. “TH” means this work.	57
6.5	Hydrogen molecule ion. The analytical results are equal to the experimental results. “TH” means this work.	58
6.6	Lithium hydride molecule. All our and BigDFT computations were done with the HGH pseudopotential. The CCCBDB all-electron total energies are not presented in the table. “TH” means this work.	59

ABBREVIATIONS

$L^2(\mathbb{R}^n)$	space of complex-valued square-integrable functions on $\mathbb{R}^n$
$C_{\text{com}}(\mathbb{R}^n, K)$	space of continuous and compactly supported functions from $\mathbb{R}^n$ into K
$C_{\text{u}}(\mathbb{R}^n, K)$	space of uniformly continuous and bounded functions from $\mathbb{R}^n$ into K
$C_0(\mathbb{R}^n, K)$	space of continuous functions from $\mathbb{R}^n$ into K vanishing at the infinity
<i>e.g.</i>	for example, from Latin <i>exempli gratia</i>
<i>et al.</i>	and others, from Latin <i>et alii</i>
<i>i.e.</i>	that is, from Latin <i>id est</i>
DFT	Density Functional Theory
HF	Hartree–Fock
MRA	Multi-Resolution Analysis
OIW	Ordinary Interpolating Wavelet

ORIGINAL PUBLICATIONS

- Publication I Tommi Höynälänmaa, Tapio T. Rantala, and Keijo Ruotsalainen. “Solution of atomic orbitals in an interpolating wavelet basis”. In: *Physical Review E* 70 (2004), p. 066701. DOI: 10.1103/PhysRevE.70.066701.
- Publication II Tommi Höynälänmaa. “Multiresolution Analysis for Compactly Supported Interpolating Tensor Product Wavelets”. In: *International Journal of Wavelets, Multiresolution and Information Processing* 13.2 (2015), p. 1550010. DOI: 10.1142/S0219691315500101.
- Publication III Tommi Höynälänmaa and Tapio T. Rantala. “Electronic Structure Calculations with the Exact Pseudopotential and Interpolating Wavelet Basis”. In: *Atoms* 11 (2023). DOI: <https://doi.org/10.3390/atoms11010009>.
- Publication IV Tommi Höynälänmaa and Tapio T. Rantala. “Electronic structure calculations with interpolating tensor product wavelet basis”. In: *Physical Review E* 108 (2023), p. 025307. DOI: <https://doi.org/10.1103/PhysRevE.108.025307>.
- Publication V Tommi Höynälänmaa. “Fourier transform and wavelet approaches to the path integral formulation”. In: *Communications in Computational Physics* (2024), submitted.

These articles are publications [1, 2, 3, 4, 5] in the References.

Author's contribution

- Publication I The author developed the algorithm to convert NSOF form of an operator to SOF and the operator formulation of the atomic Hartree–Fock method in an interpolating wavelet basis. The author also wrote the program code performing the numerical computations and ran it for several atoms.
- Publication II The author developed multivariate multiresolution analyses for function spaces $C_u(\mathbb{R}^n, K)$ and $C_0(\mathbb{R}^n, K)$ where $K = \mathbb{C}$ or $K = \mathbb{R}$. The author also defined multivariate dual interpolating MRA and generalized the Besov space norm equivalence result by Donoho to multiple dimensions.
- Publication III The author applied the exact pseudopotential method to a wavelet basis on the half-infinite real axis. The author applied the idea of Dr. Tapio T. Rantala to Schrödinger equation of the hydrogen atom and HF equations of helium ground state and excited states $\text{He } 1s2s \ ^1S$ and $1s2s \ ^3S$. The author combined the EPP method with the Finite Difference Method. The author also wrote the program code to make the numerical computations and ran it for the hydrogen and helium atoms.
- Publication IV The author developed the formulation for calculations of atoms and molecules using HF and DFT methods with three-dimensional Deslauriers–Dubuc wavelet basis. The author also developed the interpolated pseudopotential. The author wrote the program code to perform the numerical calculations and ran it for several atoms and molecules.
- Publication V The author developed an own approximation to the path integral kernel and a method to compute wavefunctions using the path integral formulation. The author wrote and ran programs to compute one- and three-dimensional harmonic oscillator and hydrogen atom using the path integral formulation and wavelets.

1 INTRODUCTION

The purpose of this study is to combine wavelets with the existing calculation methods of quantum physics. Interpolating wavelet family called Deslauriers–Dubuc wavelets is used in most of the calculations but Daubechies orthonormal wavelets are used in some path integral calculations and as reference results from the BigDFT computer program.

Research questions are “are the Deslauriers–Dubuc wavelets a good basis set for the calculations of atoms and two-atom molecules using a Galerkin method?” and “are the Deslauriers–Dubuc and Daubechies wavelets good basis sets for the calculations of the harmonic oscillator and hydrogen atom using the path integral formulation?”.

Research objectives are:

- Calculation of the wavefunctions and energies of the hydrogen atom ground state and excited states with Deslauriers–Dubuc wavelets.
- Representation of Hartree–Fock method for atoms in a Deslauriers–Dubuc wavelet basis set and use it to compute the atom energies and orbital energies of some atoms.
- Development of mathematical formulation for multivariate Deslauriers–Dubuc wavelets and check that it satisfies proper convergence properties.
- Calculation of hydrogen and helium atoms and some two-atom molecules in three dimensions using Hartree–Fock and DFT methods and three-dimensional Deslauriers–Dubuc wavelets.
- Combination of the Exact Pseudopotential method with Deslauriers–Dubuc wavelets and Finite Differences Method.
- Calculation of energies and wavefunctions of the harmonic oscillator and hydrogen atom using the path integral formulation and wavelets.

2 QUANTUM PHYSICAL CALCULATIONS OF ELECTRONIC SYSTEMS

2.1 General

Detailed electronic structure theory is introduced in references [6, 7, 8, 9]. Quantum physics explains the behaviour of very small systems. General theory of relativity explains the dynamics of very large systems. Both of these theories yield Newtonian mechanics as a special case for medium sized systems. Quantum physics was developed at the beginning of the 20th century as some physical phenomena could not be explained by classical physics. These included

- black-body radiation
- photoelectric effect
- structure of the atomic spectra

One key feature of quantum physics is that many physical observables are *quantized*, *i.e.* they can only have discrete values. The most fundamental property of quantum physics is that observables are *statistical*. This means that we can only compute probabilities to find a system in a given state. However, the laws of the nature are statistically causal even though they are not deterministically causal: although we cannot determine the value of an observable exactly we are able to calculate exact probabilities of its possible values. Quantum physics contains also *wave-particle duality*. It means that matter particles have wave properties and electromagnetic waves have particle properties, *i.e.* they consist of photons. In electron double slit experiment a beam of electrons generates an interference pattern when it is directed through a double slit. On the other hand, in photoelectric effect electromagnetic radiation behaves like a beam of particles.

The state of a quantum physical system is specified by its wavefunction $\Phi(\mathbf{r}, t)$, which is a complex valued function of the coordinate(s) $\mathbf{r}$ of the particles and time t .

Here $\mathbf{r} = (\mathbf{r}_1, \dots, \mathbf{r}_N)$. The probability to find particles in the volume $V = V_1 \times \dots \times V_N$, where $V_k = [x_k, x_k + \Delta x_k] \times [y_k, y_k + \Delta y_k] \times [z_k, z_k + \Delta z_k]$ and N is the number of coordinates, is [9]

$$P = \int_V |\Phi(\mathbf{r}, t)|^2 d^{3N} \mathbf{r}. \quad (2.1)$$

The wavefunction is determined by the time dependent Schrödinger equation

$$\hat{H}\Phi(\mathbf{r}, t) = i\hbar \frac{\partial \Phi}{\partial t}, \quad (2.2)$$

where $\hat{H}$ is the Hamiltonian operator of the system [10]. In case the potential is independent of time the eigenstates ϕ are defined by the time independent Schrödinger equation

$$\hat{H}\phi = E\phi \quad (2.3)$$

and the wavefunction

$$\Phi(\mathbf{r}, t) = \sum_{n \in \mathbb{N}} A_n \exp(-iE_n t / \hbar) \phi_n(\mathbf{r}) \quad (2.4)$$

where A_n are complex numbers, ϕ_n are the eigenfunctions yielded by equation (2.3), and E_n the corresponding eigenvalues (energies) [10].

We use atomic units in the rest of this thesis, which means that some natural constants are set to 1 so that quantum physical formulas take a simpler form. To be more precise, we have $e = m_e = \hbar = 4\pi\epsilon_0 = 1$, where e is the elementary charge, m_e the mass of the electron, $\hbar$ the reduced Planck constant, and ϵ_0 the permittivity of free space.

The Hamiltonian operator of a system consisting of N nuclei and M electrons is

$$\begin{aligned} \hat{H}(\mathbf{R}_1, \dots, \mathbf{R}_N; \mathbf{r}_1, \dots, \mathbf{r}_M) = & - \sum_{n=1}^N \frac{\nabla_n^2}{2M_n} + \frac{1}{2} \sum_{n,n'=1; n \neq n'}^N \frac{Z_n Z_{n'}}{|\mathbf{R}_n - \mathbf{R}_{n'}|} - \sum_{i=1}^M \frac{\nabla_i^2}{2} \\ & - \sum_{n=1}^N \sum_{i=1}^M \frac{Z_n}{|\mathbf{R}_n - \mathbf{r}_i|} + \frac{1}{2} \sum_{i,j=1; i \neq j}^M \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \end{aligned} \quad (2.5)$$

where $\mathbf{R}_n$ are the coordinates of the n th nucleus, $\mathbf{r}_i$ are the coordinates of the i th electron, ∇_n involves differentiation with the coordinates of the n th nucleus, ∇_i with the i th electron, Z_n is the atomic number of the n th nucleus, and M_n is the mass

of the n th nucleus in atomic units [9]. Solutions to Eq. (2.2) are the many-body wavefunctions $\Psi(\mathbf{R}_1, \dots, \mathbf{R}_N; \mathbf{r}_1, \dots, \mathbf{r}_M)$.

Due to the large relative mass of nuclei compared to electrons, the coordinates of the nuclei can be fixed. This is called the *Born–Oppenheimer approximation* and it allows us to separate the nuclear coordinates from the electronic coordinates. When we apply this approximation the Hamiltonian of the electrons is given by [9]

$$\hat{H}(\mathbf{r}_1, \dots, \mathbf{r}_M) = - \sum_{i=1}^M \frac{\nabla_i^2}{2} - \sum_{n=1}^N \sum_{i=1}^M \frac{Z_n}{|\mathbf{R}_n - \mathbf{r}_i|} + \frac{1}{2} \sum_{i,j=1; i \neq j}^M \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}. \quad (2.6)$$

2.2 Orbitals of Hydrogen-like Atoms

Due to spherical symmetry of atoms the three dimensional one-electron Schrödinger equation $\hat{H}\phi = \varepsilon\phi$ of the hydrogen-like atoms is separated to the one dimensional radial part and the two dimensional angular part. Exact solutions to the latter are spherical harmonics $Y_{\ell m_\ell}$ where ℓ and m_ℓ are the orbital quantum number (angular momentum quantum number) and orbital magnetic quantum number, respectively. Writing $R_{n\ell}$ for the radial wavefunction the hydrogen-like orbitals are $\psi_{n\ell m_\ell}(r, \theta, \varphi) = R_{n\ell}(r) Y_{\ell m_\ell}(\theta, \varphi)$, where n is the principal quantum number. The radial Schrödinger equation for a hydrogen-like atom is [6]

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} - \frac{Z}{r} + \frac{\ell(\ell+1)}{2r^2} \right] P_{n\ell}(r) = \varepsilon_{n\ell} P_{n\ell}(r), \quad (2.7)$$

where Z is the atomic number, $\varepsilon_{n\ell}$ are the orbital energies, and $P_{n\ell}(r) = rR_{n\ell}(r)$ are the radial wavefunctions multiplied by r . Functions $P_{n\ell}(r)$ are called one-electron wavefunctions or orbitals. We also define the kinetic energy operator

$$\hat{T} = -\frac{1}{2} \frac{d^2}{dr^2}, \quad (2.8)$$

the potential energy operator

$$\hat{V} = -\frac{Z}{r}, \quad (2.9)$$

and the centrifugal potential operator

$$\hat{C}_\ell = \frac{\ell(\ell+1)}{2r^2}, \quad (2.10)$$

where $\ell \in \mathbb{Z}_+$ is the angular momentum quantum number.

2.3 Hartree–Fock Method

Detailed introduction to the Hartree–Fock method can be found in reference [9]. Electrons have the *spin coordinate* in addition to the positional coordinates. The spin of an electron can take two values: $1/2$ (spin up) or $-1/2$ (spin down). We define the coordinates $\mathbf{x}_i = (\mathbf{r}_i, s_i)^T$, where $\mathbf{r}_i$ is the position of the i th electron and s_i its spin. We also define the spin vector

$$\sigma(s) := \begin{cases} \begin{pmatrix} 1 \\ 0 \end{pmatrix}; & s = 1/2 \\ \begin{pmatrix} 0 \\ 1 \end{pmatrix}; & s = -1/2 \end{cases} \quad (2.11)$$

We define $s_i = 1/2$ for odd i and $s_i = -1/2$ for even i and $\chi_i(\mathbf{x}_i) = \phi_i(\mathbf{r}_i)\sigma(s_i)$. Now we define the *Slater determinant* by

$$\Phi(\mathbf{x}_1, \dots, \mathbf{x}_M) = (M)^{-1/2} \begin{vmatrix} \chi_1(\mathbf{x}_1) & \cdots & \chi_1(\mathbf{x}_M) \\ \vdots & \ddots & \vdots \\ \chi_M(\mathbf{x}_1) & \cdots & \chi_M(\mathbf{x}_M) \end{vmatrix} \quad (2.12)$$

This wavefunction has two following important properties:

- If two electrons occupy the same orbital the value of the determinant is zero, *i.e.* the probability to find two electrons in the same orbit is zero so that the *Pauli exclusion principle* is fulfilled.
- When two orbital coordinates are interchanged the determinant changes its sign. Thus one of the basic postulates of quantum physics for the fermions is fulfilled. Consequently the probability to find two electrons in the same position is zero.

The Hartree–Fock equations are derived by minimizing the energy $\langle \Phi | \hat{H} | \Phi \rangle$ of

the Slater determinant Φ by varying the orbitals. The equations are

$$\hat{F}\chi_i = \varepsilon_i \chi_i, \quad (2.13)$$

where the *Fock operator* is

$$\hat{F} = \hat{h} + \sum_{j=1}^M (\hat{J}_j - \hat{K}_j), \quad (2.14)$$

the *Coulomb operator*

$$(\hat{J}_j \chi_i)(\mathbf{x}) := \left(\int \chi_j^*(\mathbf{x}') \frac{1}{|\mathbf{r} - \mathbf{r}'|} \chi_j(\mathbf{x}') d\mathbf{x}' \right) \chi_i(\mathbf{x}), \quad (2.15)$$

and the *exchange operator*

$$(\hat{K}_j \chi_i)(\mathbf{x}) := \left(\int \chi_j^*(\mathbf{x}') \frac{1}{|\mathbf{r} - \mathbf{r}'|} \chi_i(\mathbf{x}') d\mathbf{x}' \right) \chi_j(\mathbf{x}). \quad (2.16)$$

The Hartree–Fock energy of the system is

$$E_{\text{HF}} = \sum_{i=1}^M \varepsilon_i - \frac{1}{2} \sum_{i=1}^M \sum_{j=1}^M \int \chi_i^*(\mathbf{r}) (\hat{J}_j - \hat{K}_j) \chi_i(\mathbf{r}) d\mathbf{r}. \quad (2.17)$$

The Hartree–Fock energy can also be computed by

$$E_{\text{HF}} = \sum_{i=1}^M \langle i | \hat{h} | i \rangle + \frac{1}{2} \sum_{i,j=1}^M ([ii|jj] - [ij|ji]), \quad (2.18)$$

where the one-electron integral is

$$\langle i | \hat{h} | j \rangle = \int \chi_i^*(\mathbf{x}) \hat{h}(\mathbf{r}) \chi_j(\mathbf{x}) d\mathbf{x}, \quad (2.19)$$

the nuclear potential

$$V_{\text{nucl}}(\mathbf{r}) = - \sum_{n=1}^N \frac{Z_n}{|\mathbf{R}_n - \mathbf{r}|}, \quad (2.20)$$

the one-electron Hamiltonian

$$\hat{h}(\mathbf{r}) = -\frac{1}{2}\nabla^2 + V_{\text{nucl}}, \quad (2.21)$$

and the two-electron integral

$$[ij|kl] = \int \chi_i^*(\mathbf{x}_1)\chi_j(\mathbf{x}_1) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \chi_k^*(\mathbf{x}_2)\chi_l(\mathbf{x}_2) d\mathbf{x}_1 d\mathbf{x}_2. \quad (2.22)$$

The *restricted Hartree–Fock method* (RHF) uses a single orbital twice with spin $s = \pm 1/2$, *i.e.* $\phi_{2i-1} = \phi_{2i}$, $s_{2i-1} = 1/2$, and $s_{2i} = -1/2$ for all $i = 1, \dots, M/2$. If we do not apply this condition we have the *unrestricted Hartree–Fock method* (UHF). We use RHF in this study.

2.4 Hartree–Fock Calculations of Atoms

The Schrödinger equation $\hat{H}\Phi = E\Phi$ of a many-electron atom leads to Hartree–Fock equations in the *central field approximation* and with Slater determinant wavefunctions [6, 7, 8]. Central field approximation means that we assume the potential seen by each electron due to the nuclei and other electrons is averaged to be rotationally symmetric. Consequently, the angular parts of the orbitals are similar to the ones in hydrogen-like atoms. Slater integrals between the two radial wavefunctions $P_{n_i\ell_i}$ and $P_{n_j\ell_j}$ are defined as

$$Y_{ij}^\kappa(r) = \int_0^\infty P_i(r')\gamma^\kappa(r, r')P_j(r')dr', \quad (2.23)$$

where

$$\gamma^\kappa(r, r') = \frac{r_{<}^\kappa}{r_{>}^{\kappa+1}}, \quad (2.24)$$

$$r_{<} = \min\{r, r'\}, \quad (2.25)$$

$$r_{>} = \max\{r, r'\}. \quad (2.26)$$

The HF equation of the orbital P_i with the principal quantum number n_i and

orbital quantum number ℓ_i is [6, 7, 8]

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} - \frac{Z}{r} + \frac{\ell_i(\ell_i + 1)}{2r^2} + D_i(r) \right] P_i(r) = \varepsilon_i P_i(r) + \sum_{j(\neq i)=1}^Q w_j \delta_{\ell_i \ell_j} \varepsilon_{ij} P_j(r) + E_i(r) \quad (2.27)$$

where

$$D_i(r) = \sum_{j=1}^Q (w_j - \delta_{ij}) Y_{jj}^0(r) - (w_i - 1) A_i(r), \quad (2.28)$$

$$E_i(r) = \sum_{j(\neq i)=1}^Q w_j B_{ij}(r) P_i(r), \quad (2.29)$$

and

$$A_i(r) = \frac{2\ell_i + 1}{4\ell_i + 1} \sum_{\kappa > 0} \begin{pmatrix} \ell_i & \kappa & \ell_i \\ 0 & 0 & 0 \end{pmatrix}^2 Y_{ii}^\kappa(r), \quad (2.30)$$

$$B_{ij}(r) = \frac{1}{2} \sum_{\kappa} \begin{pmatrix} \ell_i & \kappa & \ell_j \\ 0 & 0 & 0 \end{pmatrix}^2 Y_{ji}^\kappa(r), \quad (2.31)$$

$$Z = \text{atomic number}, \quad (2.32)$$

$$Q = \text{number of orbitals}, \quad (2.33)$$

$$w_i = \text{number of electrons in orbital } i, \quad (2.34)$$

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \text{Wigner 3-j symbol}. \quad (2.35)$$

Wavefunctions $P_i(r)$ are normalized with the condition

$$\int_0^\infty (P_i(r))^2 dr = 1. \quad (2.36)$$

The nondiagonal Lagrange multipliers ε_{ij} , $i \neq j$, that ensure orthogonality of the orbitals may be neglected for closed-shell atoms. We neglect the nondiagonal Lagrange multipliers for open-shell atoms, too, and the exact orthogonality of atomic orbitals is not preserved for them.

2.5 Density Functional Theory

The Density Functional Theory has been discussed in references [9, 11, 12]. We assume that the wavefunction is represented as the Slater determinant here, too. Then the charge density is

$$\rho(\mathbf{r}) = \sum_{i=1}^M |\phi_i(\mathbf{r})|^2. \quad (2.37)$$

The Hartree potential is given by

$$V_H(\mathbf{r}) = \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}'. \quad (2.38)$$

The Kohn–Sham energy functional of an electronic system is

$$\begin{aligned} E[\rho] = & -\frac{1}{2} \sum_{i=1}^M \int \phi_i^*(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}) d\mathbf{r} + \int \rho(\mathbf{r}) V_{\text{nucl}}(\mathbf{r}) d\mathbf{r} \\ & + \frac{1}{2} \int \int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}' + E_{\text{xc}}[\rho(\mathbf{r})] \end{aligned} \quad (2.39)$$

The Kohn–Sham equations are obtained by minimizing the functional (2.39) by varying the orbitals and they are

$$\left(-\frac{1}{2} \nabla^2 + V_{\text{nucl}}(\mathbf{r}) + V_H(\mathbf{r}) + V_{\text{xc}}[\rho] \right) \phi_i(\mathbf{r}) = E_i \phi_i(\mathbf{r}) \quad (2.40)$$

where $V_{\text{xc}}[\rho]$ is the *exchange-correlation potential*. We have

$$V_{\text{xc}}[\rho] = V_{\text{x}}[\rho] + V_{\text{c}}[\rho], \quad (2.41)$$

where $V_{\text{x}}[\rho]$ is the *exchange potential* and $V_{\text{c}}[\rho]$ is the *correlation potential*. In this thesis we ignore the correlation potential. The exchange-correlation energy is defined by

$$E_{\text{xc}}[\rho] = E_{\text{x}}[\rho] + E_{\text{c}}[\rho] \quad (2.42)$$

where $E_{\text{x}}[\rho]$ is the *exchange energy* and $E_{\text{c}}[\rho]$ is the *correlation energy*. In this thesis we ignore the correlation energy.

Within the Local Density Approximation (LDA) we define

$$E_x[\rho] = \int \rho(\mathbf{r}) \varepsilon_x[\rho](\mathbf{r}) d^3\mathbf{r} \quad (2.43)$$

where $\varepsilon_x[\rho](\mathbf{r})$ is the exchange energy per particle of a uniform electron gas at a density of ρ . It follows from the Kohn–Sham theorem [9, section 3.1] that the exchange potential is

$$V_x[\rho] = \frac{\delta E_x[\rho]}{\delta \rho}. \quad (2.44)$$

We have

$$E_x[\rho] = -\frac{3}{4} \left(\frac{3}{\pi} \right)^{1/3} \int (\rho(\mathbf{r}))^{4/3} d^3\mathbf{r} \quad (2.45)$$

and

$$V_x[\rho](\mathbf{r}) = - \left(\frac{3}{\pi} \rho(\mathbf{r}) \right)^{1/3}. \quad (2.46)$$

The total energy of the system is

$$E_{\text{KS}} = \sum_{i=1}^n E_i - \frac{1}{2} \int \rho(\mathbf{r}) V_{\text{H}}(\mathbf{r}) d^3\mathbf{r} + E_{\text{xc}}[\rho] - \int \rho(\mathbf{r}) V_{\text{xc}}[\rho](\mathbf{r}) d^3\mathbf{r}. \quad (2.47)$$

The Kohn–Sham equations are solved by a similar self-consistent iteration as the HF equations.

2.6 Path Integral Formulation

The time-evolution operator defines the evolution of quantum mechanical system [10]:

$$\Psi(\mathbf{x}, t_b) = \hat{U}(t_b, t_a) \Psi(\mathbf{x}, t_a) \quad (2.48)$$

where t_a is the initial time and t_b is the final time. For a stationary system it is given by

$$\hat{U}(t_b, t_a) = \exp(-i(t_b - t_a)\hat{H}) \quad (2.49)$$

where $\hat{H}$ is the Hamiltonian operator of the system. The time evolution of an eigenstate of a stationary system is given by

$$\Psi_a(\mathbf{x}, t) = \exp(-iE_a t) \psi_a(\mathbf{x}) \quad (2.50)$$

where ψ_a is an eigenstate of the time-independent Hamiltonian and E_a is its energy.

The time-evolution operator can be represented as [10]

$$\hat{U}(t_b, t_a)\Psi_a = \int_{\mathbb{R}^d} K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a)\Psi_a(\mathbf{x}_a, t_a)d\mathbf{x}_a \quad (2.51)$$

where d is the dimensionality of the system (1, 2, or 3) and function K is called the kernel, and also propagator or Green's function. In path integral formulation the kernel is given by

$$K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \lim_{N \rightarrow \infty} \sqrt{\frac{m}{2\pi i \varepsilon}}^{Nd} \int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d} \exp(iS_N) d\mathbf{x}_1 \cdots d\mathbf{x}_{N-1}. \quad (2.52)$$

For a one-particle system the action S_N is given by [13]

$$S_N = \varepsilon \sum_{n=1}^N \left(\frac{m}{2} \left(\frac{\mathbf{x}_n - \mathbf{x}_{n-1}}{\varepsilon} \right)^2 - V(\mathbf{x}_n, t_n) \right) \quad (2.53)$$

and

$$\varepsilon = \frac{t_b - t_a}{N}. \quad (2.54)$$

We also define $\Delta t = t_b - t_a$. The Trotter kernel

$$K(\mathbf{x}_b, \mathbf{x}_a; \Delta t) = \left(\frac{m}{2\pi i \Delta t} \right)^{d/2} \exp \left(i \left(\frac{m}{2\Delta t} |\mathbf{x}_b - \mathbf{x}_a|^2 - \frac{\Delta t}{2} (V(\mathbf{x}_b) + V(\mathbf{x}_a)) \right) \right). \quad (2.55)$$

is an approximation of the path-integral kernel [14].

3 WAVELETS

3.1 General

Fourier transform of a function is localized well in frequency domain but not so well in time domain. Wavelets are basis function sets that are localized both in time and frequency domains. That makes wavelets an interesting basis for solving partial differential equations. In this study we use Deslauriers–Dubuc wavelets, which are a special case of interpolating wavelets, and Daubechies wavelets, which are orthonormal wavelets.

3.2 Orthonormal Wavelets

Univariate orthonormal wavelets [15] are defined by the *mother scaling function* $\bar{\varphi} \in L^2(\mathbb{R})$ satisfying the *refinement equation*

$$\bar{\varphi}(x) = \sum_{k=0}^{N-1} \bar{h}_k \bar{\varphi}(2x - k). \quad (3.1)$$

The *mother wavelet* is defined by

$$\bar{\psi}(x) = \sum_{k=0}^{M-1} \bar{g}_k \bar{\varphi}(2x - k) \quad (3.2)$$

In case $M = N$ we have

$$\bar{g}_k = (-1)^k \bar{h}_{N-1-k} \quad (3.3)$$

where $k = 0, \dots, N - 1$. We define the *scaling functions* by

$$\bar{\varphi}_{j,k}(x) = 2^{-j/2} \bar{\varphi}(2^j x - k) \quad (3.4)$$

and the *wavelets* by

$$\bar{\psi}_{j,k}(x) = 2^{-j/2} \bar{\psi}(2^j x - k) \quad (3.5)$$

where $j, k \in \mathbb{Z}$. These functions have to obey the orthogonality relations

$$\int_{\mathbb{R}} \bar{\varphi}_{j,k}(x) \bar{\varphi}_{j,l}(x) dx = \delta_{k,l} \quad \text{for all } j, k, l \in \mathbb{Z}, \quad (3.6)$$

$$\int_{\mathbb{R}} \bar{\varphi}_{j,k}(x) \bar{\psi}_{j',l}(x) dx = 0 \quad \text{for all } j, j', k, l \in \mathbb{Z} \text{ and } j' \geq j, \quad (3.7)$$

and

$$\int_{\mathbb{R}} \bar{\psi}_{j,k}(x) \bar{\psi}_{j',l}(x) dx = \delta_{jj'} \delta_{k,l} \quad \text{for all } j, j', k, l \in \mathbb{Z}. \quad (3.8)$$

Now any function $f \in L^2(\mathbb{R})$ can be represented as

$$f = \sum_{k \in \mathbb{Z}} s_{j_0,k} \bar{\varphi}_{j_0,k} + \sum_{j' \geq j_0} \sum_{k \in \mathbb{Z}} d_{j,k} \bar{\psi}_{j,k} \quad (3.9)$$

where $j_0 \in \mathbb{Z}$,

$$s_{j_0,k} = \int_{\mathbb{R}} \bar{\varphi}_{j_0,k}(x) f(x) dx, \quad (3.10)$$

and

$$d_{j,k} = \int_{\mathbb{R}} \bar{\psi}_{j,k}(x) f(x) dx \quad (3.11)$$

for all $j, k \in \mathbb{Z}, j \geq j_0$.

3.3 Compactly Supported Interpolating Wavelets

Detailed introduction to univariate compactly supported interpolating wavelets can be found in [16, 17]. These are generalized to the multivariate case in [2].

3.3.1 Mother Scaling Function

Let $K = \mathbb{R}$ or $K = \mathbb{C}$ and $n \in \mathbb{Z}_+$. A *compactly supported interpolating mother scaling function* is a function $\varphi \in C_{\text{com}}(\mathbb{R}^n, K)$ satisfying the following conditions:

(MSF.1)

$$\forall \mathbf{k} \in \mathbb{Z}^n : \varphi(\mathbf{k}) = \delta_{\mathbf{k},0}$$

(MSF.2)

$$\forall \mathbf{x} \in \mathbb{R}^n : \varphi(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{Z}^n} \varphi\left(\frac{\mathbf{k}}{2}\right) \varphi(2\mathbf{x} - \mathbf{k}).$$

The mother scaling function of the 8th order Deslauriers–Dubuc wavelets is plotted in Fig. 3.1.

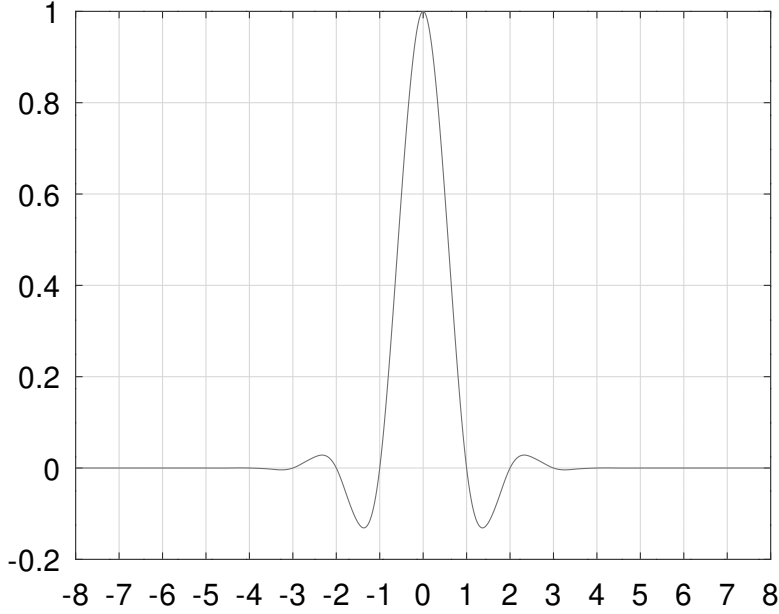


Figure 3.1 The 8th order Deslauriers–Dubuc fundamental function

3.3.2 General Definitions for Univariate MRA's

We shall denote the function space for which the MRA is defined by E in this section. We have either $E = C_u(\mathbb{R}, K)$ or $E = C_0(\mathbb{R}, K)$ where $K = \mathbb{R}$ or $K = \mathbb{C}$. We shall assume that $\varphi \in C_{\text{com}}(\mathbb{R}, K)$ is a compactly supported interpolating mother scaling function throughout this subsection.

Definition 3.1. Define function $\psi \in C_{\text{com}}(\mathbb{R}, K)$ by

$$\psi(x) := \varphi(2x - 1) \tag{3.12}$$

for all $x \in \mathbb{R}$. Function ψ is called *the mother wavelet*.

Definition 3.2. Define

$$\zeta_s := \begin{cases} \varphi; & s = 0 \\ \psi; & s = 1 \end{cases} \quad (3.13)$$

where $s \in \{0, 1\}$.

Definition 3.3. Define

$$\varphi_{j,k} := \varphi(2^j \cdot -k) \quad (3.14)$$

and

$$\psi_{j,k} := \psi(2^j \cdot -k) \quad (3.15)$$

for all $j \in \mathbb{Z}$ and $k \in \mathbb{Z}$.

Definition 3.4. When $k \in \mathbb{Z}$ define

$$h_k := \varphi\left(\frac{k}{2}\right) \quad (3.16)$$

$$g_k := \delta_{k,1} \quad (3.17)$$

$$\tilde{h}_k := \delta_{k,0} \quad (3.18)$$

$$\tilde{g}_k := (-1)^{k-1} h_{1-k}. \quad (3.19)$$

Definition 3.5. Define $\tilde{\varphi} := \delta \in E^*$ and $\tilde{\psi} \in E^*$ by

$$\tilde{\psi} := 2 \sum_{k \in \mathbb{Z}} \tilde{g}_k \tilde{\varphi}(2 \cdot -k). \quad (3.20)$$

Define $\tilde{\varphi}_{j,k} := 2^j \tilde{\varphi}(2^j \cdot -k)$ and $\tilde{\psi}_{j,k} := 2^j \tilde{\psi}(2^j \cdot -k)$ where $j, k \in \mathbb{Z}$.

As φ is compactly supported only a finite number of numbers $h_k, k \in \mathbb{Z}$, and the other three filters defined by Definition 3.4 are nonzero. Consequently the series in Eq. (3.20) has a finite number of nonzero terms.

Definition 3.6. Define

$$\tilde{\zeta}_s := \begin{cases} \tilde{\varphi}; & s = 0 \\ \tilde{\psi}; & s = 1 \end{cases} \quad (3.21)$$

where $s \in \{0, 1\}$.

3.3.3 General Definitions for Multivariate MRA's

We will assume that $n \in \mathbb{Z}_+$ and either $K = \mathbb{R}$ or $K = \mathbb{C}$ throughout this subsection. We will also assume that $E =_{\text{n.s.}} C_u(\mathbb{R}, K)$ or $E =_{\text{n.s.}} C_0(\mathbb{R}, K)$. Furthermore, $\varphi \in C_{\text{com}}(\mathbb{R}, K)$ shall be a compactly supported interpolating mother scaling function throughout this subsection.

We set

$$F :=_{\text{n.s.}} \begin{cases} C_u(\mathbb{R}^n, K); & E = C_u(\mathbb{R}, K) \\ C_0(\mathbb{R}^n, K); & E = C_0(\mathbb{R}, K) \end{cases} \quad (3.22)$$

Definition 3.7. Define function $\varphi^{[n]} \in C_{\text{com}}(\mathbb{R}^n, K)$ by

$$\varphi^{[n]} := \bigotimes_{k=1}^n \varphi. \quad (3.23)$$

Function $\varphi^{[n]}$ is called *an n -dimensional tensor product mother scaling function generated by φ* . Define also $\varphi_{j,\mathbf{k}}^{[n]} := \varphi^{[n]}(2^j \cdot -\mathbf{k})$ where $j \in \mathbb{Z}$ and $\mathbf{k} \in \mathbb{Z}^n$.

Function $\varphi^{[n]}$ is a compactly supported interpolating mother scaling function on $\mathbb{R}^n$.

Definition 3.8. When $\mathbf{s} \in \{0, 1\}^n$ define function $\psi_{\mathbf{s}}^{[n]} \in C_{\text{com}}(\mathbb{R}^n, K)$ by

$$\psi_{\mathbf{s}}^{[n]} := \bigotimes_{k=1}^n \tilde{\zeta}_{\mathbf{s}[k]} \quad (3.24)$$

and $\psi_{\mathbf{s},j,\mathbf{k}}^{[n]} := \psi_{\mathbf{s}}^{[n]}(2^j \cdot -\mathbf{k})$.

Definition 3.9. Define $\tilde{\varphi}^{[n]} \in F^*$ by

$$\tilde{\varphi}^{[n]} := \bigotimes_{l=1}^n \tilde{\varphi} \quad (3.25)$$

and $\tilde{\varphi}_{j,\mathbf{k}}^{[n]} \in F^*$ by $\tilde{\varphi}_{j,\mathbf{k}}^{[n]} := 2^j \tilde{\varphi}^{[n]}(2^j \cdot -\mathbf{k})$ where $j \in \mathbb{Z}$ and $\mathbf{k} \in \mathbb{Z}^n$. Define also $\tilde{\psi}_{\mathbf{s}}^{[n]} \in F^*$ by

$$\tilde{\psi}_{\mathbf{s}}^{[n]} := \bigotimes_{l=1}^n \tilde{\zeta}_{\mathbf{s}[l]} \quad (3.26)$$

where $\mathbf{s} \in \{0, 1\}^n$ and $\tilde{\psi}_{\mathbf{s},j,\mathbf{k}}^{[n]} \in F^*$ by $\tilde{\psi}_{\mathbf{s},j,\mathbf{k}}^{[n]} := 2^j \tilde{\psi}_{\mathbf{s}}^{[n]}(2^j \cdot -\mathbf{k})$ where $\mathbf{s} \in \{0, 1\}^n, j \in \mathbb{Z}$, and $\mathbf{k} \in \mathbb{Z}^n$.

3.4 Compactly Supported Interpolating MRA of $C_u(\mathbb{R}^n, K)$

We will assume that $n \in \mathbb{Z}_+$ and $K = \mathbb{R}$ or $K = \mathbb{C}$ throughout this section. We will also assume that $\varphi^{[n]} \in C_{\text{com}}(\mathbb{R}^n, K)$ is an n -dimensional tensor product mother scaling function in this section. Unless otherwise stated, we shall assume that the same values of n , K , and $\varphi^{[n]}$ are used throughout this section. Chui and Li [16] have developed a MRA in the univariate case $C_u(\mathbb{R})$.

Definition 3.10. Define

$$V_{n,j}^{(u)} := \left\{ \mathbf{x} \in \mathbb{R}^n \mapsto \sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{a}[\mathbf{k}] \varphi^{[n]}(2^j \mathbf{x} - \mathbf{k}) : \mathbf{a} \in l^\infty(\mathbb{Z}^n, K) \right\} \quad (3.27)$$

$$\|f|V_{n,j}^{(u)}\| := \|f\|_\infty, \quad f \in V_{n,j}^{(u)}$$

for all $j \in \mathbb{Z}$.

Definition 3.11. Let spaces $V_{n,j}^{(u)}, j \in \mathbb{Z}$, be defined by (3.27). We call $\{V_{n,j}^{(u)} : j \in \mathbb{Z}\}$ an *interpolating tensor product MRA* of $C_u(\mathbb{R}^n, K)$ generated by $\varphi^{[n]}$ provided that the following conditions are satisfied:

- (MRA1.1) $\forall j \in \mathbb{Z} : V_{n,j}^{(u)} \subset V_{n,j+1}^{(u)}$
(MRA1.2) $\overline{\bigcup_{j \in \mathbb{Z}} V_{n,j}^{(u)}} = C_u(\mathbb{R}^n, K)$

$$(MRA1.3) \quad \bigcap_{j \in \mathbb{Z}} V_{n,j}^{(u)} = K$$

$$(MRA1.4) \quad \forall j \in \mathbb{Z}, f \in K^{\mathbb{R}^n} : f \in V_{n,j}^{(u)} \iff f(2 \cdot) \in V_{n,j+1}^{(u)}$$

$$(MRA1.5) \quad \forall j \in \mathbb{Z}, \mathbf{k} \in \mathbb{Z}^n, f \in K^{\mathbb{R}^n} : f \in V_{n,j}^{(u)} \iff f(\cdot - 2^{-j}\mathbf{k}) \in V_{n,j}^{(u)}$$

$$(MRA1.6) \quad \forall \mathbf{k} \in \mathbb{Z}^n : \varphi^{[n]}(\mathbf{k}) = \delta_{\mathbf{k},0}$$

Our requirements for the definition of interpolating multiresolution analysis are stricter and simpler than those in [16]. Condition (MRA1.6) is replaced by a weaker condition for φ in [16] but it is possible to construct function φ_L that satisfies condition (MRA1.6) and generates the same subspaces $V_{1,j}^{(u)}$ as function φ .

Under the conditions given at the start of this section ($\varphi^{[n]}$ is an n -dimensional tensor product mother scaling function) all the conditions (MRA1.1), (MRA1.2), (MRA1.3), (MRA1.4), (MRA1.5), and (MRA1.6) are true.

Spaces $V_{n,j}^{(u)}$, $j \in \mathbb{Z}$, are topologically isomorphic to $l^\infty(\mathbb{Z}^n, K)$. It has been proved in [18] that

$$\sum_{\mathbf{k} \in \mathbb{Z}^n} \varphi^{[n]}(\mathbf{y} - \mathbf{k}) = \widehat{\varphi^{[n]}}(0) \quad (3.28)$$

for all $\mathbf{y} \in \mathbb{R}^n$. It follows from the cardinal interpolation property (MSF.1) that

$$\sum_{\mathbf{k} \in \mathbb{Z}^n} \varphi^{[n]}(\mathbf{y} - \mathbf{k}) = 1 \quad (3.29)$$

for all $\mathbf{y} \in \mathbb{R}^n$.

The series in Eq. (3.27) converges (pointwise) for all $\mathbf{a} \in l^\infty(\mathbb{Z}^n, K)$ but the series $\sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{a}[\mathbf{k}] \varphi^{[n]}(2^j \cdot - \mathbf{k})$ need not converge in the norm topology of $C_u(\mathbb{R}^n, K)$. For example, consider sequence $\mathbf{a}[\mathbf{k}] = 1$, $\mathbf{k} \in \mathbb{Z}^n$. Now $\sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{a}[\mathbf{k}] \varphi^{[n]}(2^j \mathbf{x} - \mathbf{k}) = 1$ for all $\mathbf{x} \in \mathbb{R}^n$ but the series $\sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{a}[\mathbf{k}] \varphi^{[n]}(2^j \cdot - \mathbf{k})$ does not converge in the norm topology of $C_u(\mathbb{R}^n, K)$.

Definition 3.12. When $j \in \mathbb{Z}$ and $\mathbf{s} \in \{0, 1\}^n$ define

$$\mathcal{W}_{n,\mathbf{s},j}^{(u)} := \left\{ \mathbf{x} \in \mathbb{R}^n \mapsto \sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{a}[\mathbf{k}] \psi_{\mathbf{s},j,\mathbf{k}}^{[n]}(\mathbf{x}) : \mathbf{a} \in l^\infty(\mathbb{Z}^n, K) \right\} \quad (3.30)$$

$$\|f| \mathcal{W}_{n,\mathbf{s},j}^{(u)}\| := \|f\|_\infty, \quad f \in \mathcal{W}_{n,\mathbf{s},j}^{(u)}. \quad (3.31)$$

Spaces $W_{n,s,j}^{(u)}$, $\mathbf{s} \in \{0,1\}^n$, $j \in \mathbb{Z}$, are topologically isomorphic to $l^\infty(\mathbb{Z}^n, K)$.

Definition 3.13. When $\mathbf{s} \in \{0,1\}^n$ and $j \in \mathbb{Z}$ define

$$\left(Q_{n,s,j}^{(u)}f\right)(\mathbf{x}) := \sum_{\mathbf{k} \in \mathbb{Z}^n} \left\langle \tilde{\psi}_{s,j,\mathbf{k}}^{[n]}, f \right\rangle \psi_{s,j,\mathbf{k}}^{[n]}(\mathbf{x}) \quad (3.32)$$

for all $\mathbf{x} \in \mathbb{R}^n$ and $f \in C_u(\mathbb{R}^n, K)$. When $j \in \mathbb{Z}$ define $P_{n,j}^{(u)} := Q_{n,0_{n,j}}^{(u)}$.

Operator $Q_{n,s,j}^{(u)}$ is a continuous projection of $C_u(\mathbb{R}^n, K)$ onto $W_{n,s,j}^{(u)}$ for each $\mathbf{s} \in \{0,1\}^n$ and $j \in \mathbb{Z}$.

When $j \in \mathbb{Z}$ we have

$$V_{n,j+1}^{(u)} =_{\text{n.s.}} V_{n,j}^{(u)} + \sum_{\mathbf{s} \in I_+(n)} W_{n,s,j}^{(u)} =_{\text{n.s.}} \sum_{\mathbf{s} \in \{0,1\}^n} W_{n,s,j}^{(u)}. \quad (3.33)$$

Theorem 3.1. There exist $c_1 \in \mathbb{R}_+$ and $c_2 \in \mathbb{R}_+$ so that

$$\left\| f - P_{n,j}^{(u)}f \right\|_\infty \leq c_1 \omega(f; 2^{-j}c_2) \quad (3.34)$$

for all $f \in C_u(\mathbb{R}^n)$ and $j \in \mathbb{Z}$.

Proof. Let $f \in C_u(\mathbb{R}^n)$ and $j \in \mathbb{Z}$. Define $r_1 := r_{\text{supp}}(\varphi^{[n]})$. Let $\mathbf{x} \in \mathbb{R}^n$. Define $I := I_{\text{trans}}(\varphi^{[n]}, 2^j\mathbf{x})$. Now by Eq. (3.29) we have

$$\left(f - P_{n,j}^{(u)}f\right)(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{Z}^n} \left(f(\mathbf{x}) - f\left(\frac{\mathbf{k}}{2^j}\right)\right) \varphi^{[n]}(2^j\mathbf{x} - \mathbf{k}) \quad (3.35)$$

$$= \sum_{\mathbf{k} \in I} \left(f(\mathbf{x}) - f\left(\frac{\mathbf{k}}{2^j}\right)\right) \varphi^{[n]}(2^j\mathbf{x} - \mathbf{k}) \quad (3.36)$$

Let $\ell \in I$. Now $2^j\mathbf{x} - \ell \in \overline{B}_{\mathbb{R}^n}(0; r_1)$ from which it follows that $\mathbf{x} - 2^{-j}\ell \in \overline{B}_{\mathbb{R}^n}(0; 2^{-j}r_1)$.

Hence

$$\left| f(\mathbf{x}) - f\left(\frac{\ell}{2^j}\right) \right| \leq \omega(f; 2^{-j}r_1). \quad (3.37)$$

Let $c_1 := N_{\text{cover}}(\varphi^{[n]}) \|\varphi^{[n]}\|_\infty$ and $c_2 := r_1 = r_{\text{supp}}(\varphi^{[n]})$. By Eq. (3.37) we have

$$\left| \left(f - P_{n,j}^{(u)}f\right)(\mathbf{x}) \right| \leq c_1 \omega(f; 2^{-j}c_2). \quad (3.38)$$

□

It follows that

$$\lim_{j \rightarrow \infty} \|f - P_{n,j}^{(u)} f\|_{\infty} = 0 \quad (3.39)$$

for all $f \in C_u(\mathbb{R}^n)$.

Define $\mathbf{0}_n := (0)_{k \in Z(n)}$ and $J_+(n) := \{0, 1\}^n \setminus \{\mathbf{0}_n\}$. We have

$$f(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{Z}^n} s_{j_0, \mathbf{k}} \varphi_{j_0, \mathbf{k}}^{[n]}(\mathbf{x}) + \sum_{j=j_0}^{\infty} \sum_{\mathbf{s} \in J_+(n)} \sum_{\mathbf{k} \in \mathbb{Z}^n} d_{\mathbf{s}, j, \mathbf{k}} \psi_{\mathbf{s}, j, \mathbf{k}}^{[n]}(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^n, \quad (3.40)$$

where $s_{j_0, \mathbf{k}} = \langle \tilde{\varphi}_{j_0, \mathbf{k}}^{[n]}, f \rangle$ and $d_{\mathbf{s}, j, \mathbf{k}} = \langle \tilde{\psi}_{\mathbf{s}, j, \mathbf{k}}^{[n]}, f \rangle$. This can be simplified in one-dimensional case as

$$f(x) = \sum_{k \in \mathbb{Z}} s_{j_0, k} \varphi_{j_0, k}(x) + \sum_{j=j_0}^{\infty} \sum_{k \in \mathbb{Z}} d_{j, k} \psi_{j, k}(x), \quad x \in \mathbb{R}, \quad (3.41)$$

where $s_{j_0, k} = \langle \tilde{\varphi}_{j_0, k}, f \rangle$ and $d_{j, k} = \langle \tilde{\psi}_{j, k}, f \rangle$. Note that expansions Eqs. (3.40) and (3.41) are not true for all $f \in C_u(\mathbb{R}^n, K)$ if we replace the pointwise convergence with the convergence in the supremum norm.

It follows from Eq. (3.39) that

$$\bigotimes_{j=1}^n \varepsilon C_u(\mathbb{R}, K) =_{\text{n.s.}} C_u(\mathbb{R}^n, K) \quad (3.42)$$

for all $n \in \mathbb{Z}_+$.

3.5 Compactly Supported Interpolating MRA of $C_0(\mathbb{R}^n, K)$

A MRA of space $C_0(\mathbb{R}^n, K)$ can be developed in the same way as the MRA of space $C_u(\mathbb{R}^n, K)$. Donoho [17] has developed a MRA for the one-dimensional case $C_0(\mathbb{R})$. We will assume that $n \in \mathbb{Z}_+$ and $K = \mathbb{R}$ or $K = \mathbb{C}$ throughout this section. We will also assume that $\varphi^{[n]} \in C_{\text{com}}(\mathbb{R}^n, K)$ is an n -dimensional tensor product mother scaling function in this section. Unless otherwise stated, we shall assume that the same values of n , K , and $\varphi^{[n]}$ are used throughout this section. Note that many of the series that are pointwise convergent with $C_u(\mathbb{R}^n, K)$ converge in the norm in $C_0(\mathbb{R}^n, K)$. We are also able to represent many subspaces and operators related to the MRA of $C_0(\mathbb{R}^n, K)$ as tensor products of the corresponding one-dimensional cases.

Definition 3.14. Define

$$V_{n,j}^{(0)} := \left\{ \sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{a}[\mathbf{k}] \varphi^{[n]}(2^j \cdot -\mathbf{k}) : \mathbf{a} \in c_0(\mathbb{Z}^n, K) \right\} \quad (3.43)$$

$$\|f|V_{n,j}^{(0)}\| := \|f\|_\infty, \quad f \in V_{n,j}^{(0)} \quad (3.44)$$

for each $j \in \mathbb{Z}$.

Definition 3.15. Let spaces $V_{n,j}^{(0)}, j \in \mathbb{Z}$, be defined by Definition 3.14. We call $\{V_{n,j}^{(0)} : j \in \mathbb{Z}\}$ an interpolating tensor product MRA of $C_0(\mathbb{R}^n, K)$ generated by $\varphi^{[n]}$ provided that the following conditions are satisfied:

$$(MRA2.1) \quad \forall j \in \mathbb{Z} : V_{n,j}^{(0)} \subset V_{n,j+1}^{(0)}$$

$$(MRA2.2) \quad \overline{\bigcup_{j \in \mathbb{Z}} V_{n,j}^{(0)}} = C_0(\mathbb{R}^n, K)$$

$$(MRA2.3) \quad \bigcap_{j \in \mathbb{Z}} V_{n,j}^{(0)} = \{0\}$$

$$(MRA2.4) \quad \forall j \in \mathbb{Z}, f \in K^{\mathbb{R}^n} : f \in V_{n,j}^{(0)} \iff f(2 \cdot) \in V_{n,j+1}^{(0)}$$

$$(MRA2.5) \quad \forall j \in \mathbb{Z}, \mathbf{k} \in \mathbb{Z}^n, f \in K^{\mathbb{R}^n} : f \in V_{n,j}^{(0)} \iff f(\cdot - 2^{-j}\mathbf{k}) \in V_{n,j}^{(0)}$$

$$(MRA2.6) \quad \forall \mathbf{k} \in \mathbb{Z}^n : \varphi^{[n]}(\mathbf{k}) = \delta_{\mathbf{k},0}$$

Note that in this definition the intersection of spaces $V_{n,j}^{(0)}$ is $\{0\}$ instead of $\mathbb{C}$ (all complex valued constant functions on $\mathbb{R}^n$) as in [16] since here the MRA is constructed for functions vanishing at infinity. Donoho [17] does not require the mother scaling function φ to be compactly supported but φ has to be of rapid decay in his construction. He also includes requirements for the regularity and polynomial span of φ , which are needed for the norm equivalences to Besov and Triebel-Lizorkin spaces, into the definition of the MRA. Under the conditions given at the start of this section ($\varphi^{[n]}$ is an n -dimensional tensor product mother scaling function) the conditions (MRA2.1), (MRA2.2), (MRA2.3), (MRA2.4), (MRA2.5), and (MRA2.6) are true.

Definition 3.16. Let $j \in \mathbb{Z}$ and $\mathbf{s} \in \{0, 1\}^n$. Define

$$W_{n, \mathbf{s}, j}^{(0)} := \left\{ \sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{a}[\mathbf{k}] \psi_{\mathbf{s}, j, \mathbf{k}}^{[n]} : \mathbf{a} \in \ell_0(\mathbb{Z}^n, K) \right\} \quad (3.45)$$

$$\|f\|_{W_{n, \mathbf{s}, j}^{(0)}} := \|f\|_{\infty}, \quad f \in W_{n, \mathbf{s}, j}^{(0)}. \quad (3.46)$$

Definition 3.17. Let $j \in \mathbb{Z}$. Define operator $P_{n, j}^{(0)} : C_0(\mathbb{R}^n, K) \rightarrow V_{n, j}^{(0)}$ by

$$P_{n, j}^{(0)} f = \sum_{\mathbf{k} \in \mathbb{Z}^n} \langle \tilde{\varphi}_{j, \mathbf{k}}^{[n]}, f \rangle \varphi_{j, \mathbf{k}}^{[n]} \quad (3.47)$$

for all $f \in C_0(\mathbb{R}^n, K)$. Define operator $Q_{n, \mathbf{s}, j}^{(0)} : C_0(\mathbb{R}^n, K) \rightarrow W_{n, \mathbf{s}, j}^{(0)}$ by

$$Q_{n, \mathbf{s}, j}^{(0)} f = \sum_{\mathbf{k} \in \mathbb{Z}^n} \langle \tilde{\psi}_{\mathbf{s}, j, \mathbf{k}}^{[n]}, f \rangle \psi_{\mathbf{s}, j, \mathbf{k}}^{[n]} \quad (3.48)$$

for all $f \in C_0(\mathbb{R}^n, K)$ and $\mathbf{s} \in \{0, 1\}^n$.

We get the following equation as a direct consequence of Eq. (3.39):

$$\lim_{j \rightarrow \infty} \|f - P_{n, j}^{(0)} f\|_{\infty} = 0 \quad (3.49)$$

for all $f \in C_0(\mathbb{R}^n)$. We also have the wavelet expansions

$$f = \sum_{\mathbf{k} \in \mathbb{Z}^n} s_{j_0, \mathbf{k}} \varphi_{j_0, \mathbf{k}}^{[n]} + \sum_{j=j_0}^{\infty} \sum_{\mathbf{s} \in J_+(n)} \sum_{\mathbf{k} \in \mathbb{Z}^n} d_{\mathbf{s}, j, \mathbf{k}} \psi_{\mathbf{s}, j, \mathbf{k}}^{[n]} \quad (3.50)$$

where $s_{j_0, \mathbf{k}} = \langle \tilde{\varphi}_{j_0, \mathbf{k}}^{[n]}, f \rangle$ and $d_{\mathbf{s}, j, \mathbf{k}} = \langle \tilde{\psi}_{\mathbf{s}, j, \mathbf{k}}^{[n]}, f \rangle$. This can be simplified in one-dimensional case as

$$f = \sum_{k \in \mathbb{Z}} s_{j_0, k} \varphi_{j_0, k} + \sum_{j=j_0}^{\infty} \sum_{k \in \mathbb{Z}} d_{j, k} \psi_{j, k} \quad (3.51)$$

where $s_{j_0, k} = \langle \tilde{\varphi}_{j_0, k}, f \rangle$ and $d_{j, k} = \langle \tilde{\psi}_{j, k}, f \rangle$.

It follows from Eq. (3.49) that

$$\bigotimes_{j=1}^n \varepsilon C_0(\mathbb{R}, K) =_{\text{n.s.}} C_0(\mathbb{R}^n, K). \quad (3.52)$$

3.6 Polynomial Span and Regularity

The polynomial span and regularity of interpolating wavelets has been discussed in [17].

Definition 3.18. Let $f \in \mathbb{C}^{\mathbb{R}^n}$, $r_1 \in \mathbb{R}_+$, and $\tilde{f} \in C(\overline{B_{\mathbb{R}^n}}(0; r_1))^*$. Let $D \in \mathbb{N}$. We say that pair $(\tilde{f}, f)$ spans all the polynomials of degree at most D iff

$$\sum_{\mathbf{k} \in \mathbb{Z}^n} \left\langle \tilde{f}, p(\cdot + \mathbf{k})|_{\overline{B_{\mathbb{R}^n}}(0; r_1)} \right\rangle f(\mathbf{x} - \mathbf{k}) = p(\mathbf{x}) \quad (3.53)$$

for all $\mathbf{x} \in \mathbb{R}^n$ and for all polynomials p of n variables that are of degree at most D .

The polynomial span D of the interpolating wavelet family generated by the compactly supported mother scaling function φ is the largest integer D so that pair (δ, φ) spans all the polynomials of degree at most D . Here δ is the Dirac delta. When φ is the m th order Deslauriers–Dubuc fundamental function we have $D = m - 1$.

The regularity R of the interpolating wavelet family is define so that φ is Hölder continuous of order R . Let $R(D)$ be the regularity of the Deslauriers–Dubuc wavelets of order $D + 1$. We have [17]

$$R(D) \geq \text{const} \cdot D, \quad D = 3, 5, 7, \dots \quad (3.54)$$

3.7 Deslauriers–Dubuc Wavelets on a Half-Infinite Interval

This derivation is based on section 3 in [17]. We construct a basis set on half-infinite interval $\mathbb{R}_0 = \{r \geq 0 | r \in \mathbb{R}\}$. We define φ to be a Deslauriers–Dubuc scaling function of some order D (the polynomial span of the wavelet family) and $\varphi_{j,k}(x) := \varphi(2^j x - k)$ for $j, k \in \mathbb{Z}$.

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 define

$$\tilde{\beta}_{j,k} := \pi_j^\#(2^{-j}k) \quad (3.55)$$

for $k < 0$ and

$$\tilde{\beta}_{j,k} := \beta_{j,k} \quad (3.56)$$

for $k \geq 0$. Now, f can be extrapolated onto the whole real line by

$$\tilde{f} = \sum_{k=-\infty}^{\infty} \tilde{\beta}_{j,k} \varphi_{j,k}. \quad (3.57)$$

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

$$\tilde{\beta}_{j,k} = \sum_{k'=0}^D e_{k,k'}^\# \beta_{j,k'} \quad (3.58)$$

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

$$\tilde{\beta}_{j,k} = e_{k,l}^\# \quad (3.59)$$

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

$$\text{supp } \varphi_{j,k} \subset 2^{-j}[k - D, k + D] \quad (3.60)$$

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

$$\varphi_{j,k}^\# := \varphi_{j,k} + \sum_{l < 0} e_{l,k}^\# \varphi_{j,l} \quad (3.61)$$

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

$$\langle \tilde{\varphi}_{j,k}, \varphi_{j,l}^\# \rangle = \delta_{k,l} \quad (3.62)$$

for $k \geq 0$ and $0 \leq l \leq D$.

We define a wavelet expansion of function f by

$$\tilde{f} := \sum_{k=0}^D \beta_{j,k} \varphi_{j,k}^{\#} + \sum_{k=D+1}^{\infty} \beta_{j,k} \varphi_{j,k}. \quad (3.63)$$

When we use a finite basis of size W , we have

$$\tilde{f} := \sum_{k=0}^D \beta_{j,k} \varphi_{j,k}^{\#} + \sum_{k=D+1}^{W-1} \beta_{j,k} \varphi_{j,k} \quad (3.64)$$

We must have $W > 2D$ so that functions $\varphi_{j,k}^{\#}(x)$, $0 \leq k \leq D$, vanish for $x \geq 2^{-j}W$. This kind of truncation of the basis requires that the function f approximately vanishes for $x > 2^{-j}W$.

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

$$\left\langle \tilde{\varphi}_{j,k}, A \varphi_{j,l}^{\#} \right\rangle = \left\langle \tilde{\varphi}_{j,k}, A \varphi_{j,l} \right\rangle + \sum_{\alpha < 0} e_{\alpha,l}^{\#} \left\langle \tilde{\varphi}_{j,k}, A \varphi_{j,\alpha} \right\rangle. \quad (3.65)$$

4 CALCULATIONS OF RADIAL WAVEFUNCTIONS OF ATOMS USING DESLAURIERS–DUBUC WAVELETS

4.1 General

We solve the Schrödinger equations of hydrogen-like atoms and the Hartree–Fock equations of some many-electron atoms, see section 2.4. The HF equations are solved for helium, beryllium, neon, magnesium, argon, lithium, and sodium. The lithium and sodium atoms are open shell and the rest of the atoms are closed shell. See Ref. [1] for more.

4.2 Construction of the Basis Function Set

To preserve orthogonality relations of basis functions the scaling functions and wavelets in the basis cannot be chosen arbitrarily. The basis set $B = \{\zeta_1, \dots, \zeta_N\}$ consists of scaling functions ϕ_i^k of resolution level $k = k_{\min}$ and wavelets ψ_i^k of resolution levels $k = k_{\min}, \dots, k_{\max}$. The dual basis functions are defined by

$$\tilde{\zeta}_j = \begin{cases} \tilde{\phi}_i^k & \text{if } \zeta_j = \phi_i^k \\ \tilde{\psi}_i^k & \text{if } \zeta_j = \psi_i^k \end{cases}. \quad (4.1)$$

Different resolution levels of the basis are denoted as $S_{k_{\min}}, D_{k_{\min}}, \dots, D_{k_{\max}}$, where S means a set consisting of scaling functions and D a set consisting of wavelets. This kind of basis is used directly for standard operator form. For nonstandard operator form, S_k parts with indices $k = k_{\min} + 1, \dots, k_{\max}$ are inserted in the basis. We define N_k to be the number of basis functions in S_k and M_k to be the number of basis functions in D_k . For $S_k = \{\phi_{i_1}^k, \dots, \phi_{i_{N_k}}^k\}$ we define $\mu_{k,\alpha} = i_\alpha$ and for $D_k = \{\psi_{i_1}^k, \dots, \psi_{i_{M_k}}^k\}$

we define $\nu_{k,\alpha} = i_\alpha$. The NSOF basis function set $B_{\text{NSOF}} = \{\zeta_1, \dots, \zeta_{N_{\text{NSOF}}}\}$ consists of parts $S_{k_{\min}}, D_{k_{\min}}, \dots, S_{k_{\max}}, D_{k_{\max}}$. Basis functions in parts $S_{k_{\min}}, D_{k_{\min}}, \dots, D_{k_{\max}}$ are the same as in the corresponding parts of the basis set B . Basis functions in parts $S_{k_{\min}+1}, \dots, S_{k_{\max}}$ are chosen so that $L(S_k, D_k) \subset L(S_{k+1})$. The radial wavefunction we want to expand should be zero at the nucleus.

Scaling function $\phi_0^{k_{\min}}$ is excluded from B due to the boundary conditions of wavefunctions at zero and singularities of potential, centrifugal potential, and functions $1/r^{k+1}$ (occurring in Slater integrals) at $r = 0$. This also makes the matrix of operator $\hat{R}$, defined by

$$(\hat{R}f)(r) = |r|f(r), \quad (4.2)$$

nonsingular (an empirical observation).

However, since the Slater integrals do not generally vanish at $r = 0$ we include $\phi_0^{k_{\min}}$ in the basis set $B_0 = B \cup \{\phi_0^{k_{\min}}\} = \{\zeta_1^{(0)}, \dots, \zeta_{N'}^{(0)}\}$. Basis change matrix from B to B_0 is denoted by $L_{1 \rightarrow 0}$ and basis change matrix from B_0 to B by $L_{0 \rightarrow 1}$. We do not need to compute the matrix of operator $\hat{R}_{-1}$ (corresponding division by r) in basis B_0 .

4.3 Forward and Backward Wavelet Transforms

Forward wavelet transform is defined by equations [19]

$$s_i^{k-1} = \sum_{j=-m}^m \tilde{h}_j s_{j+2i}^k, \quad (4.3)$$

$$d_i^{k-1} = \sum_{j=-m}^m \tilde{g}_j s_{j+2i}^k. \quad (4.4)$$

where s_i^k is the coefficient for basis function ϕ_i^k and d_i^k is the coefficient for basis function ψ_i^k . Backward wavelet transform is defined by equations [19]:

$$s_{2i}^{k+1} = \sum_{j=-m/2}^{m/2} \left(b_{2j} s_{i-j}^k + g_{2j} d_{i-j}^k \right), \quad (4.5)$$

$$s_{2i+1}^{k+1} = \sum_{j=-m/2}^{m/2} \left(b_{2j+1} s_{i-j}^k + g_{2j+1} d_{i-j}^k \right). \quad (4.6)$$

The forward wavelet transform defined by (4.3) and (4.4) can be written in matrix form as

$$v^{(k-1)} = \tilde{Z}_{S_k}^{S_{k-1}} v^{(k)}, \quad (4.7)$$

$$w^{(k-1)} = \tilde{Z}_{S_k}^{D_{k-1}} v^{(k)}, \quad (4.8)$$

where

$$\tilde{Z}_{S_k}^{S_{k-1}} = \left(\tilde{h}_{\mu_{k,\beta}-2\mu_{k-1,\alpha}} \right)_{\alpha=1, \beta=1}^{N_{k-1}, N_k}, \quad (4.9)$$

$$\tilde{Z}_{S_k}^{D_{k-1}} = \left(\tilde{g}_{\mu_{k,\beta}-2\nu_{k-1,\alpha}} \right)_{\alpha=1, \beta=1}^{M_{k-1}, N_k}. \quad (4.10)$$

The backward wavelet transform defined by (4.5) and (4.6) can be similarly written in matrix form as

$$v^{(k+1)} = B_{S_k}^{S_{k+1}} v^{(k)} + B_{D_k}^{S_{k+1}} w^{(k)}, \quad (4.11)$$

where [19]

$$B_{S_k}^{S_{k+1}} = \left(Z_{S_{k+1}}^{S_k} \right)^T, \quad (4.12)$$

$$B_{D_k}^{S_{k+1}} = \left(Z_{S_{k+1}}^{D_k} \right)^T, \quad (4.13)$$

and

$$Z_{S_{k+1}}^{S_k} = \left(h_{\mu_{k+1,\beta}-2\mu_{k,\alpha}} \right)_{\alpha=1, \beta=1}^{N_k, N_{k+1}}, \quad (4.14)$$

$$Z_{S_{k+1}}^{D_k} = \left(g_{\mu_{k+1,\beta}-2\nu_{k,\alpha}} \right)_{\alpha=1, \beta=1}^{M_k, N_{k+1}}. \quad (4.15)$$

We use symbols $\tilde{Z}$ and Z for forward wavelet transform instead of $\tilde{F}$ and F (as in Ref. [19]) to avoid confusion with the Fock operator F .

4.4 Standard Operator Form and Nonstandard Operator Form

The eigenvalue equations are solved using the standard operator form, which represents the operator in the chosen basis. Elements of matrix $\mathcal{A}$ of an operator $\hat{A}$ in

SOF are defined by

$$A_{ij} = \int_{-\infty}^{\infty} \tilde{\zeta}_i(x) \hat{A} \zeta_j(x) dx, \quad (4.16)$$

where ζ_j , $j = 1, \dots, N$ are the basis functions and $\tilde{\zeta}_i$, $i = 1, \dots, N$ are the dual basis functions defined by Eq. (4.1).

The standard operator form of an operator can be obtained from the matrix elements in nonstandard operator form. Nonstandard operator form decouples different resolution levels in the basis set and makes derivation of explicit formulas for the matrix elements easier [19, 20, 21]. The nonzero blocks of nonstandard operator form A of the operator $\hat{A}$ are defined by

$$A_{\alpha\beta}^{S_{k_{\min}}S_{k_{\min}}} = \int_{-\infty}^{\infty} \tilde{\phi}_{\mu_{k_{\min},\alpha}}^{k_{\min}}(x) \hat{A} \phi_{\mu_{k_{\min},\beta}}^{k_{\min}}(x) dx, \quad \alpha = 1, \dots, N_{k_{\min}}, \beta = 1, \dots, N_{k_{\min}}, \quad (4.17)$$

and

$$A_{\alpha\beta}^{S_k D_k} = \int_{-\infty}^{\infty} \tilde{\phi}_{\mu_{k,\alpha}}^k(x) \hat{A} \psi_{\nu_{k,\beta}}^k(x) dx, \quad \alpha = 1, \dots, N_k, \beta = 1, \dots, M_k, \quad (4.18)$$

$$A_{\alpha\beta}^{D_k S_k} = \int_{-\infty}^{\infty} \tilde{\psi}_{\nu_{k,\alpha}}^k(x) \hat{A} \phi_{\mu_{k,\beta}}^k(x) dx, \quad \alpha = 1, \dots, M_k, \beta = 1, \dots, N_k, \quad (4.19)$$

$$A_{\alpha\beta}^{D_k D_k} = \int_{-\infty}^{\infty} \tilde{\psi}_{\nu_{k,\alpha}}^k(x) \hat{A} \psi_{\nu_{k,\beta}}^k(x) dx, \quad \alpha = 1, \dots, M_k, \beta = 1, \dots, M_k, \quad (4.20)$$

where $k = k_{\min} + 1, \dots, k_{\max}$.

We introduce an algorithm for converting a matrix from NSOF to SOF. The NSOF blocks ($S_k S_k$, $S_k D_k$, $D_k S_k$ and $D_k D_k$) are computed on the fly. The algorithm is:

Input:

- NSOF basis $B = (S_{k_{\min}}, D_{k_{\min}}, \dots, S_{k_{\max}}, D_{k_{\max}})$.
- Function M that calculates the NSOF matrix elements according to formulas (4.17) – (4.20).

Output: Matrix in standard operator form.

Algorithm:

1. If the basis contains only parts $S_{k_{\min}}$ and $D_{k_{\min}}$ the SOF matrix is

$$A = \begin{pmatrix} A^{S_{k_{\min}} S_{k_{\min}}} & A^{S_{k_{\min}} D_{k_{\min}}} \\ A^{D_{k_{\min}} S_{k_{\min}}} & A^{D_{k_{\min}} D_{k_{\min}}} \end{pmatrix}, \quad (4.21)$$

where the blocks are computed with formulas (4.17) – (4.20).

else

2. Compute matrix A_{prev} by calling algorithm recursively with basis $B_{\text{prev}} = (S_{k_{\min}}, D_{k_{\min}}, \dots, S_{k_{\max}-1}, D_{k_{\max}-1})$.
3. Compute $A^{S_{k_{\max}} D_{k_{\max}}}$ with function M according to formula (4.18).
4. Compute $A^{D_{k_{\max}} S_{k_{\max}}}$ with function M according to formula (4.19).
5. Compute $A^{D_{k_{\max}} D_{k_{\max}}}$ with function M according to formula (4.20).
6. Calculate matrices $A^{S_{k_{\min}} D_{k_{\max}}}$ and $A^{D_q D_{k_{\max}}}$ where $q = k_{\min}, \dots, k_{\max} - 1$ by applying forward wavelet transforms to matrix $A^{S_{k_{\max}} D_{k_{\max}}}$ using formulas

$$A^{S_{k_{\min}} D_{k_{\max}}} = \tilde{Z}_{S_{k_{\min}+1}}^{S_{k_{\min}}} \tilde{Z}_{S_{k_{\min}+2}}^{S_{k_{\min}+1}} \dots \tilde{Z}_{S_{k_{\max}-1}}^{S_{k_{\max}-2}} \tilde{Z}_{D_{k_{\max}}}^{S_{k_{\max}-1}} A^{S_{k_{\max}} D_{k_{\max}}}, \quad (4.22)$$

$$A^{D_q D_{k_{\max}}} = \tilde{Z}_{S_{q+1}}^{D_q} \tilde{Z}_{S_{q+2}}^{S_{q+1}} \dots \tilde{Z}_{S_{k_{\max}-1}}^{S_{k_{\max}-2}} \tilde{Z}_{D_{k_{\max}}}^{S_{k_{\max}-1}} A^{S_{k_{\max}} D_{k_{\max}}}. \quad (4.23)$$

7. Calculate matrices $A^{D_{k_{\max}} S_{k_{\min}}}$ and $A^{D_{k_{\max}} D_q}$ where $q = k_{\min}, \dots, k_{\max} - 1$ by applying backward wavelet transforms to matrix $A^{D_{k_{\max}} S_{k_{\max}}}$ using formulas

$$A^{D_{k_{\max}} S_{k_{\min}}} = A^{D_{k_{\max}} S_{k_{\max}}} B_{S_{k_{\max}-1}}^{D_{k_{\max}}} B_{S_{k_{\max}-2}}^{S_{k_{\max}-1}} \dots B_{S_{k_{\min}+1}}^{S_{k_{\min}+2}} B_{S_{k_{\min}}}^{S_{k_{\min}+1}}, \quad (4.24)$$

$$A^{D_{k_{\max}} D_q} = A^{D_{k_{\max}} S_{k_{\max}}} B_{S_{k_{\max}-1}}^{D_{k_{\max}}} B_{S_{k_{\max}-2}}^{S_{k_{\max}-1}} \dots B_{S_{q+1}}^{S_{q+2}} B_{D_q}^{S_{q+1}}. \quad (4.25)$$

8. Construct the result A from matrices calculated in steps 2, 5, 6, and 7 using

formulas

$$A_{\text{vert}} = \begin{pmatrix} A^{S_{k_{\min}} D_{k_{\max}}} \\ A^{D_{k_{\min}} D_{k_{\max}}} \\ \vdots \\ A^{D_{k_{\max}-1} D_{k_{\max}}} \end{pmatrix}, \quad (4.26)$$

$$A_{\text{horiz}} = \begin{pmatrix} A^{D_{k_{\max}} S_{k_{\min}}} \\ A^{D_{k_{\max}} D_{k_{\min}}} \\ \dots \\ A^{D_{k_{\max}} D_{k_{\max}-1}} \end{pmatrix}^T, \quad (4.27)$$

$$A = \begin{pmatrix} A_{\text{prev}} & A_{\text{vert}} \\ A_{\text{horiz}} & A^{D_{k_{\max}} D_{k_{\max}}} \end{pmatrix}. \quad (4.28)$$

4.5 Evaluation of Matrix Elements

We use the following notation for matrix elements of an operator $\hat{A}$ in nonstandard operator form [20]

$$\alpha_{ij}^k = \int_{-\infty}^{\infty} \tilde{\psi}_i^k(x) \hat{A} \psi_j^k(x) dx, \quad (4.29)$$

$$\beta_{ij}^k = \int_{-\infty}^{\infty} \tilde{\psi}_i^k(x) \hat{A} \phi_j^k(x) dx, \quad (4.30)$$

$$\gamma_{ij}^k = \int_{-\infty}^{\infty} \tilde{\phi}_i^k(x) \hat{A} \psi_j^k(x) dx, \quad (4.31)$$

$$s_{ij}^k = \int_{-\infty}^{\infty} \tilde{\phi}_i^k(x) \hat{A} \phi_j^k(x) dx. \quad (4.32)$$

In this chapter we denote the matrix of an operator $\hat{A}$ in an arbitrary wavelet basis B (with or without function $\phi_0^{k_{\min}}$) by A .

4.6 Solving the Hartree–Fock Equations

We use a standard (damped) self-consistent field method [6] to solve the HF equations. For an arbitrary operator $\hat{A}$, we denote matrix of $\hat{A}$ in basis B by A and matrix in basis B_0 by $A^{(0)}$. We define some operators to be used:

$$(\hat{R}f)(r) = |r|f(r), \quad (4.33)$$

$$(\hat{R}_{-1}f)(r) = f(r)/|r|, \quad (4.34)$$

$$(\hat{U}_0f)(r) = \int_0^{|r|} f(r')dr', \quad (4.35)$$

$$(\hat{U}_\infty f)(r) = \int_{|r|}^\infty f(r')dr', \quad (4.36)$$

$$\hat{S}_\kappa = \hat{R}_{-1}^{\kappa+1} \hat{U}_0 \hat{R}^\kappa + \hat{R}^\kappa \hat{U}_\infty \hat{R}_{-1}^{\kappa+1}, \quad (4.37)$$

where $\kappa \in \mathbb{Z}$, $\kappa \geq 0$ and $\hat{A}^n f = \hat{A} \cdots \hat{A} f$ where $\hat{A}$ is applied n times. We define multiplication operator $\hat{M}(f) = \hat{A}$ by setting

$$(\hat{A}g)(r) = f(r)g(r) \quad (4.38)$$

for an arbitrary function $g(r)$. If f is a vector (function) in a wavelet basis B' we define matrix $M(f)$ to be the matrix of operator $\hat{M}(f)$ in the basis B' (f is kept constant). Let f and g be arbitrary vectors (functions) in wavelet basis B' . We define $f \star g$ to be the projection of function $h(r) = f(r)g(r)$ to $L(B')$.

We omit the nondiagonal Lagrange multipliers and equations (2.27) can be written as matrix eigenvalue equations [22]

$$F_i c_i = \varepsilon_i c_i, \quad (4.39)$$

where the Fock operator F_i for orbital i is defined by

$$F_i = H_i^0 + J_i - K_i. \quad (4.40)$$

Wavefunctions P_i are given by

$$P_i = \sum_{p=1}^N c_i^{(p)} \zeta_p. \quad (4.41)$$

The single-electron Hamiltonian operator is defined as

$$H_i^0 = T + V + C_{\ell_i}, \quad (4.42)$$

where the components are defined as in the case of hydrogen-like atoms, Eqs. (2.8), (2.9), and (2.10).

The Slater direct integral operator is defined by

$$\hat{J}_i = \sum_{j=1}^q (w_j - \delta_{ij}) \hat{J}_j^0 - (w_i - 1) \frac{2\ell_i + 1}{4\ell_i + 1} \sum_{\kappa > 0} \begin{pmatrix} \ell_i & \kappa & \ell_i \\ 0 & 0 & 0 \end{pmatrix}^2 \hat{J}_i^\kappa \quad (4.43)$$

where

$$(\hat{J}_i^\kappa P_j)(r) = Y_{ii}^\kappa(r) P_j(r) \quad (4.44)$$

and the Slater exchange integral operator by

$$\hat{K}_i = \frac{1}{2} \sum_{j(\neq i)=1}^q w_j \sum_{\kappa} \begin{pmatrix} \ell_i & \kappa & \ell_j \\ 0 & 0 & 0 \end{pmatrix}^2 \hat{K}_j^\kappa \quad (4.45)$$

where

$$(\hat{K}_j^\kappa P_i)(r) = Y_{ij}^\kappa(r) P_j(r). \quad (4.46)$$

Note that in the definition of operator $\hat{K}_j^\kappa$ the argument of the operator occurs only in the Slater integral $Y_{ij}^\kappa(r)$. This operator is linear, though. For matrices of direct Slater integral operators we have

$$J_i^\kappa = L_{0 \rightarrow 1} \mathcal{M}^{(0)} \left(S_\kappa^{(0)} (P_i \star P_i) \right) L_{1 \rightarrow 0} \quad (4.47)$$

and for matrices of exchange integral operators

$$K_j^\kappa = L_{0 \rightarrow 1} \mathcal{M}^{(0)} (P_j) S_\kappa^{(0)} \mathcal{M}^{(0)} (P_j) L_{1 \rightarrow 0}, \quad (4.48)$$

where

$$S_0^{(0)} = L_{1 \rightarrow 0} R^{-1} U_0 L_{0 \rightarrow 1} + U_\infty^{(0)} L_{1 \rightarrow 0} R^{-1} L_{0 \rightarrow 1} \quad (4.49)$$

and

$$S_\kappa^{(0)} = L_{1 \rightarrow 0} (R^{-1})^{\kappa+1} U_0 R^\kappa L_{0 \rightarrow 1} + (R^{(0)})^\kappa U_\infty^{(0)} L_{1 \rightarrow 0} (R^{-1})^{\kappa+1} L_{0 \rightarrow 1}$$

for $\kappa > 0$.

4.7 Results

We use 8th order interpolating wavelets for numerical results. The unit of length is the atomic unit unless otherwise stated. We examine the convergence of the essential physical quantities towards the known exact or accurate values when the number of resolution levels is increased. We also examine the effect of the number of basis functions in each resolution level. Various parameters affecting the computations are also reported.

The basis sets were formed so that there are S type basis functions $\phi_{-2B}^{k_{\min}}, \dots, \phi_{2B}^{k_{\min}}$ in resolution level $k_{\min}$ and D type basis functions $\psi_{-B}^k, \dots, \psi_{B-1}^k$ for $k = k_{\min}, \dots, k_{\min} + L - 2$. Here L is the number of resolution levels and B is a parameter describing the number of basis functions in each resolution level. We count $S_{k_{\min}}$ and $D_{k_{\min}}$ as two separate resolution levels. The total number of basis functions is

$$N = 4B + 2(L - 1)B = 2B(L + 1). \quad (4.50)$$

In principle, the number of resolution levels L determines the maximum possible accuracy of the computations with fixed $k_{\min}$ and unit of length u .

The most accurate energy for the hydrogen 1s orbital is $E = -0.499996$ Ha, which has been computed with $L = 9$. The results for the calculated closed-shell atoms are presented in Table 4.1. The results for the open-shell atoms are presented in Table 4.2.

Table 4.1 Results from Hartree–Fock calculations for helium, beryllium, neon, magnesium, and argon. Deviation from the accurate value [23] is given in parentheses so that negative deviation means that the computed value is less than the accurate value.

	He	Be	Ne	Mg	Ar
E	-2.86157(11)	-14.571(3)	-128.45(10)	-198.8(9)	-525.8(11)
n_{iter}	21	23	31	27	25
ε_{1s}	-0.91793(3)	-4.7318(9)	-32.73(5)	-48.7(4)	-118.2(5)
ε_{2s}		-0.30925(2)	-1.928(3)	-3.75(2)	-12.29(4)
ε_{2p}			-0.8508(-4)	-2.287(-5)	-9.577(-6)
ε_{3s}				-0.2525(6)	-1.274(4)
ε_{3p}					-0.5916(-6)
$\langle 1s 2s \rangle$		-2.6×10^{-7}	-4.2×10^{-6}	-5.6×10^{-8}	-1.8×10^{-8}
$\langle 1s 3s \rangle$				-1.6×10^{-8}	-7.8×10^{-9}
$\langle 2s 3s \rangle$				-8.9×10^{-8}	-2.5×10^{-8}
$\langle 2p 3p \rangle$					-1.4×10^{-8}

Table 4.2 Results from Hartree-Fock calculations for lithium and sodium. Deviation from the accurate value [23] is given in parentheses so that negative deviation means that the computed value is less than the accurate value.

	Li	Na
E	-7.4321(7)	-161.3(6)
n_{iter}	17	27
ε_{1s}	-2.4775(3)	-40.2(3)
ε_{2s}	-0.196309(14)	-2.78(2)
ε_{2p}		-1.521(-3)
ε_{3s}		-0.1817(5)
$\langle 1s 2s \rangle$	-5.7×10^{-4}	-5.9×10^{-8}
$\langle 1s 3s \rangle$		-1.4×10^{-6}
$\langle 2s 3s \rangle$		-2.8×10^{-4}

5 EXACT PSEUDOPOTENTIAL

5.1 General

Suppose that we have a system consisting of a positively charged nucleus at the origin and N electrons. In the exact pseudopotential method, we choose a small radius r_0 so that inside the sphere with radius r_0 , the wavefunctions of the system are approximated by hydrogenic wavefunctions, and the actual computations are performed only for values $r \geq r_0$. Actually, we define a basis set for the half-infinite interval $[0, \infty]$ and make a change of the variables $s = r - r_0$. For Hartree–Fock calculations, the Slater integrals are computed by

$$\begin{aligned} \tilde{J}_{ab}^0(s) &= \frac{Q_{ab}}{s + r_0} + \frac{1}{s + r_0} \int_0^s \bar{P}_a(s') \bar{P}_b(s') ds' \\ &\quad + \int_s^\infty \frac{1}{s' + r_0} \bar{P}_a(s') \bar{P}_b(s') ds' \end{aligned} \quad (5.1)$$

where $s \geq 0$ and Q_{ab} is a system-dependent quantity that approximates the contribution of the EPP core region to the Slater integral.

Let $v(f)$ denote the coefficient vector $(\beta_{j,k})_{k=0}^{W-1}$ defined by Equation (3.64) and define

$$M(f) := \left(f(2^{-j}k) \delta_{k,k'} \right)_{k,k'=0}^{W-1, W-1} \quad (5.2)$$

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

5.2 Hydrogen-like Atoms

The Schrödinger equation of the hydrogen atom and Hartree–Fock equations of atoms [6] and their representation in the interpolating wavelet basis [1] denote our starting point. With a change in variables $s := r - r_0$, the Schrödinger equation of a

hydrogen-like atom in interval $r \geq r_0$ takes the form

$$\left(-\frac{1}{2} \frac{d^2}{ds^2} - \frac{Z}{s+r_0} + \frac{l(l+1)}{2(s+r_0)^2} \right) \bar{P}(s) = E\bar{P}(s), \quad s \geq 0 \quad (5.3)$$

where Z is the charge of the nucleus, l is the angular momentum quantum number, and $\bar{P}(s) = P(r_0 + s)$ for $s \geq 0$.

We define the second derivative filter by

$$a_k := \langle \tilde{\varphi}, D^2 \varphi(\cdot - k) \rangle \quad (5.4)$$

Matrix elements of the Laplacian operator L are computed by

$$L_{k,l} := \langle \tilde{\varphi}_{j,k}, L\varphi_{j,l}^\# \rangle = 2^{2j} \left(a_{l-k} + \sum_{\alpha=-D}^{-1} e_{\alpha,l}^\# a_{\alpha-k} \right) \quad (5.5)$$

for $0 \leq l \leq D$ and

$$L_{k,l} := \langle \tilde{\varphi}_{j,k}, L\varphi_{j,l} \rangle = 2^{2j} a_{l-k} \quad (5.6)$$

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

$$\hat{V}_{k,k} = V(2^{-j}k) \quad (5.7)$$

where

$$V(y) = -\frac{Z}{y+a} \quad (5.8)$$

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

5.3 Hartree–Fock Equations for Helium Atom

Define the Slater integrals as

$$\gamma_{ab}^0(r) = \int_{r'=0}^{\infty} P_a(r') \gamma(r, r') P_b(r') dr' \quad (5.9)$$

where a and b denote the atomic orbitals and

$$\gamma(r, r') = \frac{1}{\max\{r, r'\}}. \quad (5.10)$$

We use symbol y instead of Y to avoid confusion with spherical harmonics. By carrying out a similar change in 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

$$\left(-\frac{1}{2} \frac{d^2}{ds^2} - \frac{2}{s + r_0} + \gamma_{1s1s}^0(s + r_0) \right) \bar{P}_{1s}(s) = \varepsilon_{1s} \bar{P}_{1s}(s), \quad s \geq 0. \quad (5.11)$$

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

$$\left(-\frac{1}{2} \frac{d^2}{ds^2} - \frac{2}{s + r_0} + \gamma_{2s2s}^0(s + r_0) \right) \bar{P}_{1s}(s) = \varepsilon_{1s} \bar{P}_{1s}(s) \quad (5.12)$$

$$\left(-\frac{1}{2} \frac{d^2}{ds^2} - \frac{2}{s + r_0} + \gamma_{1s1s}^0(s + r_0) \right) \bar{P}_{2s}(s) = \varepsilon_{2s} \bar{P}_{2s}(s) \quad (5.13)$$

and for helium $1s2s$ ^3S configuration

$$\begin{aligned} \left(-\frac{1}{2} \frac{d^2}{ds^2} - \frac{2}{s + r_0} + \gamma_{2s2s}^0(s + r_0) \right) \bar{P}_{1s}(s) &= \varepsilon_{1s} \bar{P}_{1s}(s) + \\ &\quad \gamma_{1s2s}^0(s + r_0) \bar{P}_{2s}(s) \end{aligned} \quad (5.14)$$

$$\begin{aligned} \left(-\frac{1}{2} \frac{d^2}{ds^2} - \frac{2}{s + r_0} + \gamma_{1s1s}^0(s + r_0) \right) \bar{P}_{2s}(s) &= \varepsilon_{2s} \bar{P}_{2s}(s) + \\ &\quad \gamma_{2s1s}^0(s + r_0) \bar{P}_{1s}(s) \end{aligned} \quad (5.15)$$

5.4 EPP of Helium Atom

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

$$(\hat{U}_0 f)(s) = \int_0^s f(s') ds' \quad (5.16)$$

and

$$(\hat{U}_\infty f)(s) = \int_s^\infty f(s') ds' \quad (5.17)$$

Define $P_{1s,H}(r')$ and $P_{2s,H}(r')$ to be the hydrogenic orbitals of the helium atom. Then, we have

$$\langle \tilde{\varphi}_{j,k} \hat{U}_0 \varphi_{j,l} \rangle = 2^{-j} (\Phi(|k| - l) - \Phi(-l)) \quad (5.18)$$

and

$$\langle \tilde{\varphi}_{j,k} \hat{U}_\infty \varphi_{j,l} \rangle = 2^{-j} (1 - \Phi(|k| - l)) \quad (5.19)$$

where

$$\Phi(x) = \int_{-\infty}^x \varphi(\gamma) d\gamma. \quad (5.20)$$

The Slater integrals in the shifted variables are obtained from Equation (5.1) where we set

$$Q_{ab} := \frac{\bar{P}_a(0)}{P_{a,H}(r_0)} \frac{\bar{P}_b(0)}{P_{b,H}(r_0)} \int_0^{r_0} P_{a,H}(r') P_{b,H}(r') dr'. \quad (5.21)$$

for the helium ground state, and

$$Q_{ab} := \int_0^{r_0} P_{a,H}(r') P_{b,H}(r') dr'. \quad (5.22)$$

for the excited states of helium. Define

$$q(s) := \frac{1}{s + r_0} \quad (5.23)$$

and

$$S_0 := M(q) U_0 + U_\infty M(q). \quad (5.24)$$

Now,

$$v(\tilde{y}_{ab}^0) = Q_{ab} v(q) + S_0 (v(\bar{P}_a \star \bar{P}_b)) \quad (5.25)$$

where U_0 and U_∞ are the matrices of operators $\hat{U}_0$ and $\hat{U}_\infty$ in the basis set constructed in Section 3.7. We define $\mathbf{v}_a = v(\bar{P}_a)$ and $\mathbf{v}_b = v(\bar{P}_b)$. The matrix of the exchange integral operator

$$(\hat{K}_a \bar{P}_a)(s) := \tilde{y}_{ab}^0(s) \bar{P}_b(s) \quad (5.26)$$

is computed by

$$K_a := W_a + M(\mathbf{v}_b) S_0 M(\mathbf{v}_b) \quad (5.27)$$

The term $W_a \mathbf{v}_a$ approximates the first term in Equation (5.1) as a linear function of $\mathbf{v}_a$. For 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

$$\frac{Q_{ab}}{s + r_0} \bar{P}_b(s) \approx \frac{1}{s + r_0} \bar{P}_a(0) \left(\int_{s'=-r_0}^0 \left(1 + \frac{s'}{r_0} \right) P_{b,H}(s' + r_0) ds' \right) \bar{P}_b(s) \quad (5.28)$$

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 find the hydrogenic Slater integrals

$$\gamma_{1s1s,H}^0(r) = \frac{1}{r} - e^{-2Zr} \left(\frac{1}{r} + Z \right) \quad (5.29)$$

$$\gamma_{2s2s,H}^0(r) = \frac{1}{r} + e^{-Zr} \left(-\frac{Z^3}{8} r^2 - \frac{1}{4} Z^2 r - \frac{3Z}{4} - \frac{1}{r} \right) \quad (5.30)$$

$$\gamma_{1s2s,H}^0(r) = \frac{1}{27\sqrt{2}} (12Z^2 r + 8Z) e^{-3Zr/2} \quad (5.31)$$

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

$$\begin{aligned} \langle P_a | \gamma_{ab}^0 | P_b \rangle &\approx \left(\frac{\bar{P}_a(0)}{P_{a,H}(r_0)} \right)^2 \left(\frac{\bar{P}_b(0)}{P_{b,H}(r_0)} \right)^2 \\ &\cdot \int_{r'=0}^{r_0} P_{a,H}(r') \gamma_{ab,H}^0(r') P_{b,H}(r') dr' \\ &+ \int_{s=0}^{\infty} \bar{P}_a(s) \bar{\gamma}_{ab}^0(s) \bar{P}_b(s) ds \end{aligned} \quad (5.32)$$

for the helium ground state and

$$\begin{aligned} \langle P_a | \gamma_{ab}^0 | P_b \rangle &\approx \int_{r'=0}^{r_0} P_{a,H}(r') \gamma_{ab,H}^0(r') P_{b,H}(r') dr' \\ &+ \int_{s=0}^{\infty} \bar{P}_a(s) \bar{\gamma}_{ab}^0(s) \bar{P}_b(s) ds. \end{aligned} \quad (5.33)$$

for the excited states of helium.

5.5 Total Energy of Helium Atom

The total energy of the ground state of the helium atom is

$$E(\text{He } 1s^2) = 2\varepsilon_{1s} - \langle P_{1s} | \gamma_{1s1s}^0 | P_{1s} \rangle \quad (5.34)$$

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

$$\begin{aligned} E(\text{He } 1s2s \ ^1S) &= \varepsilon_{1s} + \varepsilon_{2s} \\ &\quad - \frac{1}{2} \langle P_{1s} | \gamma_{2s2s}^0 | P_{1s} \rangle - \frac{1}{2} \langle P_{2s} | \gamma_{1s1s}^0 | P_{2s} \rangle \end{aligned} \quad (5.35)$$

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

$$\begin{aligned} E(\text{He } 1s2s \ ^3S) &= \varepsilon_{1s} + \varepsilon_{2s} \\ &\quad - \frac{1}{2} \langle P_{1s} | \gamma_{2s2s}^0 | P_{1s} \rangle - \frac{1}{2} \langle P_{2s} | \gamma_{1s1s}^0 | P_{2s} \rangle \\ &\quad + \langle P_{1s} | \gamma_{1s2s}^0 | P_{2s} \rangle. \end{aligned} \quad (5.36)$$

5.6 Combination of EPP with Finite Difference Method

The Schrödinger and Hartree–Fock equations are converted to matrix equations using the biorthogonality relations of interpolating wavelets [1]. We compare these calculations with the Finite Difference Method, which is a straightforward method for solving differential equations. The spatial and time domains are discretized, and the derivative at a point is computed with a stencil applied to the nearby points. This way the differential equation is converted to a matrix equation. The Laplacian operator is approximated by

$$u''(x) \approx \frac{u(x-b) - 2u(x) + u(x+b)}{b^2} \quad (5.37)$$

where b is the discretization step size.

We discretize the Schrödinger Equation (5.3) at points $p_j = jb, j = 0, \dots, J+1$, where J is the number of actual numerical calculation points and $b \in \mathbb{R}_+$ is the grid spacing. We define the discretized potential by $v_j = \bar{V}(s_j)$. The boundary condition

at the end of the interval is set by $p_{J+1} = 0$. We have

$$-\frac{p_{j+1} + (-2 - 2b^2 v_j)p_j + p_{j-1}}{2b^2} = Ep_j \quad (5.38)$$

for $j = 2, \dots, J$. We handle case $j = 1$ by extrapolating p_0 linearly from p_1 and p_2 . We obtain $p_0 = 2p_1 - p_2$ from which it follows that $p_2 + (-2 - 2b^2 v_j)p_1 + p_0 = -2b^2 v_1 p_1$. Hence, the difference equation for $j = 1$ is

$$v_1 p_1 = Ep_1. \quad (5.39)$$

In order to discretize the exchange operator $\hat{K}_a$ we need to discretize the integral operators

$$(\hat{I}_g(f))(s) = \int_0^s g(s')f(s')ds' \quad (5.40)$$

and

$$(\hat{I}_g^{\text{compl}}(f))(s) = \int_s^\infty g(s')f(s')ds'. \quad (5.41)$$

We define

$$(I(g))_{j,k} := \begin{cases} hg_k; & k < j \\ 0; & k \geq j \end{cases} \quad (5.42)$$

and

$$(I^{\text{compl}}(g))_{j,k} := \begin{cases} hg_k; & k \geq j \\ 0; & k < j \end{cases} \quad (5.43)$$

where $g_k = g(s_k)$. When f is a real function, we define $w(f) := (f(s_k))_{k=1}^J$. Now, the matrix of the exchange integral operator is computed by

$$K_a := W_a + K_a^0 \quad (5.44)$$

where W_a is computed as in the case of wavelets,

$$K_a^0 := \text{diag}(w(f_1))I(\bar{P}_b) + I^{\text{compl}}(f_1 \star \bar{P}_b), \quad (5.45)$$

and

$$f_1(s) := \frac{1}{s + r_0}, \quad s \geq 0. \quad (5.46)$$

5.7 Results

We demonstrate the EPP method by performing calculations where the EPP radius r_0 and the basis size W are varied. We actually select a length scale $u = R/W$ and conduct a change of variables $s = us'$ in Equations (5.3) and (5.11)–(5.15). The length scale u specifies how many atomic units of length a length unit in our own coordinate system is. Here, R is the size of the computation domain. For hydrogen 1s, we have $R = 15$ a.u., for hydrogen 2s and 2p $R = 25$ a.u., for He 1s² $R = 15$ a.u., and for He 1s2s ¹S and ³S $R = 20$ a.u.. We also set $j = 0$ for the basis set (see Section 3.7), and hence u is equal to the grid spacing h_{EPP} .

The best of the calculated energies are presented in table 5.1. OIW means the interpolating wavelet Galerkin method that uses a pseudopotential to handle the singularity of the Coulomb potential. Using 200 basis functions for the helium ground state and computing the atom energies for $r_0 = 10^k$, $k = -10, \dots, -1$ shows that atom energies are equal up to seven decimal places for $r_0 \leq 10^{-6}$. Similar computation for the hydrogen 1s orbital shows that the H 1s energy is equal to -0.5 Ha up to seven decimal places for $r_0 \leq 0.01$. For hydrogen 2s and 2p, the corresponding limit is $r_0 \leq 0.01$, too.

We also found that when the number of basis functions is sufficiently large for a given system, there is an approximate threshold value so that reducing r_0 below it does not make the accuracy of the computed energy better. When the number of basis functions is sufficiently large and r_0 is sufficiently small, the hydrogenic orbitals are approximately continuous at r_0 .

Table 5.1 Hartree–Fock total energies of H and He occupation configurations. E_{ref} are chosen reference values. E_{EPP} is the energy given by the EPP–Galerkin-method, h_{EPP} is the grid spacing in the EPP–Galerkin method, E_{OIW} is the energy given by the OIW–Galerkin method, and E_{FDM} is the energy given by the Finite Difference Method. For EPP, the most accurate results are given. For OIW approach, the number of basis functions is 201 and the finest grid spacing is 0.00625 a.u.. The number of FDM computation points is 2001 for the second and third systems and 1001 for the other ones.

System	E_{ref}/Ha	E_{EPP}/Ha	$h_{\text{EPP}}/\text{a.u.}$	E_{OIW}/Ha	E_{FDM}/Ha
H 1s	$-0.5 *^{\dagger}$	-0.500000	0.075	-0.50	-0.49803
H 2s	$-0.125 *^{\dagger}$	-0.125000	0.125	-0.125	-0.124741
H 2p	$-0.125 *^{\dagger}$	-0.125000	0.125	-0.124998	-0.124995
He 1s ²	$-2.8616800^{\dagger}$ [23] $-2.903724 *$ [24]	-2.862	0.075	-2.834868	-2.839
He 1s2s ¹ S	-2.147° [25] $-2.145974 *$ [24]	-2.1531	0.1	-2.133579	-2.132
He 1s2s ³ S	-2.171° [25] $-2.175229 *$ [24]	-2.174	0.1	-2.154536	-2.155

* : exact energy; † : HF limit; $^{\circ}$: HF result.

6 CALCULATIONS OF ATOMS AND MOLECULES USING THREE-DIMENSIONAL DESLAURIERS–DUBUC WAVELETS

6.1 Interpolating Wavelet Basis Set

Let $n \in \mathbb{Z}_+$ be the dimensionality of the basis set. We use here $n = 3$ but this formulation works for other values of n , too. Let $j_{\min}$ and $j_{\max}$ be the minimum and maximum resolution levels of the point grid. Let

$$Z_j = \left\{ \frac{k}{2^j} \mid k \in \mathbb{Z} \right\} \quad (6.1)$$

and

$$V_j = Z_j^n \quad (6.2)$$

where $j \in \mathbb{Z}$. Define sets Q_j by

$$Q_{j_{\min}} = V_{j_{\min}} \quad (6.3)$$

$$Q_j = V_j \setminus V_{j-1} \text{ for } j > j_{\min} \quad (6.4)$$

The point grid G shall be some finite subset of $V_{j_{\max}}$. We define

$$G_j := G \cap Q_j \quad (6.5)$$

for $j \geq j_{\min}$. The functions $\varphi_{j,k}$ and $\psi_{j,k}$ are scaling functions and wavelets belonging to an interpolating wavelet family. Functions $\tilde{\varphi}_{j,k}$ and $\tilde{\psi}_{j,k}$ are dual basis functions of interpolating wavelets.

Define

$$\psi_{s,j,k} := \begin{cases} \varphi_{j,k}; & \text{if } s = 0 \\ \psi_{j,k}; & \text{if } s = 1 \end{cases} \quad (6.6)$$

$$\tilde{\psi}_{s,j,k} := \begin{cases} \tilde{\varphi}_{j,k}; & \text{if } s = 0 \\ \tilde{\psi}_{j,k}; & \text{if } s = 1 \end{cases} \quad (6.7)$$

and

$$\eta_{j,k} := \begin{cases} \varphi_{j_{\min},k}; & \text{if } j = j_{\min} \\ \varphi_{j-1,k/2}; & \text{if } j > j_{\min} \text{ and } k \text{ even} \\ \psi_{j-1,(k-1)/2}; & \text{if } j > j_{\min} \text{ and } k \text{ odd} \end{cases} \quad (6.8)$$

$$\tilde{\eta}_{j,k} := \begin{cases} \tilde{\varphi}_{j_{\min},k}; & \text{if } j = j_{\min} \\ \tilde{\varphi}_{j-1,k/2}; & \text{if } j > j_{\min} \text{ and } k \text{ even} \\ \tilde{\psi}_{j-1,(k-1)/2}; & \text{if } j > j_{\min} \text{ and } k \text{ odd} \end{cases} \quad (6.9)$$

When $\alpha \in Q_j$ and $j \geq j_{\min}$ define

$$\zeta_\alpha := \eta_{j,\mathbf{k}[1]} \otimes \cdots \otimes \eta_{j,\mathbf{k}[n]} \quad (6.10)$$

and

$$\tilde{\zeta}_\alpha := \tilde{\eta}_{j,\mathbf{k}[1]} \otimes \cdots \otimes \tilde{\eta}_{j,\mathbf{k}[n]} \quad (6.11)$$

where $\mathbf{k} = 2^j \alpha$. We also define

$$\varphi_{j,\mathbf{k}} := \varphi_{j,\mathbf{k}[1]} \otimes \cdots \otimes \varphi_{j,\mathbf{k}[n]} \quad (6.12)$$

where $j \in \mathbb{Z}$ and $\mathbf{k} \in \mathbb{Z}^n$.

We use notation

$$Z_\pm(n) := \{k \in \mathbb{Z} : |k| \leq n\} \quad (6.13)$$

in the definitions of basis functions sets.

Laplacian operator

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (6.14)$$

is approximated by linear operator $L = L^{(x)} + L^{(y)} + L^{(z)}$ where

$$L_{\alpha,\alpha'}^{(x)} = \int_{\mathbb{R}^3} \tilde{\zeta}_\alpha(\mathbf{x}) \frac{\partial^2}{\partial x^2} \zeta_{\alpha'}(\mathbf{x}) d\tau \quad (6.15)$$

$$L_{\alpha,\alpha'}^{(y)} = \int_{\mathbb{R}^3} \tilde{\zeta}_\alpha(\mathbf{x}) \frac{\partial^2}{\partial y^2} \zeta_{\alpha'}(\mathbf{x}) d\tau \quad (6.16)$$

$$L_{\alpha,\alpha'}^{(z)} = \int_{\mathbb{R}^3} \tilde{\zeta}_\alpha(\mathbf{x}) \frac{\partial^2}{\partial z^2} \zeta_{\alpha'}(\mathbf{x}) d\tau \quad (6.17)$$

for $\alpha, \alpha' \in G$.

6.2 Interpolating Wavelet Transforms

Let

$$f = \sum_{\alpha \in G} c_\alpha \zeta_\alpha \quad (6.18)$$

where $c_\alpha \in \mathbb{R}$ for all $\alpha \in G$. Let $c = (c_\alpha)_{\alpha \in G}$. Define $v = (v_\alpha)_{\alpha \in G}$ by setting

$$v_\alpha = f(\alpha). \quad (6.19)$$

We define forward wavelet transform U and backward wavelet transform W by setting $U(v) = c$ and $W(c) = v$. Mappings U and W are linear. We compute the forward wavelet transform U using an algorithm somewhat similar to [26]. Define matrix $P^{(j)}$ by

$$P_{\alpha,\beta}^{(j)} = \delta_{\alpha,\beta} \quad (6.20)$$

where $\alpha \in G_j$ and $\beta \in G$ and matrix $E^{(j)}$ by

$$E_{\alpha,\beta}^{(j)} = \delta_{\alpha,\beta} \quad (6.21)$$

where $\alpha \in G$ and $\beta \in G_j$. Define

$$W_{\alpha,\beta}^{(j,j')} = \zeta_\beta(\alpha) \quad (6.22)$$

where $\alpha \in G_j$ and $\beta \in G_{j'}$. See equation (6.5) for definition of G_j and equation (6.10) for definition of ζ_β . We have

$$W = \sum_{j=j_{\min}}^{j_{\max}} \sum_{j'=j_{\min}}^j E^{(j)} W^{(jj')} P^{(j')}. \quad (6.23)$$

For forward wavelet transform we have

$$U = \sum_{j=j_{\min}}^{j_{\max}} E^{(j)} U^{(j)} \quad (6.24)$$

$$U^{(j)} = J^{(j)} \left(P^{(j)} - \sum_{j'=j_{\min}}^{j-1} W^{(jj')} U^{(j')} \right), \quad (6.25)$$

for $j > j_{\min}$

$$U^{(j_{\min})} = P^{(j_{\min})} \quad (6.26)$$

$$J^{(j)} = \left(W^{(jj)} \right)^{-1} \quad (6.27)$$

When

$$f = \sum_{\beta \in G_j} c_\beta \zeta_\beta \quad (6.28)$$

we have

$$c_\alpha = \langle \zeta_\alpha f \rangle = \left\langle \zeta_\alpha \sum_{\beta \in G_j} f(\beta) \varphi_{j,2^j\beta} \right\rangle = \sum_{\beta \in G_j} \langle \zeta_\alpha \varphi_{j,2^j\beta} \rangle f(\beta). \quad (6.29)$$

Consequently

$$J_{\alpha,\beta}^{(j)} = \langle \zeta_\alpha \varphi_{j,2^j\beta} \rangle \quad (6.30)$$

and we do not have to invert matrix $W^{(jj)}$.

An operator representing pointwise multiplication of a function f by another in the given computation grid is

$$M = UDW \quad (6.31)$$

where D is a diagonal matrix with values of the function f at the grid points in the diagonal.

6.3 Constant and Interpolated Pseudopotentials

The Coulomb potential arising from a single nucleus is

$$V(r) = -\frac{Z}{r} \quad (6.32)$$

where Z is the charge of the nucleus.

We avoid the singularity by using a pseudopotential. We define c to be the cutoff point of the pseudopotential and D to be the degree of the interpolating polynomial used in the pseudopotential. Actually we use $c = 2^{-j_{\max}}$ where $j_{\max}$ is the highest resolution level in the wavelet basis. Parameter D has to be an odd integer and we define $n = (D + 1)/2$. We define

$$V_1(r) := -\frac{1}{r}, \quad r \geq 0, \quad (6.33)$$

$$\mathbf{s} := (-nc, -(n-1)c, \dots, -2c, -c, c, 2c, \dots, (n-1)c, nc), \quad (6.34)$$

and

$$\mathbf{t}[i] := V_1(\mathbf{s}[i]) \quad (6.35)$$

where $i = 1, \dots, 2n$. Let P be the interpolating polynomial of degree at most D having value $\mathbf{t}[i]$ at point $\mathbf{s}[i]$ for $i = 1, \dots, 2n$. Now we define the interpolated pseudopotential with

$$V_{\text{interp}}(r) := \begin{cases} V_1(r), & r \geq c \\ P(r), & r < c \end{cases} \quad (6.36)$$

The actual pseudopotential of a nucleus with charge Z and location $\mathbf{R}$ is then

$$V(\mathbf{r}) = ZV_{\text{interp}}(|\mathbf{r} - \mathbf{R}|). \quad (6.37)$$

Function V_{interp} with different values of c is plotted in Fig. 6.1. We may also use the cut pseudopotential defined by

$$V_{\text{cut}}(r) := \begin{cases} V_1(r), & r \geq c \\ -\frac{1}{c}, & r < c \end{cases} \quad (6.38)$$

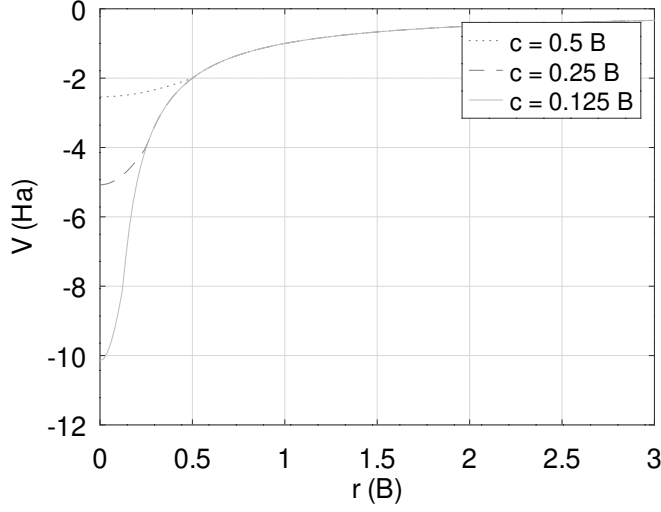


Figure 6.1 Pseudopotentials V_{interp} with $D = 7$. Parameter c is the cutoff value, see section 6.3.

where $c = 2^{-j_{\text{max}}-1}$.

6.4 HGH Pseudopotential

By using pseudopotentials the number of computed orbitals can be reduced and since the pseudo wavefunctions are smoother than all-electron wavefunctions the basis function set can also be reduced. In a pseudopotential computation only the valence electrons are actually computed and the effect of the core electrons is handled by replacing the nuclear potential with a pseudopotential. We use the Hartwigsen-Goedecker-Hutter (HGH) pseudopotential [27, 28] in these computations.

The HGH pseudopotential consists of a local and nonlocal part. The local part is a function of the position as the nuclear potential. The nonlocal part is a linear operator and it is not a function of position. The local pseudopotential is given by

$$V_{\text{loc}}(r) = \frac{-Z_{\text{ion}}}{r} \text{erf}\left(\frac{r}{\sqrt{2}\eta_{\text{loc}}}\right) + \exp\left(-\frac{1}{2}\left(\frac{r}{\eta_{\text{loc}}}\right)^2\right) \times \left(C_1 + C_2\left(\frac{r}{\eta_{\text{loc}}}\right)^2 + C_3\left(\frac{r}{\eta_{\text{loc}}}\right)^4 + C_4\left(\frac{r}{\eta_{\text{loc}}}\right)^6\right) \quad (6.39)$$

where r is the distance from the nucleus. Note that

$$\lim_{r \rightarrow 0} \frac{-Z_{\text{ion}}}{r} \operatorname{erf}\left(\frac{r}{\sqrt{2}r_{\text{loc}}}\right) = \frac{-Z_{\text{ion}}}{r_{\text{loc}}} \sqrt{\frac{2}{\pi}} \quad (6.40)$$

and the local pseudopotential is defined at the origin (nucleus), too.

The nonlocal pseudopotential is defined by

$$V_{\text{nonlocal}}[\phi] = \mathbf{r} \in \mathbb{R}^3 \mapsto \sum_l \int V_l(\mathbf{r}, \mathbf{r}') \phi(\mathbf{r}') d^3 \mathbf{r}' \quad (6.41)$$

where

$$V_l(\mathbf{r}, \mathbf{r}') = \sum_{i=1}^3 \sum_{j=1}^3 \sum_{m=-l}^l Y_{l,m}(\hat{\mathbf{r}}) p_i^l(r) b_{i,j}^l p_j^l(r') Y_{l,m}^*(\hat{\mathbf{r}}') \quad (6.42)$$

for each nucleus. The origin of the coordinate system in (6.42) is located at the nucleus. The functions p_i^l are defined by

$$p_i^l(r) = \frac{\sqrt{2} r^{l+2(i-1)} \exp\left(-\frac{r^2}{2r_l^2}\right)}{r_l^{l+(4i-1)/2} \sqrt{\Gamma\left(l + \frac{4i-1}{2}\right)}} \quad (6.43)$$

where parameter r_l is given in Bohrs. The range of values l is determined by the actual pseudopotential. The spherical harmonics $Y_{l,m}$ in equation (6.42) can be replaced by orthonormal linear combinations of $Y_{l,m}$, $m = -l, \dots, l$. This allows us to avoid computation with complex valued functions.

6.5 Atomic and Molecular Orbitals

The grid spacing for a wavelet basis is defined to be $g = 2^{-j_{\text{max}}} a$ where j_{max} is the maximum resolution level in the basis and a is the size of one unit in resolution level 0 in the wavelet basis in atomic units.

The data presented in the tables in this article was obtained from our own software (denoted by TH), our own computations with BigDFT [28, 29], and CCCBDB [30]. BigDFT is a quantum mechanical computation package using Daubechies wavelets. CCCBDB is large database containing atomic and molecular data. The CCCBDB energies and internuclear distances in this article use the STO-3G basis

set. Quantity g is the distance between grid points in the highest resolution level and quantity d is the distance between the nuclei in the result tables. E_{system} is the total energy of the system and E_{binding} is the binding energy. Note that the total energy does not include the energies of the core electrons in the lithium hydride HGH computations.

When binding energies of molecules were computed the energies of atoms were usually computed with the same basis set as the molecule. When the basis was unsymmetric it was modified. For example, grid $Z_{\pm}(4) \times Z_{\pm}(4) \times Z_{\pm}(10)$ becomes $Z_{\pm}(4) \times Z_{\pm}(4) \times Z_{\pm}(4)$ for the atoms.

The results for hydrogen atom ground state are presented in Table 6.1. The calculation of hydrogen excited states uses HGH pseudopotential and grid spacing $g = 0.25$ B. Results are presented in Table 6.2. The names of the excited states were obtained by computing inner products between the computed states and analytical states. The resulting orbitals are approximately orthonormal and the computed 2p states are approximately linear combinations of the analytical 2p states.

Helium atom has been computed using the HGH pseudopotential. Results are presented in Table 6.3. Grid spacing $g = 0.5$ B does not give sensible results with the HGH pseudopotential. We suppose that Froese Fischer’s results [23] can be regarded as the Hartree–Fock limit for helium. The computed total energies of the helium atom are quite good.

We calculated the hydrogen molecule with the interpolated and HGH pseudopotentials. The computation results for the hydrogen molecule are presented in Table 6.4. The resulting dissociation curve with the HF method, HGH pseudopotential, and grid spacing $g = 0.25$ B is plotted in Fig. 6.2. When the HGH pseudopotential was used the computation worked for grid spacing $g = 0.25$ B but did not work for spacing $g = 0.5$ B. The minimum energy of the curve is $E_0 = -1.188$ Ha and it is located at internuclear distance $d_0 = 1.398$ B. The corresponding values for the BigDFT reference curve are $E_0 = -1.132$ Ha and $d_0 = 1.385$ B. The results for the hydrogen molecule ion are presented in Table 6.5.

The calculations for lithium hydride molecule are presented in Table 6.6. Grid spacing $g = 0.5$ B did not yield a physical dissociation curve for the HGH pseudopotential. Neither $g = 0.5$ B nor $g = 0.25$ B yielded a physical dissociation curve for the interpolated pseudopotential. The dissociation curve of lithium hydride computed with the Hartree–Fock method and grid spacing $g = 0.25$ B is plotted in Fig. 6.3.

Table 6.1 Total energy of the hydrogen atom. Quantity g is the distance between grid points in the highest resolution level. “TH” means this work.

source	g (B)	pseudopot.	E (Ha)
TH	0.125	const.	-0.496380
TH	0.125	interp.	-0.493471
TH	0.125	HGH	-0.499899
CCCBDB [30]			-0.466582
BigDFT [28, 29]		HGH	-0.499969
exact		none	-0.5

Table 6.2 Hydrogen atom orbital energies with the HGH pseudopotential. We labelled the resulting $2p$ orbitals with a, b, and c. All the orbitals presented are approximately orthogonal.

Orbital	Computed energy (Ha)	Exact energy (Ha)
1s	-0.499295	-0.5
2s	-0.120957	-0.125
2p _a	-0.123045	-0.125
2p _b	-0.123045	-0.125
2p _c	-0.123045	-0.125

The minimum energy of the curve is $E_0 = -0.817$ Ha and it is located at internuclear distance $d_0 = 2.880$ B. The corresponding values for the BigDFT reference curve are $E_0 = -0.760$ Ha and $d_0 = 2.921$ B.

Note that having no more than two resolution levels in the basis makes the computation of the Laplacian operator simpler and faster, because in that case the $s(\dots)$ terms in the Laplacian operator, formulas (60) – (62) in publication IV, are either Kronecker deltas or zero.

Table 6.3 Energetics of the helium atom. All our and BigDFT computations use HGH pseudopotential. “TH” means this work.

source	g (B)	exchange potential	E (Ha)	E_{orb} (Ha)
TH	0.25	HF	-2.901180	-0.970247
TH	0.25	LDA	-2.819951	-0.628152
TH	0.125	HF	-2.916129	-0.974768
CCCBDB [30]		HF	-2.807584	
CCCBDB [30]		LSDA	-2.809599	
BigDFT [28, 29]		HF	-2.862303	
BigDFT [28, 29]		LDA	-2.833895	
HF limit [23]		HF	-2.862	-0.918

Table 6.4 Hydrogen molecule. “TH” means this work.

source	g (B)	pseudopot. interp.	exch.	E_{system} (Ha)	E_{binding} (Ha)	d (B)
TH	0.125	interp.	HF	-1.186176	0.210390	1.454593
TH	0.25	HGH	HF	-1.187995	0.189405	1.397991
TH	0.20	HGH	HF	-1.188547	0.189383	1.389890
TH	0.25	HGH	LDA	-1.155960	0.157378	1.485851
CCCBDB [30]			HF	-1.117506	0.184342	1.345
CCCBDB [30]			LSDA	-1.157014	0.248654	1.391
BigDFT [28, 29]		HGH	HF	-1.133393	0.133455	1.386175
BigDFT [28, 29]		HGH	LDA	-1.136870	0.136932	1.445097
experimental [31, chapter 5.2]					0.166	1.40

Table 6.5 Hydrogen molecule ion. The analytical results are equal to the experimental results. “TH” means this work.

source	g (B)	pseudopot.	E_{system} (Ha)	E_{binding} (Ha)	d (B)
TH	0.125	interp.	-0.589135	0.101242	2.015143
TH	0.125	HGH	-0.602448	0.102549	1.999338
CCCBDB [30]			-0.582697	0.116115	2.005
BigDFT [28, 29]		HGH	-0.602489	0.102520	1.995677
exp. [31]				0.103	2.00

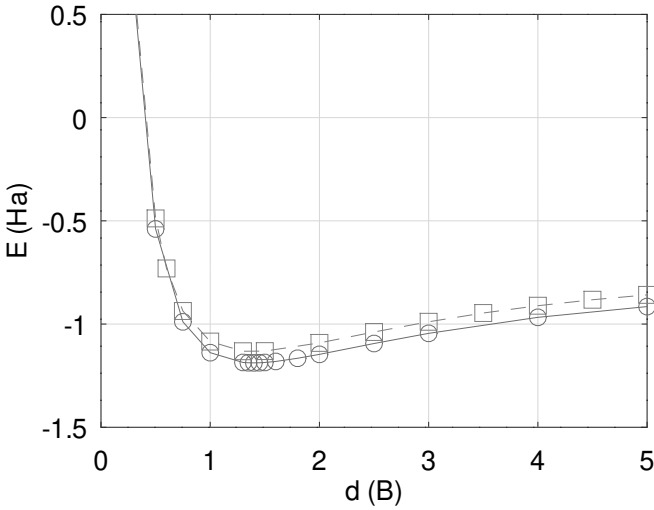


Figure 6.2 Energy of H_2 as a function of internuclear distance calculated with Hartree–Fock method and HGH pseudopotential. The solid line is our computation with interpolating wavelets and grid spacing $g = 0.25$ B and the dashed line is computed with BigDFT and (fine) grid spacing $g = 0.225$ B.

Table 6.6 Lithium hydride molecule. All our and BigDFT computations were done with the HGH pseudopotential. The CCCBDB all-electron total energies are not presented in the table. “TH” means this work.

source	a (B)	g (B)	exch.	E_{system} (Ha)	E_{binding} (Ha)	d (B)
TH	1.0	0.25	HF	-0.817030	0.116686	2.880018
TH	1.0	0.25	LDA	-0.809904	0.109560	3.013474
TH	0.4	0.2	HF	-0.817007	0.116370	2.863496
CCCBDB [30]			HF		0.081274	2.855
CCCBDB [30]			LSDA		0.135698	2.899
BigDFT [28, 29]			HF	-0.760938	0.059911	2.866004
BigDFT [28, 29]			LDA	-0.776416	0.075389	2.930745

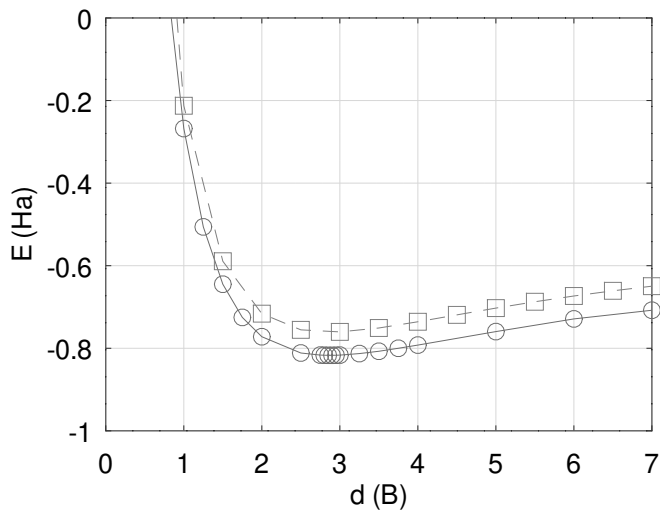


Figure 6.3 Total energy of the lithium hydride molecule as a function of the internuclear distance calculated with the Hartree–Fock method and HGH pseudopotential. The solid line has been computed with interpolating wavelets and grid spacing $g = 0.25$ B and the dashed line with BigDFT and (fine) grid spacing $g = 0.225$ B.

7 FOURIER TRANSFORM AND WAVELET APPROACHES TO THE PATH INTEGRAL FORMULATION

7.1 Stationary State Energies and Wavefunctions

Fourier transform has been used to determine the energy spectrum of a quantum mechanical system with path integral formulation *e.g.* by Gholizadehkalkhoran *et al.* [32].

A stationary state ψ of a quantum mechanical system can be represented by

$$\psi(\mathbf{x}) = \sum_{k=0}^{\infty} c_k f_k(\mathbf{x}) \quad (7.1)$$

where functions f_k are the eigenstates of the Hamiltonian operator of the system and c_k are complex numbers. The time evolution of the stationary states is given by

$$\Psi(\mathbf{x}, t) = \sum_{k=0}^{\infty} c_k \exp(-iE_k t) f_k(\mathbf{x}) \quad (7.2)$$

where E_k are the energies of the eigenstates. Suppose that we have a fixed point $\mathbf{x}_0 \in \mathbb{R}^d$ and define $g(t) := \Psi(\mathbf{x}_0, t)$. By making a Fourier transform of eq. (7.2) we obtain

$$\hat{g}(\omega) = \sqrt{2\pi} \sum_{k=0}^{\infty} c_k f_k(\mathbf{x}_0) \delta(\omega + E_k). \quad (7.3)$$

Thus, we may compute the eigenenergies of the system from the Fourier spectrum of function g .

The initial function of the time evolution should be chosen so that it has a broad Fourier spectrum and it should also contain both even and odd terms. So we chose to

approximate the sum of delta function and its derivative at the origin with a scaling function centred at the origin and its derivative in the one-dimensional case. In some calculations we use function $-\varphi_{j_{\min},-1} + \varphi_{j_{\min},1}$ instead of the derivative. In three dimensions we use the tensor products of functions $(-1 - i)\varphi_{j_{\min},-1} + (1 + i)\varphi_{j_{\min},0} + (1 + i)\varphi_{j_{\min},1}$.

Let $\mathbf{x}_j, j = 1, \dots, N$ be the points where we calculate the wavefunction of state k . Let $g_j(t) := \Psi(\mathbf{x}_j, t)$ and ΔE be the spacing between points in the Fourier spectrum $\hat{g}_j(E)$. Let $d_{k,j} = |c_k f_k(\mathbf{x}_j)|^2$ be the undefined variables. Define

$$p_{k,j} = |\hat{g}_j(-E_k)|^2 \quad (7.4)$$

and

$$p'_{k,j} = \frac{1}{2} \left(|\hat{g}_j(-E_k + \Delta E)|^2 + |\hat{g}_j(-E_k - \Delta E)|^2 \right). \quad (7.5)$$

Now, we fit peak k to the Lorentzian distribution

$$L_{k,j}(E) = \frac{1}{\pi} \frac{\gamma_{k,j}}{(E + E_k)^2 + \gamma_{k,j}^2} \quad (7.6)$$

by setting

$$p_{k,j} = d_{k,j} L_{k,j}(-E_k) = d_{k,j} \frac{1}{\pi} \frac{1}{\gamma_{k,j}} \quad (7.7)$$

and

$$p'_{k,j} = d_{k,j} L_{k,j}(-E_k + \Delta E) = d_{k,j} \frac{1}{\pi} \frac{\gamma_{k,j}}{\Delta E^2 + \gamma_{k,j}^2}. \quad (7.8)$$

It follows that

$$d_{k,j} = \pi \gamma_{k,j} p_{k,j} \quad (7.9)$$

where

$$\gamma_{k,j} = \sqrt{\frac{q_{k,j}}{1 - q_{k,j}}} |\Delta E| \quad (7.10)$$

and

$$q_{k,j} = \frac{p'_{k,j}}{p_{k,j}}. \quad (7.11)$$

Note that $|\hat{g}_j(E)|^2$ is the Fourier transform of the autocorrelation function of $g_j(t)$ multiplied by a constant.

We assume that the potential V does not depend on time in the sequel. We ap-

proximate the kernel (2.52) by setting $N = 2$ and we have

$$K_2(\mathbf{x}_b, \mathbf{x}_a; \varepsilon) := \left(\frac{m}{2\pi i \varepsilon} \right)^d \int_{\mathbb{R}^d} \exp(iS_2) d\mathbf{x}_1. \quad (7.12)$$

We get

$$K_2(\mathbf{x}_b, \mathbf{x}_a; \varepsilon) = \left(\frac{m}{2\pi i \varepsilon} \sqrt{2\pi} \right)^d \exp \left(i \left(\frac{m}{2\varepsilon} (\mathbf{x}_b^2 + \mathbf{x}_a^2) - \varepsilon V(\mathbf{x}_b) \right) \right) \hat{b} \left(\frac{m}{\varepsilon} (\mathbf{x}_b + \mathbf{x}_a) \right) \quad (7.13)$$

where

$$b(\mathbf{x}_1) := \exp \left(i \left(\frac{m}{\varepsilon} \mathbf{x}_1^2 - \varepsilon V(\mathbf{x}_1) \right) \right). \quad (7.14)$$

We call kernel (7.13) the *midpoint kernel*.

If function b is radially symmetric (*i.e.* the potential is radially symmetric) we have

$$\hat{b}(\mathbf{k}) = \frac{i}{2k} \left(\hat{f}(k) - \hat{f}(-k) \right), \quad (7.15)$$

where $f(r) = r b_{\text{rad}}(|r|)$ and $b(\mathbf{r}) = b_{\text{rad}}(|\mathbf{r}|)$. Note that the Fourier transform of f in equation (7.15) is one-dimensional.

7.2 Quantum Harmonic Oscillator and Hydrogen-like Atom

The potential of the one-dimensional harmonic oscillator is

$$V(x) = \frac{m\omega_0^2}{2} x^2 \quad (7.16)$$

where m is the mass of the particle and ω_0 is the angular frequency. The potential of the isotropic three-dimensional harmonic oscillator is

$$V(\mathbf{x}) = \frac{m\omega_0^2}{2} |\mathbf{x}|^2. \quad (7.17)$$

The kernel for the one-dimensional harmonic oscillator can be computed exactly [10]. We have

$$K(x_b, x_a; t) = \left(\frac{m\omega_0}{2\pi i \sin(\omega_0 t)} \right)^{1/2} \exp(iS_{\text{cl}}), \quad (7.18)$$

where S_{cl} is the classical action given by

$$S_{\text{cl}} = \frac{m\omega_0}{2 \sin(\omega_0 t)} ((x_b^2 + x_a^2) \cos(\omega_0 t) - 2x_b x_a). \quad (7.19)$$

By substituting the potential of the one-dimensional harmonic oscillator to equation (7.14) we obtain

$$b(x_1) = \exp \left(i \frac{m}{\varepsilon} \left(1 - \frac{\omega_0^2}{2} \right) x_1^2 \right). \quad (7.20)$$

Define

$$a := \frac{m}{\varepsilon} \left(1 - \frac{\omega_0^2}{2} \right) \quad (7.21)$$

and assume that $a > 0$. Now

$$\hat{b}(k) = \frac{1}{2} (1 + i) \frac{1}{\sqrt{a}} \exp \left(-i \frac{k^2}{4a} \right). \quad (7.22)$$

Similarly, in the three-dimensional case we have

$$\hat{b}(\mathbf{k}) = \frac{1}{4} (-1 + i) a^{-3/2} \exp \left(-i \frac{k^2}{4a} \right) \quad (7.23)$$

using equation (7.15).

The potential of a hydrogen-like atom is

$$V(x) = -\frac{Z}{|x|} \quad (7.24)$$

in one dimension and

$$V(\mathbf{x}) = -\frac{Z}{|\mathbf{x}|} \quad (7.25)$$

in three dimensions. Here Z is the atomic number.

7.3 Wavelet Bases

7.3.1 Interpolating Wavelets

We construct the basis set as in section 6.1. The interpolating mother scaling function can be represented as [16, 2]

$$\varphi(x) = \sum_{\alpha \in \mathbb{Z}} s[\alpha] \varphi(2^J x - \alpha) \quad (7.26)$$

where J is some nonnegative integer and $s[\alpha]$, $\alpha \in \mathbb{Z}$, are constants that depend on the mother scaling function and J . We define $s_0[\alpha]$ to be the coefficients for J and $s_1[\alpha]$ for $J - 1$.

The matrix of the time evolution operator in the interpolating wavelet basis is Note that the dual wavelets $\tilde{\zeta}_{\mathbf{r}}$ are finite sums of delta distributions and consequently the integration over $\mathbf{y}$ is actually a weighted sum of values of the function

$$\int_{\mathbb{R}^d} K(\mathbf{y}, \mathbf{x}) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x}$$

in finite number of points $\mathbf{y}$. When $\mathbf{r} = 2^{-j_{\min}} \ell \in G_{j_{\min}}$ we have

$$K_{\mathbf{r}, \mathbf{q}} = \int_{\mathbb{R}^d} K(2^{-j_{\min}} \ell, \mathbf{x}) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x}. \quad (7.27)$$

In one-dimensional case the integral over x is approximated by

$$\int_{\mathbb{R}} K(y, x) \zeta_q(x) dx \approx 2^{-j_{\min} - J} \sum_{p \in \mathbb{Z}} K(y, 2^{-j_{\min} - J} p) s_{t(q)}(p - 2^{J-t(q)} k) \quad (7.28)$$

where $k \in \mathbb{Z}$, $q = 2^{-j_{\min}} k \in G_{j_{\min}}$ or $q = 2^{-j_{\min} - 1} k \in G_{j_{\min} + 1}$, and

$$t(q) := \begin{cases} 1 & \text{if } q \in G_{j_{\min} + 1} \\ 0 & \text{if } q \in G_{j_{\min}}. \end{cases} \quad (7.29)$$

For the three-dimensional case define

$$t_i(\mathbf{q}) := \begin{cases} 1 & \text{if } \mathbf{q} \in G_{j_{\min}+1} \text{ and } 2^{j_{\min}+1}\mathbf{q}[i] \text{ odd} \\ 0 & \text{otherwise} \end{cases} \quad (7.30)$$

for $i = 1, 2, 3$ and $\mathbf{t}(\mathbf{q}) := (t_1(\mathbf{q}), t_2(\mathbf{q}), t_3(\mathbf{q}))$. Define also

$$s_{\mathbf{t}}(\mathbf{z}) := s_{t[1]}(\mathbf{z}[1])s_{t[2]}(\mathbf{z}[2])s_{t[3]}(\mathbf{z}[3]). \quad (7.31)$$

Now we can approximate

$$\int_{\mathbb{R}^3} K(\mathbf{y}, \mathbf{x}) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x} \approx 2^{-3(j_{\min}+J)} \sum_{\mathbf{p} \in \mathbb{Z}^3} K(\mathbf{y}, 2^{-j_{\min}-J}\mathbf{p}) s_{\mathbf{t}(\mathbf{q})}(\mathbf{p} - \mathbf{w} \cdot \mathbf{k}) \quad (7.32)$$

where $\mathbf{k} \in \mathbb{Z}^3$ and $\mathbf{q} = 2^{-j_{\min}}\mathbf{k} \in G_{j_{\min}}$ or $\mathbf{q} = 2^{-j_{\min}-1}\mathbf{k} \in G_{j_{\min}+1}$, and $\mathbf{w} := (2^{J-t_1(\mathbf{q})}, 2^{J-t_2(\mathbf{q})}, 2^{J-t_3(\mathbf{q})})^T$. We pick some value $J_0 \geq 2$ and for $\mathbf{r} \in G_{j_{\min}+1}$ we use value $J = J_0 - 1$ in equation (7.26) and $J = J_0$ otherwise. The lower accuracy is used because the matrix elements where $\mathbf{q}$ belongs to the finer grid are significantly more complex to compute as the ones in the coarser grid.

We use 8th order Deslauriers–Dubuc wavelets for one-dimensional calculations and 4th order functions for three-dimensional calculations.

7.3.2 Orthonormal Wavelets

See [15] for more information on orthonormal wavelets. We define the basis indices by $I = I_{j_{\min}} \cup I_{j_{\min}+1}$ where $I_j = \{(j, k) : k \in K_j\}$ and K_j is a finite set of integer numbers (usually a range of integers). Now the basis functions are defined by

$$\zeta_{j,k} = \begin{cases} \varphi_{j_{\min},k} = 2^{j/2} \varphi(2^j \cdot -k) & j = j_{\min} \\ \psi_{j-1,k} = 2^{(j-1)/2} \psi(2^{j-1} \cdot -k) & j > j_{\min} \end{cases} \quad (7.33)$$

where $(j, k) \in I$, φ is the mother scaling function of the wavelet family, and ψ is the mother wavelet of the wavelet family. The matrix elements of the time-evolution operator are given by

$$K_{j,k,j',k'} = \int_{\mathbb{R}} \int_{\mathbb{R}} \zeta_{j,k}(y) K(y, x) \zeta_{j',k'}(x) dx dy \quad (7.34)$$

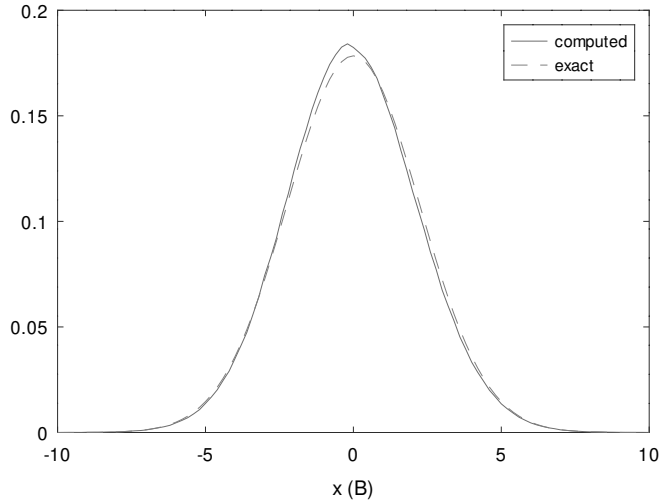


Figure 7.1 Probability density function $|\psi(x)|^2$ of the one-dimensional harmonic oscillator computed with the exact kernel.

with orthonormal wavelets. We use the 20th order Daubechies wavelets in this study. We use only one-dimensional orthonormal wavelets.

7.4 Application to the Harmonic Oscillator and Hydrogen Atom

Unless otherwise stated the calculations use Deslauriers–Dubuc wavelets.

We make calculations for the one-dimensional harmonic oscillator with the exact kernel, Trotter kernel, and midpoint kernel. We compute all these systems with both one and two resolution levels of the basis functions for $\Delta t = 1.0$ a.u. and one resolution level for $\Delta t = 0.5$ a.u. and $\Delta t = 0.25$ a.u. The mass of the particle is 1 a.u. and the angular frequency 0.1 radians. All these calculations yield the ground state energy 0.050265 Ha and first excited state 0.150796 Ha or 0.149226 Ha. We use the basis $(1/4)\{-48, \dots, 48\}$ for one-level calculations and $(1/4)\{-48, \dots, 48\} \cup (1/8)\{-5, \dots, 5\}$ for two-level calculations. We use scaling function resolution $J = 3$. Both of these calculations use two resolution levels. The wavefunction of the one-dimensional harmonic oscillator calculated with the method described in section 7.1 is plotted in Fig. 7.1.

When the Deslauriers–Dubuc (interpolating) wavelets are used for the hydrogen atom the calculations work for parameter $\Delta t = 1$ a.u. but not for $\Delta t = 0.5$ a.u. So we calculated this system with Daubechies (orthonormal) wavelets using both

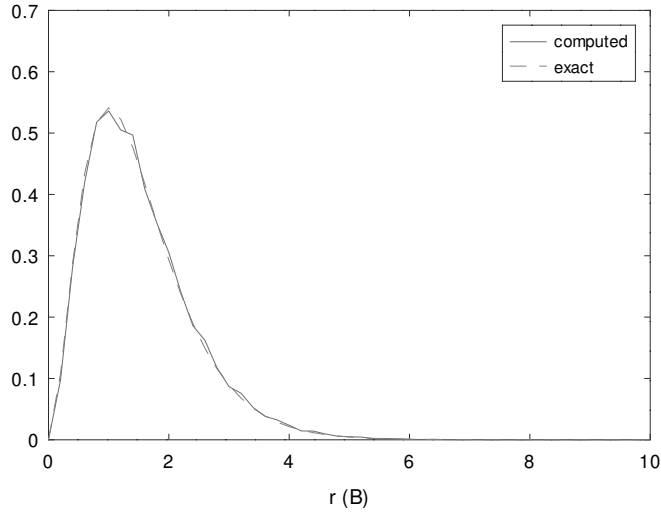


Figure 7.2 Radial probability density function $|P_{1s}(r)|^2$ of the hydrogen atom computed with the midpoint kernel in one dimension.

Trotter and midpoint kernels. For one resolution level calculations we use the basis $\{(2, -48), \dots, (2, 48)\}$ and for the two-level calculations $\{(1, -24), \dots, (1, 24)\} \cup \{(2, -6), \dots, (2, 6)\}$. We set the mother scaling function resolution to $J = 5$. We found that for the same time parameter the midpoint kernel yields usually better energy compared to the Trotter kernel but the Trotter kernel accepts smaller time parameters. The best energy for the Trotter kernel is $E_0 = -0.502655$ Ha and if the energies smaller than the exact energy are neglected we get $E_0 = -0.494801$ Ha. The best energy for the midpoint kernel is $E_0 = -0.496372$ Ha. The radial probability density function of the hydrogen atom calculated in one dimension with the method described in section 7.1 is plotted in Fig. 7.2.

We make calculations for the three-dimensional harmonic oscillator using the midpoint kernel and the Trotter kernel. The mass of the particle is 1 a.u. and the angular frequency 0.1 radians. We use basis $\{-10, \dots, 10\}^3$ and mother scaling function resolution $J = 2$. The resulting ground state energy for the midpoint kernel is $E_0 = 0.150796$ Ha and the first excited state $E_1 = 0.249757$ Ha for $\Delta t = 4.0$ a.u.. For $\Delta t = 2.0$ a.u. the energies are $E_0 = 0.150796$ Ha and $E_1 = 0.251327$ Ha. The energy spectrum for $\Delta t = 2.0$ a.u. is plotted in Fig. 7.3. For the Trotter kernel the energies are $E_0 = 0.150796$ Ha and $E_1 = 0.251327$ Ha for both $\Delta t = 4.0$ a.u. and $\Delta t = 2.0$ a.u..

We make three-dimensional calculations of the hydrogen atom using the mid-

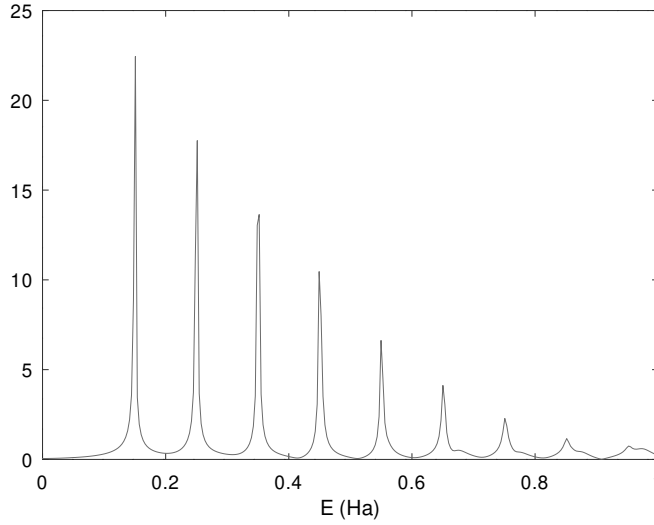


Figure 7.3 Energy spectrum of the three-dimensional harmonic oscillator calculated with the midpoint kernel.

point kernel and the Trotter kernel. The basis function set is $(1/2)\{-9, \dots, 9\} \cup (1/4)\{-4, \dots, 4\}$. The function $\hat{b}(\mathbf{k})$ for the midpoint kernel is calculated with formula (7.15). We have to invert the sign of the midpoint kernel (7.13) in order to get the energy computation to work. We get energy $E = -0.474380$ Ha for the midpoint kernel with parameter $\Delta t = 2.0$ a.u. and value $\Delta t = 1.5$ a.u. does not yield reasonable results. For the Trotter kernel we get $E = -0.477522$ Ha with parameter $\Delta t = 0.2$ a.u. and value $\Delta t = 0.125$ a.u. does not give reasonable results.

Note that we get exactly the same energy values for many different calculations because the energy spectrum $\hat{g}(-E)$ is approximated by the Discrete Fourier Transform, for which the energy values are discrete. Ruokosenmäki [13] has discussed the behavior of the path integral kernel with small values of Δt , too. It turned out that when the time step parameter Δt is the same the midpoint kernel gives usually better energy than the Trotter kernel for the hydrogen atom (one and three dimensions) but the Trotter kernel accepts smaller values for Δt . The two kernels yield approximately the same energy for the harmonic oscillator.

8 CONCLUSIONS

We have solved numerically the radial Schrödinger equations of hydrogen-like atoms and HF equations of several many-electron atoms: hydrogen, helium, beryllium, neon, magnesium, argon, lithium, and sodium. The results were very accurate and the approach worked for open-shell atoms, too, even though the nondiagonal Lagrange multipliers in the HF equations were neglected. We were able to derive analytical formulas for all the relevant matrix elements and we developed an algorithm for converting a matrix in nonstandard operator form to the standard operator form.

Multivariate compactly supported interpolating multiresolution analyses of spaces $C_u(\mathbb{R}^n, K)$ and $C_0(\mathbb{R}^n, K)$ were introduced. Here $K = \mathbb{C}$ or $K = \mathbb{R}$. We also defined compactly supported interpolating wavelets on the half-infinite real interval. We generalized the Besov-space norm equivalence from Donoho [17] to multiple dimensions, too.

The Exact Pseudopotential approach was applied to wavelet-Galerkin and Finite Difference methods. We calculated ground states of hydrogen and helium atoms and helium excited states $\text{He } 1s2s \ ^1S$ and $\text{He } 1s2s \ ^3S$. The numerical results were good. It turned out that the EPP Hartree–Fock energy of configuration $\text{He } 1s2s \ ^1S$ was lower than the exact energy including correlations. This has been observed earlier in Ref. [25], and Cohen and Kelly [33] have shown that the reason is the nonorthogonality of this particular state and the ground state $1s^2 \ ^1S$. The EPP wavelet-Galerkin method gave notably better results than the ordinary wavelet-Galerkin method described in chapter 4 and the EPP Finite Differences method. We assume that the reason for the first case is that we have computation grid points considerably closer to the origin in the EPP wavelet-Galerkin method compared to the ordinary wavelet-Galerkin method.

Atoms and diatomic molecules were calculated using three-dimensional Deslauriers–Dubuc wavelet basis. We used dual wavelets to evaluate the necessary matrix elements, which allowed us to neglect the overlap integrals. We computed the energet-

ics of the hydrogen and helium atoms, hydrogen molecule ion, hydrogen molecule, and lithium hydride molecule. The internuclear equilibrium distance is determined for the molecules, too. We obtained good numerical results for all the calculated systems.

We developed the midpoint kernel and an algorithm to compute the wavefunction of a system using path integral formulation. The energies of one and three dimensional harmonic oscillator and hydrogen atom in one and three dimensions were calculated using the path integral formulation. For the one-dimensional systems we computed the wavefunctions, too.

We conclude that the Deslauriers–Dubuc wavelets form a good basis set for calculations of wavefunctions of electronic systems using the Galerkin method. In some cases the Daubechies wavelets give better results but calculation of matrix elements of the potential energy operator is faster with the Deslauriers–Dubuc wavelets. This is significant in three-dimensional simulations. We also conclude that Daubechies wavelets are a good basis set for path-integral calculations. The most important challenge in this study turned out to be handling the singularities of the nuclear potential at nuclei. Another issue was the slowness of the three-dimensional computations due to the large number of basis functions.

Making the self-consistent field iteration with Deslauriers–Dubuc wavelets as fast as the one implemented by the BigDFT software package using orthonormal wavelets is one challenge for future research. Another thing to study is computing three-dimensional systems with more than two valence electrons with HF and DFT methods and Deslauriers–Dubuc wavelets. Molecules with more than two nuclei and more than two valence electrons are examples of this kind of system. The remaining challenge in this topic is the calculation of the exchange operator for the HF method in three dimensions.

REFERENCES

- [1] Tommi Höynälänmaa, Tapio T. Rantala, and Keijo Ruotsalainen. “Solution of atomic orbitals in an interpolating wavelet basis”. In: *Physical Review E* 70 (2004), p. 066701. DOI: 10.1103/PhysRevE.70.066701.
- [2] Tommi Höynälänmaa. “Multiresolution Analysis for Compactly Supported Interpolating Tensor Product Wavelets”. In: *International Journal of Wavelets, Multiresolution and Information Processing* 13.2 (2015), p. 1550010. DOI: 10.1142/S0219691315500101.
- [3] Tommi Höynälänmaa and Tapio T. Rantala. “Electronic Structure Calculations with the Exact Pseudopotential and Interpolating Wavelet Basis”. In: *Atoms* 11 (2023). DOI: <https://doi.org/10.3390/atoms11010009>.
- [4] Tommi Höynälänmaa and Tapio T. Rantala. “Electronic structure calculations with interpolating tensor product wavelet basis”. In: *Physical Review E* 108 (2023), p. 025307. DOI: <https://doi.org/10.1103/PhysRevE.108.025307>.
- [5] Tommi Höynälänmaa. “Fourier transform and wavelet approaches to the path integral formulation”. In: *Communications in Computational Physics* (2024), submitted.
- [6] R. D. Cowan. *The theory of atomic structure and spectra*. University of California Press, 1981.
- [7] V. Schmidt. *Electron Spectrometry of Atoms using Synchrotron Radiation*. Cambridge University Press, 1997.
- [8] Peter Atkins and Ronald Friedman. *Molecular Quantum Mechanics*. New York: Oxford University Press Inc., 2005. DOI: 10.1080/00107514.2012.678277.
- [9] Yousef Saad, James R Chelikowsky, and Suzanne M Shontz. “Numerical methods for electronic structure calculations of materials”. In: *SIAM review* 52.1 (2010), pp. 3–54. DOI: 10.1137/060651653.

- [10] Richard P. Feynman and Albert R. Hibbs and Daniel F. Styer. *Quantum Mechanics and Path Integrals*. Courier Corporation, 2010.
- [11] W. Kohn. “Nobel Lecture: Electronic structure of matter – wavefunctions and density functionals”. In: *Rev. Mod. Phys.* 71.5 (1999), pp. 1253–1266. DOI: 10.1103/RevModPhys.71.1253.
- [12] José M Soler et al. “The SIESTA method for ab initio order-N materials simulation”. In: *Journal of Physics: Condensed Matter* 14.11 (Mar. 2002), pp. 2745–2779. DOI: 10.1088/0953-8984/14/11/302.
- [13] Ilkka Ruokosenmäki. “Real Time Path Integral Simulation Methods for Quantum Particles”. PhD thesis. Tampere University, 2019.
- [14] Ilkka Ruokosenmäki and Tapio T. Rantala. “Numerical Path Integral Approach to Quantum Dynamics and Stationary Quantum States”. In: *Commun. Comput. Phys.* 18.1 (2015), pp. 91–103. DOI: 10.4208/cicp.180914.161214a.
- [15] I. Daubechies. *Ten Lectures on Wavelets*. CBMS-NSF regional conference series in applied mathematics ; 61. SIAM, 1992. DOI: 10.1137/1.9781611970104.
- [16] Charles K. Chui and Chun Li. “Dyadic affine decompositions and functional wavelet transforms”. In: *SIAM J. Math. Anal.* 27.3 (1996), pp. 865–890. DOI: 10.1137/0527046.
- [17] David L. Donoho. *Interpolating Wavelet Transforms*. Tech. rep. 408. Department of Statistics, Stanford University, 1992.
- [18] Rong Qing Jia and Charles A Micchelli. “Using the refinement equations for the construction of pre-wavelets II: Powers of two”. In: *Curves and surfaces* (1991), pp. 209–246.
- [19] S. Goedecker. *Wavelets and their application for the solution of partial differential equations in physics*. Presses Polytechniques et Universitaires Romandes, 1998.
- [20] G. Beylkin, R. Coifman, and V. Rokhlin. “Fast Wavelet Transforms and Numerical Algorithms I”. In: *Commun. Pure Appl. Math.* XLIV.6 (1991), pp. 141–183.
- [21] G. Beylkin and J. M. Keiser. “On the adaptive Numerical Solution of Non-linear Partial Differential Equations in Wavelet Bases”. In: *J. Comput. Phys.* 132 (1997), pp. 233–259.

- [22] I. N. Levine. *Quantum chemistry*. Allyn and Bacon, 1983.
- [23] Ch. Froese Fischer. *The Hartree–Fock Method for Atoms – A Numerical Approach*. New York: John Wiley & Sons, 1977. DOI: 10.1088/0031-9112/29/4/040.
- [24] Gordon WF Drake. *Atomic, Molecular, and Optical Physics Handbook*. New York: AIP Press, 1996.
- [25] T. L. Tang. “Hartree-Fock method for Helium excited state”. 2017. URL: <https://nukephysik101.wordpress.com/2017/10/22/>.
- [26] O. V. Vasilyev and P. Paolucci. “A Dynamically Adaptive Multilevel Wavelet Collocation method for Solving Partial Differential Equations in a Finite Domain”. In: *J. Comput. Phys.* 125 (1996), pp. 498–512. DOI: 10.1006/jcph.1996.0111.
- [27] C. Hartwigsen, S. Goedecker, and J. Hutter. “Relativistic separable dual-space Gaussian Pseudopotentials from H to Rn”. In: *Phys. Rev. B* 58 (1998), p. 3641. DOI: 10.1103/PhysRevB.58.3641.
- [28] L. Genovese et al. “Daubechies wavelets as a basis set for density functional pseudopotential calculations”. In: *J. Chem. Phys.* 129 (2008), p. 014149. DOI: 10.1063/1.2949547.
- [29] S. Mohr et al. “Daubechies wavelets for linear scaling density functional theory”. In: *J. Chem. Phys.* 140 (2014), p. 204110. DOI: 10.1063/1.4871876.
- [30] “Computational Chemistry Comparison and Benchmark DataBase”. URL: <http://cccbdb.nist.gov>.
- [31] Leon van Dommelen. *Quantum Mechanics for Engineers*. May 19, 2019. URL: <http://www.umich.edu/~ners312/CourseLibrary/Dommelen.pdf>.
- [32] Hossein Gholizadehkalkhoran, Ilkka Ruokosenmäki, and Tapio T. Rantala. “Eigenstates and dynamics of Hooke’s atom: Exact results and path integral simulations”. In: *J. Math. Phys.* 59 (2018), p. 052104. DOI: 10.1063/1.5028503.
- [33] Maurice Cohen and Paul S. Kelly. “Hartree–Fock Wavefunctions for Excited States: the $1S$ State of Helium”. In: *Canadian Journal of Physics* 43.10 (1965). DOI: <https://doi.org/10.1139/p65-178>.

PUBLICATIONS

PUBLICATION

I

Solution of atomic orbitals in an interpolating wavelet basis

Tommi Höynälänmaa, Tapio T. Rantala, and Keijo Ruotsalainen

Physical Review E 70 (2004), p. 066701

DOI: 10.1103/PhysRevE.70.066701

Reprinted with permission from Tommi Höynälänmaa, Tapio T. Rantala, and Keijo Ruotsalainen, *Physical Review E*, 70, 066701, 2004. Copyright (2004) by the American Physical Society.

Solution of atomic orbitals in an interpolating wavelet basis

Tommi Höynälänmaa* and Tapio T. Rantala†

Institute of Physics, Tampere University of Technology, P.O. Box 692, FI-33101 Tampere, Finland

Keijo Ruotsalainen‡

Mathematics Division, Department of Electrical Engineering, University of Oulu, P.O. Box 4500, FI-90014 Finland

(Received 7 July 2004; published 2 December 2004)

The Schrödinger equation of hydrogenic atoms and the Hartree-Fock equations of some many-electron atoms are solved using interpolating wavelets as basis functions. The nonstandard operator form is used to compute operators in basis sets including multiple resolution levels. We introduce an algorithm for converting matrices from nonstandard operator form to standard operator form. We also consider the different components of the Hamiltonian and Fock operators separately and derive analytic formulas for their evaluation. Extension to many-electron atoms is done within the Hartree-Fock formalism. Convergence of atomic parameters such as orbital eigenvalues with respect to the number of resolution levels is inspected numerically for hydrogenlike atoms (ions) and some light many-electron atoms (helium, lithium, beryllium, neon, sodium, magnesium, and argon).

DOI: 10.1103/PhysRevE.70.066701

PACS number(s): 02.60.-x, 31.15.Ne, 71.15.Ap

I. INTRODUCTION

Use of wavelets for solving differential equations and partial differential equations in physics has recently been investigated in the literature [1–8]. One particular application is solving the Schrödinger equation of a quantum mechanical system using wavelets as basis functions. Fischer and DeFranceschi have used Daubechies wavelets [9,10] to solve the Schrödinger equation of hydrogenlike atoms [2] and they have also analyzed the Hartree-Fock method with continuous wavelet transform [6]. Electronic structure calculations with the Hartree-Fock (HF) method and wavelets have also been done by Yamaguchi and Mukoyama [11].

Most authors have used compactly supported orthonormal wavelets for electronic structure calculations. Daubechies wavelets have been used by Fischer and DeFranceschi [2] and Wei and Chu [3], Meyer wavelets by Yamaguchi and Mukoyama [4], and Mexican hat wavelets by Cho *et al.* [5]. Orthonormal wavelet families provide several useful properties—they possess recursive refinement relations [10], and they lead to fast discrete wavelet transform for multi-resolution analysis.

Interpolating wavelets are a biorthogonal wavelet family. They are not an orthonormal basis of $L^2(\mathbb{R})$. Interpolating wavelets enable simple computation of matrix elements and expansion of functions in a basis function set because of the special form of the dual scaling functions and dual wavelets [8,12]. Since the dual scaling functions and dual wavelets are sums of δ functions the integrals involving these functions usually require evaluating some function in a finite set of points. Goedecker and Ivanov [7] have used interpolating

wavelets to solve the Coulomb problem. Wavelet methods are closely connected to point-grid based methods that also generalize to higher than one dimension [13,14]. Lippert *et al.* [12] have used interpolating wavelets in point-grid based methods. Mann has done Hartree-Fock calculations using point sets with logarithmic scaling [15]. The basis function sets that we have used, where the accuracy is increased by adding basis functions of finer resolution levels near the nucleus, resemble this kind of point grid. In our treatment of the HF method matrices of all the necessary operators are computed and calculations are implemented as matrix and vector operations. We are able to derive analytic formulas for the matrix elements. We handle the various singularities in a similar way as Johnson *et al.* [16].

Representation of operators in orthonormal wavelet bases has been studied, for example, by Beylkin *et al.* [17–19]. We introduce an algorithm to compute the standard operator form (SOF) of an arbitrary operator from its nonstandard operator form (NSOF). The nonstandard operator form decouples different resolution levels, which is an important aspect for numerical approaches. We chose to use standard operator form because it enables the direct use of standard matrix and vector algorithms (e.g., solution of the matrix eigenproblem). However, for large basis sets and several resolution levels the SOF computations become slow and taking advantage of the special structure of NSOF matrices might make the computations significantly faster.

In the next section we first present the relevant concepts of hydrogenlike atoms. Then the Hartree-Fock formalism for many-electron atoms is briefly summarized. We present details of the basis set in Sec. III and the formulation of HF equations using interpolating wavelets in Sec. IV. The structure of matrices in standard and nonstandard operator form is presented in Sec. V [8,17,19]. Section VI discusses details of the computation of various operators and some other computational aspects. We give some numerical results in Sec. VII and conclusions are presented in the last section.

*Corresponding author.

Electronic address: tommy.hoynalanmaa@iki.fi

†Electronic address: tapio.rantala@tut.fi

‡Electronic address: keijo.ruotsalainen@oulu.fi

We use atomic units [20,21] throughout this article ($e = m = \hbar = 4\pi\epsilon_0 = 1$). We use the symbol A to denote a matrix of an arbitrary linear operator $\hat{A}$ in the given basis. The vector space spanned by the basis function set S is denoted by $L(S)$.

II. SCHRÖDINGER EQUATIONS OF ATOMS

A. Schrödinger equation of a hydrogenlike atom

Due to the spherical symmetry of atoms the three-dimensional one-electron Schrödinger equation $\hat{H}\psi = \epsilon\psi$ of hydrogenlike atoms is separated into a one-dimensional radial part and a two-dimensional angular part. The exact solutions to the latter are spherical harmonics $Y_{\ell m_\ell}$ where ℓ and m_ℓ are the orbital quantum number (angular momentum quantum number) and orbital magnetic quantum numbers, respectively. Writing $R_{n\ell}$ for the radial wave function, the hydrogenlike orbitals are $\psi_{n\ell m_\ell}(r, \theta, \phi) = R_{n\ell}(r)Y_{\ell m_\ell}(\theta, \phi)$, where n is the principal quantum number. The radial Schrödinger equation for a hydrogenlike atom is

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} - \frac{Z}{r} + \frac{\ell(\ell+1)}{2r^2} \right] P_{n\ell}(r) = \epsilon_{n\ell} P_{n\ell}(r), \quad (1)$$

where Z is the atomic number, $\epsilon_{n\ell}$ are the orbital energies, and $P_{n\ell}(r) = rR_{n\ell}(r)$ are the radial wave functions multiplied by r . The functions $P_{n\ell}(r)$ are called wave functions too. In general, the radial wave function $P_{n\ell}$ has $n - \ell - 1$ nodes [22].

The Hamiltonian $\hat{H}$ consists of three parts as

$$\hat{H} = \hat{T} + \hat{V} + \hat{C}_\ell, \quad (2)$$

where

$$\hat{T} = -\frac{1}{2} \frac{d^2}{dr^2}, \quad (3)$$

$$\hat{V} = -\frac{Z}{r}, \quad (4)$$

$$\hat{C}_\ell = \frac{\ell(\ell+1)}{2r^2}. \quad (5)$$

With a finite basis function set $\{\zeta_p(r)\}_{p=1}^N$ the approximate solutions P_i of Eq. (1) can be expanded as

$$P_i = \sum_{p=1}^N c_i^{(p)} \zeta_p. \quad (6)$$

In case a finite biorthogonal wavelet basis set is used Eq. (1) is represented as a matrix eigenproblem

$$Hc = \epsilon c, \quad (7)$$

where H is given by

$$H = (H_{pq})_{p,q=1}^N = \int_{\mathbb{R}} \tilde{\zeta}_p(r) \hat{H} \zeta_q(r) dr \quad (8)$$

and

$$c_i = (c_i^{(p)})_{p=1}^N. \quad (9)$$

The functions $\tilde{\zeta}_p(r)$ are so called dual basis functions (see Sec. III). Equations (7) and (8) are consequences of the biorthogonality relations (26)–(29). Diagonalization of the eigenproblem (7) for each orbital i yields N eigenvectors

$$c_j = (c_j^{(p)})_{p=1}^N \quad (10)$$

and the corresponding eigenvalues ϵ_j as a solution. We choose the eigenvalue ϵ_i of eigenvector c_i so that the wave function corresponding to the eigenvector has $n_i - \ell_i - 1$ nodes and satisfies the boundary conditions at zero and infinity. Note that all functions $P_{n\ell}(r)$ vanish at both limits. If we change the unit system so that the new unit of length is u atomic units of length and the energy is not changed, the Schrödinger equation (1) of the hydrogen atom becomes

$$\left(-\frac{1}{2} \frac{1}{u^2} \frac{d^2}{dr^2} - \frac{1}{u} \frac{Z}{r} + \frac{1}{u^2} \frac{\ell(\ell+1)}{2r^2} \right) P_{n\ell}(r) = \epsilon_{n\ell} P_{n\ell}(r) \quad (11)$$

and the Hamiltonian $\hat{H}$ and its components are changed according to Eq. (11).

B. Hartree-Fock equations

The Schrödinger equation $\hat{H}\Psi = E\Psi$ of a many-electron atom leads to Hartree-Fock equations in the central field approximation and with Slater determinant wave functions [20–22]. The Slater integrals between the two radial wave functions P_i and P_j are defined as

$$Y_{ij}^\kappa(r) = \int_0^\infty P_i(r') \gamma^\kappa(r, r') P_j(r') dr', \quad (12)$$

where

$$\gamma^\kappa(r, r') = \begin{cases} r'^\kappa & r' \leq r \\ r^{\kappa+1} & r' > r \end{cases}, \quad (13)$$

$$r_{<} = \min\{r, r'\}, \quad (14)$$

$$r_{>} = \max\{r, r'\}. \quad (15)$$

The HF equation for the orbital P_i with the principal quantum number n_i and orbital quantum number ℓ_i is

$$\left(-\frac{1}{2} \frac{d^2}{dr^2} - \frac{Z}{r} + \frac{\ell_i(\ell_i+1)}{2r^2} + D_i(r) \right) P_i(r) = \epsilon_i P_i(r) + \sum_{j(i \neq j)=1}^Q w_j \delta_{\ell_i \ell_j} \epsilon_{ij} P_j(r) + E_i(r), \quad (16)$$

where

$$D_i(r) = \sum_{j=1}^Q (w_j - \delta_{ij}) Y_{jj}^0(r) - (w_i - 1) A_i(r), \quad (17)$$

$$E_i(r) = \sum_{j(\neq i)=1}^Q w_j B_{ij}(r) P_j(r), \quad (18)$$

and

$$A_i(r) = \frac{2\ell_i + 1}{4\ell_i + 1} \sum_{\kappa > 0} \begin{pmatrix} \ell_i & \kappa & \ell_i \\ 0 & 0 & 0 \end{pmatrix}^2 Y_{ii}^\kappa(r), \quad (19)$$

$$B_{ij}(r) = \frac{1}{2} \sum_{\kappa} \begin{pmatrix} \ell_i & \kappa & \ell_j \\ 0 & 0 & 0 \end{pmatrix}^2 Y_{ji}^\kappa(r), \quad (20)$$

$$Z \text{ is the atomic number,} \quad (21)$$

$$Q \text{ is the number of orbitals,} \quad (22)$$

$$w_i \text{ is the number of electrons in orbital } i, \quad (23)$$

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} \text{ is the Wigner 3-}j \text{ symbol.} \quad (24)$$

The wave functions $P_i(r)$ are normalized with the condition

$$\int_0^\infty [P_i(r)]^2 dr = 1. \quad (25)$$

The nondiagonal Lagrange multipliers ε_{ij} , $i \neq j$, that ensure orthogonality of the orbitals may be neglected for closed-shell atoms. We neglect the nondiagonal Lagrange multipliers for open-shell atoms, too, and the exact orthogonality of atomic orbitals is not preserved for them.

III. INTERPOLATING WAVELETS AS BASIS SET

A. Biorthogonal wavelet families

For a more detailed description of the biorthogonal wavelet families and interpolating wavelets, see Ref. [8]. A biorthogonal wavelet family of degree m is characterized by four filters h_j , g_j , $\tilde{h}_j$, and $\tilde{g}_j$. The degree m is chosen to be even and large enough so that all the nonzero elements of the filters are included by the indices $j = -m, \dots, m$. The two-index basis functions are

$$\varphi_i^k(x) = \varphi(2^k x - i), \quad (26)$$

$$\psi_i^k(x) = \psi(2^k x - i), \quad (27)$$

$$\tilde{\varphi}_i^k(x) = 2^k \tilde{\varphi}(2^k x - i), \quad (28)$$

$$\tilde{\psi}_i^k(x) = 2^k \tilde{\psi}(2^k x - i). \quad (29)$$

The index k is called the scaling index and the index i the translation index.

The functions φ , ψ , $\tilde{\varphi}$, and $\tilde{\psi}$ satisfy the following refinement relations:

$$\varphi(x) = \sum_{j=-m}^m h_j \varphi(2x - j), \quad (30)$$

$$\psi(x) = \sum_{j=-m}^m g_j \varphi(2x - j), \quad (31)$$

$$\tilde{\varphi}(x) = \sum_{j=-m}^m \tilde{h}_j \tilde{\varphi}(2x - j), \quad (32)$$

$$\tilde{\psi}(x) = \sum_{j=-m}^m \tilde{g}_j \tilde{\varphi}(2x - j). \quad (33)$$

The basis functions defined by Eqs. (26)–(29) satisfy the biorthogonality relations

$$\int_{-\infty}^{\infty} \tilde{\varphi}_i^k(x) \varphi_j^k(x) dx = \delta_{ij}, \quad (34)$$

$$\int_{-\infty}^{\infty} \tilde{\psi}_i^k(x) \varphi_j^q(x) dx = 0, \quad k \geq q, \quad (35)$$

$$\int_{-\infty}^{\infty} \psi_i^k(x) \tilde{\varphi}_j^q(x) dx = 0, \quad k \geq q, \quad (36)$$

$$\int_{-\infty}^{\infty} \psi_i^k(x) \tilde{\psi}_j^q(x) dx = \delta_{kq} \delta_{ij}. \quad (37)$$

B. Construction of the basis function set

To preserve the orthogonality relations of the basis functions the scaling functions and wavelets in the basis cannot be chosen arbitrarily. The basis set $B = \{\zeta_1, \dots, \zeta_N\}$ consists of scaling functions φ_i^k of resolution level $k = k_{\min}$ and wavelets ψ_i^k of resolution levels $k = k_{\min}, \dots, k_{\max}$. The dual basis functions are defined by

$$\tilde{\zeta}_j = \begin{cases} \tilde{\varphi}_i^k & \text{if } \zeta_j = \varphi_i^k, \\ \tilde{\psi}_i^k & \text{if } \zeta_j = \psi_i^k. \end{cases} \quad (38)$$

Different resolution levels of the basis are denoted as $S_{k_{\min}}, D_{k_{\min}}, \dots, D_{k_{\max}}$, where S means a set consisting of scaling functions and D a set consisting of wavelets. This kind of basis is used directly for the standard operator form. For the nonstandard operator form, S_k parts with indices $k = k_{\min} + 1, \dots, k_{\max}$ are inserted in the basis. We define N_k to be the number of basis functions in S_k and M_k to be the number of basis functions in D_k . For $S_k = \{\varphi_{i_1}^k, \dots, \varphi_{i_{N_k}}^k\}$ we define $\mu_{k,\alpha} = i_\alpha$ and for $D_k = \{\psi_{i_1}^k, \dots, \psi_{i_{M_k}}^k\}$ we define $\nu_{k,\alpha} = i_\alpha$. The NSOF basis function set $B_{\text{NSOF}} = \{\zeta_1, \dots, \zeta_{N_{\text{NSOF}}}\}$ consists of parts $S_{k_{\min}}, D_{k_{\min}}, \dots, S_{k_{\max}}, D_{k_{\max}}$. The basis functions in the parts $S_{k_{\min}}, D_{k_{\min}}, \dots, D_{k_{\max}}$ are the same as in the corresponding parts of the basis set B . The basis functions in the parts $S_{k_{\min}+1}, \dots, S_{k_{\max}}$ are chosen so that $L(S_k, D_k) \subset L(S_{k+1})$. The radial wave function we want to expand should be zero at the nucleus. We exclude the function $\varphi_{i_1}^{k_{\min}}$ from the basis in order to force the wave functions $P_{n\ell}$ to be zero at $r=0$. This

also makes the matrix of operator $\hat{R}$, defined by

$$(\hat{R}f)(r) = |r|f(r), \quad (39)$$

nonsingular (an empirical observation). See also Ref. [16] for the handling of singularities. The projection of an arbitrary function f in $L^2(\mathbb{R})$ to the space spanned by a finite number of basis functions is

$$f(x) = \sum_i v_i^{(k_{\min})} \varphi_i^{k_{\min}}(x) + \sum_{k=k_{\min}}^{k_{\max}} \sum_i w_i^{(k_{\max})} \psi_i^k(x). \quad (40)$$

In this article, a vector consisting of coefficients of S_k basis functions is denoted by $v^{(k)}$ and a vector consisting of coefficients of D_k basis functions by $w^{(k)}$.

We use a similar basis set, denoted by B , for Hartree-Fock calculations. The scaling function $\varphi_0^{k_{\min}}$ is excluded from B due to the boundary conditions of wave functions at zero and singularities of the potential, the centrifugal potential, and the functions $1/r^{\kappa+1}$ (occurring in Slater integrals) at $r=0$. However, since the Slater integrals do not generally vanish at $r=0$ we include $\varphi_0^{k_{\min}}$ in the basis set $B_0 = B \cup \{\varphi_0^{k_{\min}}\} = \{\zeta_1^{(0)}, \dots, \zeta_{N'}^{(0)}\}$. The basis change matrix from B to B_0 is denoted by $L_{1 \rightarrow 0}$ and the basis change matrix from B_0 to B by $L_{0 \rightarrow 1}$. We do not need to compute the matrix of operator $\hat{R}_{-1}$ (corresponding to division by r) in basis B_0 . We also use the basis set

$$B_s = \{\varphi_i^{k_{\max}+1} | i \in I_s\} \quad (41)$$

consisting of scaling functions of resolution level $k_{\max}+1$ where $k_{\max}$ is the maximum resolution level in basis B and $I_s \subset \mathbb{Z}$ is finite. The basis set B_s is constructed so that $L(B) \subset L(B_s)$ and $L(B_0) \subset L(B_s)$. Expansion of an arbitrary function f in the scaling function basis B_s is given by

$$f(r) = \sum_{i \in I_s} a_i \varphi_i^{k_{\max}+1}(r). \quad (42)$$

C. Forward and backward wavelet transforms

The forward wavelet transform is defined by the equations [8]

$$s_i^{k-1} = \sum_{j=-m}^m \tilde{h}_j s_{j+2i}^k, \quad (43)$$

$$d_i^{k-1} = \sum_{j=-m}^m \tilde{g}_j s_{j+2i}^k, \quad (44)$$

where s_i^k is the coefficient for the basis function φ_i^k and d_i^k is the coefficient for the basis function ψ_i^k . The backward wavelet transform is defined by the equations [8]

$$s_{2i}^{k+1} = \sum_{j=-m/2}^{m/2} (h_{2j} s_{i-j}^k + g_{2j} d_{i-j}^k), \quad (45)$$

$$s_{2i+1}^{k+1} = \sum_{j=-m/2}^{m/2} (h_{2j+1} s_{i-j}^k + g_{2j+1} d_{i-j}^k). \quad (46)$$

The forward wavelet transform defined by Eqs. (43) and (44) can be written in matrix form as

$$v^{(k-1)} = \tilde{Z}_{S_k}^{S_{k-1}} v^{(k)}, \quad (47)$$

$$w^{(k-1)} = \tilde{Z}_{S_k}^{D_{k-1}} w^{(k)}, \quad (48)$$

where

$$\tilde{Z}_{S_k}^{S_{k-1}} = (\tilde{h}_{\mu_{k,\beta}-2\mu_{k-1,\alpha}})_{\alpha=1, \beta=1}^{N_{k-1}, N_k}, \quad (49)$$

$$\tilde{Z}_{S_k}^{D_{k-1}} = (\tilde{g}_{\mu_{k,\beta}-2\mu_{k-1,\alpha}})_{\alpha=1, \beta=1}^{M_{k-1}, N_k}. \quad (50)$$

The backward wavelet transform defined by Eqs. (45) and (46) can be similarly written in matrix form as

$$v^{(k+1)} = B_{S_k}^{S_{k+1}} v^{(k)} + B_{D_k}^{S_{k+1}} w^{(k)}, \quad (51)$$

where [8]

$$B_{S_k}^{S_{k+1}} = (Z_{S_{k+1}}^{S_k})^T, \quad (52)$$

$$B_{D_k}^{S_{k+1}} = (Z_{S_{k+1}}^{D_k})^T, \quad (53)$$

and

$$Z_{S_{k+1}}^{S_k} = (h_{\mu_{k+1,\beta}-2\mu_{k,\alpha}})_{\alpha=1, \beta=1}^{N_k, N_{k+1}}, \quad (54)$$

$$Z_{S_{k+1}}^{D_k} = (g_{\mu_{k+1,\beta}-2\mu_{k,\alpha}})_{\alpha=1, \beta=1}^{M_k, N_{k+1}}. \quad (55)$$

We use the symbols $\tilde{Z}$ and Z for the forward wavelet transform instead of $\tilde{F}$ and F (as in Ref. [8]) to avoid confusion with the Fock operator F .

D. Interpolating wavelets

Interpolating wavelets are one biorthogonal wavelet family [8,12]. For an interpolating wavelet family of degree m , the mother scaling function φ is constructed by recursively applying polynomial interpolation of degree $m-1$ to data $s_i = \delta_{i,0}$ and the mother dual scaling function is

$$\tilde{\varphi}(x) = \delta(x), \quad (56)$$

where δ is the Dirac delta function. For interpolating wavelets the coefficients h_j satisfy

$$h_j = \varphi(j/2), \quad j = -m, \dots, m. \quad (57)$$

The following symmetry equations hold for interpolating scaling functions and wavelets:

$$\varphi_i^k(x) = \varphi_{-i}^k(-x), \quad (58)$$

$$\psi_i^k(x) = \psi_{-i-1}^k(-x). \quad (59)$$

IV. SOLVING HARTREE-FOCK EQUATIONS

For an arbitrary operator $\hat{A}$, we denote the matrix of $\hat{A}$ in basis B by A and the matrix in basis B_0 by $A^{(0)}$. We define some operators to be used:

$$(\hat{R}f)(r) = |r|f(r), \quad (60)$$

$$(\hat{R}_{-1}f)(r) = f(r)/|r|, \quad (61)$$

$$(\hat{U}_0f)(r) = \int_0^{|r|} f(r')dr', \quad (62)$$

$$(\hat{U}_\infty f)(r) = \int_{|r|}^\infty f(r')dr', \quad (63)$$

$$\hat{S}_\kappa = \hat{R}_{-1}^{\kappa+1} \hat{U}_0 \hat{R}^\kappa + \hat{R}^\kappa \hat{U}_\infty \hat{R}_{-1}^{\kappa+1}, \quad (64)$$

where $\kappa \in \mathbb{Z}$, $\kappa \geq 0$, and $\hat{A}^n f = \hat{A} \cdots \hat{A} f$ where $\hat{A}$ is applied n times. Let $f \in L^2(\mathbb{R})$. We define the multiplication operator $\hat{M}(f) = \hat{A}$ by setting

$$(\hat{A}g)(r) = f(r)g(r) \quad (65)$$

for an arbitrary function $g \in L^2(\mathbb{R})$. If f is a vector (function) in a wavelet basis B' we define the matrix $M(f)$ to be the matrix of operator $\hat{M}(f)$ in the basis B' (f is kept constant). Let f and g be arbitrary vectors (functions) in the wavelet basis B' . We define $f \star g$ to be the projection of the function $h(r) = f(r)g(r)$ to $L(B')$.

We omit the nondiagonal Lagrange multipliers and Eqs. (16) can be written as matrix eigenvalue equations [23]

$$F_i c_i = \varepsilon_i c_i, \quad (66)$$

where the Fock operator F_i for orbital i is defined by

$$F_i = H_i^0 + J_i - K_i. \quad (67)$$

The wave functions P_i are given by

$$P_i = \sum_{p=1}^N c_i^{(p)} \xi_p. \quad (68)$$

The single-electron Hamiltonian operator is defined as

$$H_i^0 = T + V + C_{\ell_i}, \quad (69)$$

where the components are defined as in the case of hydrogenlike atoms, Eqs. (3)–(5).

The Slater direct integral operator is defined by

$$\hat{J}_i = \sum_{j=1}^q (w_j - \delta_{ij}) \hat{J}_j^0 - (w_i - 1) \frac{2\ell_i + 1}{4\ell_i + 1} \sum_{\kappa > 0} \begin{pmatrix} \ell_i & \kappa & \ell_i \\ 0 & 0 & 0 \end{pmatrix}^2 \hat{J}_i^\kappa, \quad (70)$$

where

$$(\hat{J}_i^\kappa P_j)(r) = Y_{ii}^\kappa(r) P_j(r) \quad (71)$$

and the Slater exchange integral operator by

$$\hat{K}_i = \frac{1}{2} \sum_{j(\neq i)=1}^q w_j \sum_{\kappa} \begin{pmatrix} \ell_i & \kappa & \ell_j \\ 0 & 0 & 0 \end{pmatrix}^2 \hat{K}_j^\kappa, \quad (72)$$

where

$$(\hat{K}_j^\kappa P_i)(r) = Y_{ij}^\kappa(r) P_j(r). \quad (73)$$

Note that in the definition of operator $\hat{K}_j^\kappa$ the argument of the operator occurs only in the Slater integral $Y_{ij}^\kappa(r)$. This operator is linear, though. For matrices of direct Slater integral operators we have

$$J_i^\kappa = L_{0 \rightarrow 1} M^{(0)}(S_\kappa^{(0)}(P_i \star P_i)) L_{1 \rightarrow 0} \quad (74)$$

and for matrices of exchange integral operators

$$K_j^\kappa = L_{0 \rightarrow 1} M^{(0)}(P_j) S_\kappa^{(0)} M^{(0)}(P_j) L_{1 \rightarrow 0}, \quad (75)$$

where

$$S_\kappa^{(0)} = L_{1 \rightarrow 0} R^{-1} U_0 L_{0 \rightarrow 1} + U_\infty^{(0)} L_{1 \rightarrow 0} R^{-1} L_{0 \rightarrow 1} \quad (76)$$

and

$$S_\kappa^{(0)} = L_{1 \rightarrow 0} (R^{-1})^{\kappa+1} U_0 R^\kappa L_{0 \rightarrow 1} + (R^{(0)})^\kappa U_\infty^{(0)} L_{1 \rightarrow 0} (R^{-1})^{\kappa+1} L_{0 \rightarrow 1} \quad (77)$$

for $\kappa > 0$.

The HF equations are solved by an iterative procedure. We use the standard procedure given in [22] modified for the matrix form of the HF equations presented in this section. The following input parameters are needed for the HF iteration algorithm: the weight coefficients α_i , $i=1, \dots, Q$ [see formula (78)]; the precision parameter z_0 characterizing the desired accuracy of the solution [see formulas (79) and (80)]; and the type of matrix norm $\|\cdot\|_p$ used to test the convergence of the iteration [see formula (79)].

The algorithm for HF iteration is as follows.

(1) Compute the Fock matrices F_i for each orbital i with formula (67). We set $J_i=0$ and $K_i=0$ in the first step, i.e., hydrogenic wave functions are used as the first trial wave functions.

(2) Solve the matrix eigenvalue equations (66) for each orbital i . Each eigenvalue equation yields N solutions, where N is the number of basis functions. We choose the solution satisfying the following conditions: the wave function is odd with respect to inversion: $P_i(r) = -P_i(-r)$; the wave function has $n_i - \ell_i - 1$ nodes, where n_i and ℓ_i are the principal quantum number and orbital quantum number of the orbital i ; and, we choose the solution with lowest possible eigenvalue ε_i among the solutions satisfying the other two conditions.

Normalize the wavefunctions with Eq. (25). Let ε_i be the eigenvalue and P_i^{new} the normalized wavefunction for each orbital i . We need not explicitly test the boundary conditions of wave functions at zero and infinity in the method described in this article.

(3) Let P_i^{prev} be the old output wave functions from the previous iteration. Compute the new output wave functions as normalized linear combinations of the new wave functions and the old output wave functions as

$$P_i = C_i [\alpha_i P_i^{\text{new}} + (1 - \alpha_i) P_i^{\text{prev}}], \quad i = 1, \dots, Q. \quad (78)$$

The normalization coefficients C_i are determined by Eq. (25). According to Ref. [22] the values of α_i are usually about 0.5 but they may be anywhere from 0.05 to 1.1.

(4) Compute the matrices J_i^κ and K_i^κ for all the necessary combinations of i , j , and κ . Use the wave functions com-

puted in step 3. Compute the matrices J_i and K_i with Eqs. (70) and (72), substituting matrices in the place of operators.

(5) Compute the quantity

$$z = \max_{i=1,\dots,Q} \|F_i - F_i^{\text{prev}}\|_p, \quad (79)$$

where F_i^{prev} are the Fock operators from the previous iteration. If

$$z < z_0 \quad (80)$$

we have obtained self-consistent solutions for the HF equations and the iteration is stopped.

(6) Return to step 1.

Finally, we evaluate the total energy of the atom with the self-consistent solutions for the wave functions P_i and energies ε_i from the formula

$$E = \sum_{i=1}^Q w_i \varepsilon_i - \frac{1}{2} \sum_{i=1}^Q w_i \langle P_i | J_i - K_i | P_i \rangle, \quad (81)$$

where w_i are the occupation numbers.

V. STANDARD OPERATOR FORM AND NONSTANDARD OPERATOR FORM

The eigenvalue equations are solved using the standard operator form, which represents the operator in the chosen basis. The elements of matrix A of an operator $\hat{A}$ in the SOF are defined by

$$A_{ij} = \int_{-\infty}^{\infty} \tilde{\zeta}_i(x) \hat{A} \zeta_j(x) dx, \quad (82)$$

where ζ_j , $j=1,\dots,N$, are the basis functions and $\tilde{\zeta}_i$, $i=1,\dots,N$, are the dual basis functions defined by Eq. (38).

The standard operator form of an operator can be obtained from the matrix elements in nonstandard operator form. The nonstandard operator form decouples different resolution levels in the basis set and makes derivation of explicit formulas for the matrix elements easier [8,17,19]. The nonzero blocks of nonstandard operator form A of the operator $\hat{A}$ are defined by

$$A_{\alpha\beta}^{S_{k_{\min}} S_{k_{\min}}} = \int_{-\infty}^{\infty} \tilde{\varphi}_{\mu_{k_{\min}}\alpha}^{k_{\min}}(x) \hat{A} \varphi_{\mu_{k_{\min}}\beta}^{k_{\min}}(x) dx, \quad (83)$$

$$\alpha = 1, \dots, N_{k_{\min}}, \quad \beta = 1, \dots, N_{k_{\min}},$$

and

$$A_{\alpha\beta}^{S_k D_k} = \int_{-\infty}^{\infty} \tilde{\varphi}_{\mu_{k,\alpha}}^k(x) \hat{A} \psi_{\nu_{k,\beta}}^k(x) dx, \quad \alpha = 1, \dots, N_k, \quad (84)$$

$$\beta = 1, \dots, M_k,$$

$$A_{\alpha\beta}^{D_k S_k} = \int_{-\infty}^{\infty} \tilde{\psi}_{\nu_{k,\alpha}}^k(x) \hat{A} \varphi_{\mu_{k,\beta}}^k(x) dx, \quad \alpha = 1, \dots, M_k, \quad (85)$$

$$\beta = 1, \dots, N_k,$$

$$A_{\alpha\beta}^{D_k D_k} = \int_{-\infty}^{\infty} \tilde{\psi}_{\nu_{k,\alpha}}^k(x) \hat{A} \psi_{\nu_{k,\beta}}^k(x) dx, \quad \alpha = 1, \dots, M_k,$$

$$\beta = 1, \dots, M_k, \quad (86)$$

where $k=k_{\min}+1, \dots, k_{\max}$.

We introduce an algorithm for converting a matrix from NSOF to SOF. The NSOF blocks ($S_k S_k$, $S_k D_k$, $D_k S_k$, and $D_k D_k$) are computed on the fly. The algorithm is as follows.

Input

The NSOF basis $B = (S_{k_{\min}}, D_{k_{\min}}, \dots, S_{k_{\max}}, D_{k_{\max}})$.

The function M that calculates the NSOF matrix elements according to formulas (83)–(86).

Output. Matrix in standard operator form.

Algorithm

(1) If the basis contains only parts $S_{k_{\min}}$ and $D_{k_{\min}}$ the SOF matrix is

$$A = \begin{pmatrix} A_{S_{k_{\min}} S_{k_{\min}}} & A_{S_{k_{\min}} D_{k_{\min}}} \\ A_{D_{k_{\min}} S_{k_{\min}}} & A_{D_{k_{\min}} D_{k_{\min}}} \end{pmatrix}, \quad (87)$$

where the blocks are computed with formulas (83)–(86).

Else

(2) Compute matrix A_{prev} by calling the algorithm recursively with basis $B_{\text{prev}} = (S_{k_{\min}}, D_{k_{\min}}, \dots, S_{k_{\max}-1}, D_{k_{\max}-1})$.

(3) Compute $A_{S_{k_{\max}} D_{k_{\max}}}$ with function M according to formula (84).

(4) Compute $A_{D_{k_{\max}} S_{k_{\max}}}$ with function M according to formula (85).

(5) Compute $A_{D_{k_{\max}} D_{k_{\max}}}$ with function M according to formula (86).

(6) Calculate matrices $A_{S_{k_{\min}} D_{k_{\max}}}$ and $A_{D_{k_{\min}} S_{k_{\max}}}$ where $q = k_{\min}, \dots, k_{\max}-1$ by applying forward wavelet transforms to matrix $A_{S_{k_{\max}} D_{k_{\max}}}$ using the formulas

$$A_{S_{k_{\min}} D_{k_{\max}}} = \tilde{Z}_{S_{k_{\min}+1}}^{S_{k_{\min}}} \tilde{Z}_{S_{k_{\min}+2}}^{S_{k_{\min}+1}} \dots \tilde{Z}_{S_{k_{\max}-1}}^{S_{k_{\max}-2}} \tilde{Z}_{D_{k_{\max}}}^{S_{k_{\max}-1}} A_{S_{k_{\max}} D_{k_{\max}}}, \quad (88)$$

$$A_{D_q D_{k_{\max}}} = \tilde{Z}_{S_{q+1}}^{D_q} \tilde{Z}_{S_{q+2}}^{S_{q+1}} \dots \tilde{Z}_{S_{k_{\max}-1}}^{S_{k_{\max}-2}} \tilde{Z}_{D_{k_{\max}}}^{S_{k_{\max}-1}} A_{S_{k_{\max}} D_{k_{\max}}}. \quad (89)$$

(7) Calculate matrices $A_{D_{k_{\max}} S_{k_{\min}}}$ and $A_{D_{k_{\max}} D_q}$ where $q = k_{\min}, \dots, k_{\max}-1$ by applying backward wavelet transforms to matrix $A_{D_{k_{\max}} S_{k_{\max}}}$ using the formulas

$$A_{D_{k_{\max}} S_{k_{\min}}} = A_{D_{k_{\max}} S_{k_{\max}}} B_{S_{k_{\max}-1}}^{D_{k_{\max}}} B_{S_{k_{\max}-2}}^{S_{k_{\max}-1}} \dots B_{S_{k_{\min}+1}}^{S_{k_{\min}+2}} B_{S_{k_{\min}}}^{S_{k_{\min}+1}}, \quad (90)$$

$$A_{D_{k_{\max}} D_q} = A_{D_{k_{\max}} S_{k_{\max}}} B_{S_{k_{\max}-1}}^{D_{k_{\max}}} B_{S_{k_{\max}-2}}^{S_{k_{\max}-1}} \dots B_{S_{q+1}}^{S_{q+2}} B_{D_q}^{S_{q+1}}. \quad (91)$$

(8) Construct the result A from matrices calculated in steps 2, 5, 6, and 7 using the formulas

$$A_{\text{vert}} = \begin{pmatrix} A_{S_{k_{\min}} D_{k_{\max}}} \\ A_{D_{k_{\min}} D_{k_{\max}}} \\ \vdots \\ A_{D_{k_{\max}} D_{k_{\max}}} \end{pmatrix}, \quad (92)$$

$$A_{\text{horiz}} = \begin{pmatrix} A^{D_{k_{\max}} S_{k_{\min}}} \\ A^{D_{k_{\max}} D_{k_{\min}}} \\ \dots \\ A^{D_{k_{\max}} D_{k_{\max}-1}} \end{pmatrix}^T, \quad (93)$$

$$A = \begin{pmatrix} A_{\text{prev}} & A_{\text{vert}} \\ A_{\text{horiz}} & A^{D_{k_{\max}} D_{k_{\max}}} \end{pmatrix}. \quad (94)$$

VI. EVALUATION OF MATRIX ELEMENTS AND OTHER COMPUTATIONAL ASPECTS

A. Notation

We use the following notation for matrix elements of an operator $\hat{A}$ in nonstandard operator form [17]:

$$\alpha_{ij}^k = \int_{-\infty}^{\infty} \tilde{\psi}_i^k(x) \hat{A} \psi_j^k(x) dx, \quad (95)$$

$$\beta_{ij}^k = \int_{-\infty}^{\infty} \tilde{\psi}_i^k(x) \hat{A} \varphi_j^k(x) dx, \quad (96)$$

$$\gamma_{ij}^k = \int_{-\infty}^{\infty} \tilde{\varphi}_i^k(x) \hat{A} \psi_j^k(x) dx, \quad (97)$$

$$s_{ij}^k = \int_{-\infty}^{\infty} \tilde{\varphi}_i^k(x) \hat{A} \varphi_j^k(x) dx. \quad (98)$$

In this section we denote the matrix of an operator $\hat{A}$ in an arbitrary wavelet basis B (with or without the function $\varphi_0^{k_{\min}}$) by A .

B. Differentiation operator

The basic integral for a differentiation operator d^p/dx^p is defined as

$$a_i = \int_{-\infty}^{\infty} \tilde{\varphi}(x) \frac{d^p}{dx^p} \varphi(x-i) dx. \quad (99)$$

The matrix elements of operator d^p/dx^p in nonstandard operator form in an interpolating wavelet family are

$$\alpha_{ij}^k = -2^{(k+1)p} \sum_{\nu=-m}^m \tilde{g}_{\nu} a_{2j-2i+1-\nu}, \quad (100)$$

$$\beta_{ij}^k = 2^{(k+1)p} \sum_{\nu=-m}^m \sum_{\mu=-m}^m \tilde{g}_{\nu} h_{\mu} a_{2j-2i+\mu-\nu}, \quad (101)$$

$$\gamma_{ij}^k = -2^{(k+1)p} a_{2j-2i+1}, \quad (102)$$

$$s_{ij}^k = 2^{kp} a_{j-i}. \quad (103)$$

See Ref. [8].

C. Function operator

By a function operator we mean multiplication by a given function f as defined by Eq. (65). The NSOF matrix elements of a function operator in the interpolating wavelet basis are

$$\alpha_{ij}^k = f\left(\frac{2i+1}{2^{k+1}}\right) \delta_{ij}, \quad (104)$$

$$\beta_{ij}^k = h_{2i-2j+1} \left[f\left(\frac{j}{2^k}\right) - f\left(\frac{2i+1}{2^{k+1}}\right) \right], \quad (105)$$

$$\gamma_{ij}^k = 0, \quad (106)$$

$$s_{ij}^k = f\left(\frac{i}{2^k}\right) \delta_{ij}. \quad (107)$$

D. Operator $\hat{R}$

The operator $\hat{R}$ is a function operator with

$$(\hat{R}g)(r) = |r|g(r). \quad (108)$$

Its NSOF matrix elements are obtained from formulas (104)–(107) where we set $f(r) = |r|$. If the basis does not contain the function $\varphi_0^{k_{\min}}$ the matrix R does not become singular and we can compute R^{-1} as an inverse matrix.

We obtain the potential energy operator as

$$V = -R^{-1} \quad (109)$$

and the centrifugal potential operator as

$$C_{\ell} = \frac{\ell(\ell+1)}{2} (R^{-1})^2. \quad (110)$$

E. Operator $\hat{U}_0$

The matrix elements of operator $\hat{U}_0$ in the nonstandard operator form are

$$\alpha_{ij}^k = -2^{-k-1} \sum_{\nu=-m}^m \tilde{g}_{\nu} [\Phi(|2i+\nu|-2j-1) - \Phi(-2j-1)], \quad (111)$$

$$\beta_{ij}^k = 2^{-k} \sum_{\nu=-m}^m \tilde{g}_{\nu} \left[\Phi\left(\left|\frac{2i+\nu}{2}\right| - j\right) - \Phi(-j) \right], \quad (112)$$

$$\gamma_{ij}^k = -2^{-k-1} [\Phi(2|i|-2j-1) - \Phi(-2j-1)], \quad (113)$$

$$s_{ij}^k = 2^{-k} [\Phi(|i|-j) - \Phi(-j)], \quad (114)$$

where $\Phi(x)$ is the integral function of the mother scaling function $\varphi(x)$. We evaluated the function Φ with numerical integration using the fourth-order Runge-Kutta method. The function Φ can also be calculated analytically using the refinement equation (30). When the distance between adjacent

TABLE I. Effects of operators on the parities of functions (“o” means odd and “e” means even).

$P_{n_i \ell_i}$	$P_{n_i \ell_i}^{\text{precv}}$	$TP_{n_i \ell_i}$	$VP_{n_i \ell_i}$	$C_\ell P_{n_i \ell_i}$	$J_{n_i \ell_i} P_{n_i \ell_i}$	$K_{n_i \ell_i} P_{n_i \ell_i}$
o	o	o	o	o	o	o
o	e	o	o	o	o	e
e	o	e	e	e	e	o
e	e	e	e	e	e	e

points in numerical integration is 2^{-8} the maximum deviation of the numerical result from the analytical one is of the order of magnitude 10^{-11} .

F. Operator $\hat{U}_\infty$

The matrix elements of $\hat{U}_\infty$ in the nonstandard operator form are

$$\alpha_{ij}^k = -2^{-k-1} \sum_{\nu=-m}^m \tilde{g}_\nu [\Phi(\infty) - \Phi(|2i + \nu| - 2j - 1)], \quad (115)$$

$$\beta_{ij}^k = 2^{-k} \sum_{\nu=-m}^m \tilde{g}_\nu \left[\Phi(\infty) - \Phi\left(\left|\frac{2i + \nu}{2}\right| - j\right) \right], \quad (116)$$

$$\gamma_{ij}^k = -2^{-k-1} [\Phi(\infty) - \Phi(2|i| - 2j - 1)], \quad (117)$$

$$s_{ij}^k = 2^{-k} [\Phi(\infty) - \Phi(|i| - j)]. \quad (118)$$

G. Multiplication operator

The multiplication operator $\hat{M}(f)$ is defined in Sec. IV. Let f be a vector (function) in an arbitrary wavelet basis B . We first convert the vector f in basis B to a scaling function basis B_s using formula (42). Here B_s is defined according to Eq. (41) so that $L(B) \subset L(B_s)$. Conversion is done with backward wavelet transforms. The matrix $M(f)$ is computed using the formulas for matrix elements of a function, Eqs. (104)–(107), where we set

$$f\left(\frac{i}{2^k}\right) = a_{(2^{k_{\max}+1-k})i} \quad (119)$$

and

TABLE II. Parameters used for $1s$ orbitals of hydrogenlike atoms.

Z	u	$k_{\min}$	B
1	1.0	0	10
2	1.0	1	8
10	0.25	2	12
50	0.031 25	1	10
100	0.031 25	2	20

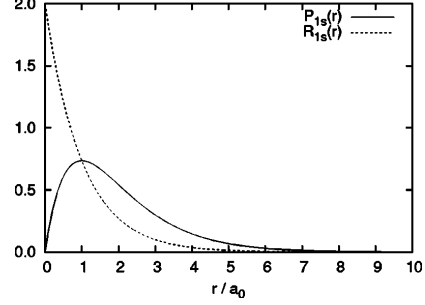


FIG. 1. Computed $1s$ radial wave functions $P_{1s}(r)$ and $R_{1s}(r)$ of the hydrogen atom with $L=8$. There is no visible deviation from the exact wave functions.

$$f\left(\frac{i}{2^{k+1}}\right) = a_{(2^{k_{\max}-k})i}. \quad (120)$$

H. Product function $f \star g$

The product function $f \star g$ is defined in Sec. IV. The vectors f and g in the arbitrary wavelet basis B are converted to the scaling function basis B_s , where $L(B) \subset L(B_s)$, so that we have

$$f(r) = \sum_i a_i \varphi_i^{k_{\max}+1}(r) \quad (121)$$

and

$$g(r) = \sum_i b_i \varphi_i^{k_{\max}+1}(r). \quad (122)$$

The expansion of the product function $h(r) = f(r)g(r)$ in the scaling function basis B_s is given by

$$h(r) = \sum_i c_i \varphi_i^{k_{\max}+1}(r), \quad (123)$$

where $c_i = a_i b_i$ for all i . To compute $f \star g$, the vector representation for the function $h(r)$ given by Eq. (123) is converted to the basis B using forward wavelet transforms.

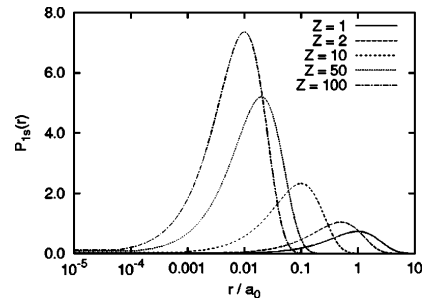


FIG. 2. Radial $1s$ wave functions $P_{1s}(r)$ of hydrogenlike atoms computed with $L=8$. Note the logarithmic scale for r .

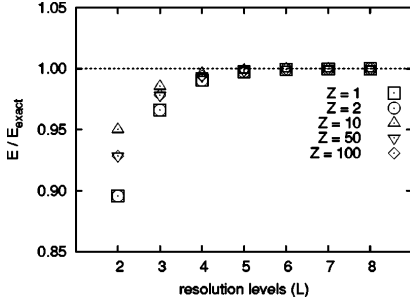


FIG. 3. The 1s eigenvalues of hydrogenlike atoms with $Z=1, 2, 10, 50$, and 100 . Ratio of the computed and exact values is shown.

I. Basis change matrices $L_{1 \rightarrow 0}$ and $L_{0 \rightarrow 1}$

The matrices $L_{1 \rightarrow 0}$ and $L_{0 \rightarrow 1}$ occur only in products with other matrices. This kind of matrix products is computed by removing the row or the column corresponding to basis function $\varphi_0^{\min}$ or inserting a zero row or a zero column corresponding to that basis function.

J. Evaluation of scalar products

When normalizing wave functions or evaluating the expectation values of operators we encounter integrals of the type

$$I = \int_0^\infty f(r)g(r)dr \quad (124)$$

or

$$I = \int_0^\infty f(r)(\hat{A}g)(r)dr. \quad (125)$$

We first compute the expansion (c_i) of the product function $h(r)=f(r)(\hat{A}g)(r)$ in the scaling function basis B_s (as in the case of a product function). The integral is then given by

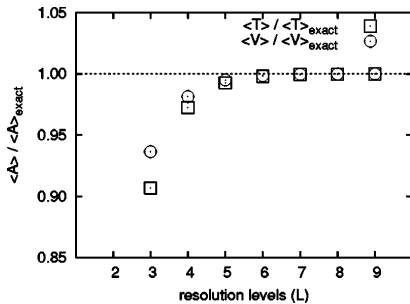


FIG. 4. Expectation values of the kinetic energy and potential energy operators for the hydrogen 1s orbital. Ratio of the computed and exact values is shown.

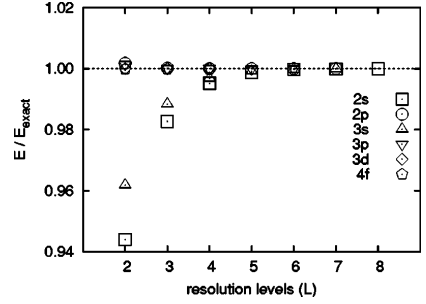


FIG. 5. Energy eigenvalues of 2s, 2p, 3s, 3p, 3d, and 4f orbitals of hydrogen with $B=15, 20, 30, 30, 30$, and 45 , respectively. Ratio of the computed and exact values is shown.

$$I = \frac{1}{2^{k_{\max}+1}} \sum_{i \geq 0} c_i. \quad (126)$$

See also Refs. [24] and [25].

K. Negative values of r

A negative r coordinate has no physical meaning for radial wave functions. However, interpolating wavelets constitute a basis set for functions space $L^2(\mathbb{R})$ and their domain is the whole real axis. Interpolating wavelets and scaling functions that are located near zero (i.e., nonzero values of the functions are concentrated near zero) do not generally vanish on the negative real axis, so we are not able to exclude the negative real axis by choosing a suitable basis set. We choose the basis set so that it is symmetrical around zero, so that for each basis function $\xi(x)$ the function $\xi(-x)$ is also in the basis set; see Eqs. (58) and (59). We actually solve the eigenproblem in both the positive and negative real axes, i.e., if $P(r)$, $r \in \mathbb{R}$, is a solution of the eigenproblem then both $P(r)$, $r \geq 0$, and $P(-r)$, $r \geq 0$, are wave functions. We may generally get either odd or even solutions to the eigenproblem, i.e., $P(r)=P(-r)$ or $P(r)=-P(-r)$. For hydrogenic computations we simply neglect the negative r part of the wave function but the situation is more complex when HF equations are solved. The operators used in HF computation yield either

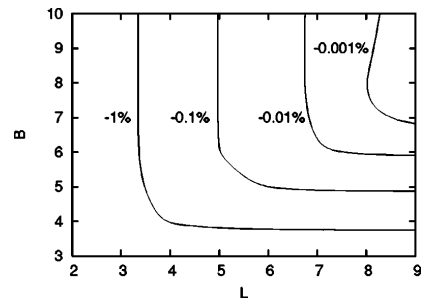


FIG. 6. Relative error of the hydrogen 1s orbital eigenvalue; unit of length $u=0.6$.

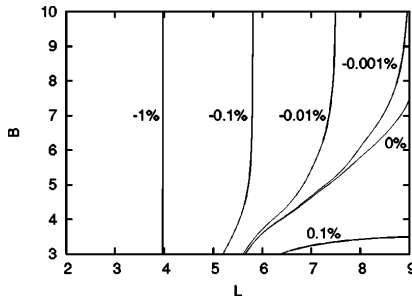


FIG. 7. Relative error of the hydrogen 1s orbital eigenvalue; unit of length $u=1.0$.

odd or even functions. The parity of the function $\hat{A}P$ depends on the parity of the function P and in the case of the direct integral and exchange integral operators also the parities of the wave functions from the previous iteration that are used to compute these operators themselves. Table I shows how the operators needed in HF computations affect the parities of the functions. The functions yielded by the exchange integral operator and the other operators would have different parities if we chose a wave function with parity different from the output wave functions of the previous iteration (second and third lines of the table). Consequently, the computation would be wrong on the negative real axis (the exchange integrals would have the wrong sign). We have to use either odd or even wave functions during the whole HF iteration. We have chosen to use odd wave functions, which have continuous first derivatives at the origin.

VII. NUMERICAL RESULTS

A. General

We use eighth-order interpolating wavelets for numerical results. The unit of length is the atomic unit unless otherwise stated. We examine the convergence of the essential physical quantities toward the known exact or accurate values when the number of resolution levels is increased. We also examine the effect of the number of basis functions in each reso-

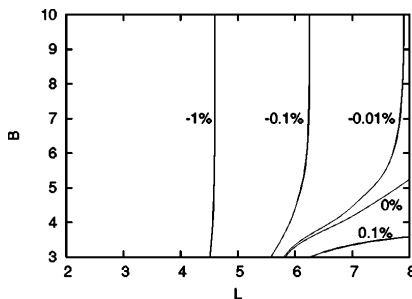


FIG. 8. Relative error of the hydrogen 1s orbital eigenvalue; unit of length $u=1.4$.

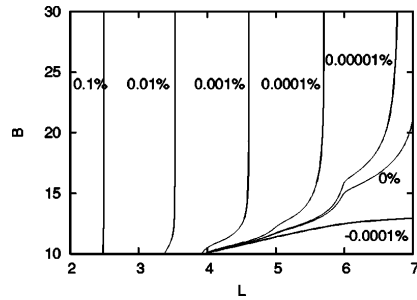


FIG. 9. Relative error of the hydrogen 2p orbital eigenvalue; unit of length $u=1.0$.

lution level. Various parameters affecting the computations are also reported.

The basis sets were formed so that there are S type basis functions $\varphi_{-2B}^{k_{\min}}, \dots, \varphi_{2B}^{k_{\min}}$ in resolution level $k_{\min}$ and D type basis functions $\psi_{-B}^k, \dots, \psi_{B-1}^k$ for $k=k_{\min}, \dots, k_{\min}+L-2$. Here L is the number of resolution levels and B is a parameter describing the number of basis functions in each resolution level. We count $S_{k_{\min}}$ and $D_{k_{\min}}$ as two separate resolution levels. The total number of basis functions is

$$N = 4B + 2(L-1)B = 2B(L+1). \quad (127)$$

In principle, the number of resolution levels L determines the maximum possible accuracy of the computations with fixed $k_{\min}$ and unit of length u .

B. Hydrogenlike orbitals

We solved the 1s orbitals for hydrogenlike atoms for atomic numbers $Z=1, 2, 10, 50$, and 100 using the basis sets and length units u given in Table II. The basis sets were chosen large enough to cover the relevant radial range of the wave functions. The resulting 1s radial wave functions are shown in Figs. 1 and 2. There is no visible deviation of these wave functions (computed with $L=8$) from the corresponding exact wave functions. Convergence of the eigenvalues $\varepsilon_{n\ell}$ as a function of resolution level is presented in Fig. 3. The exact values are

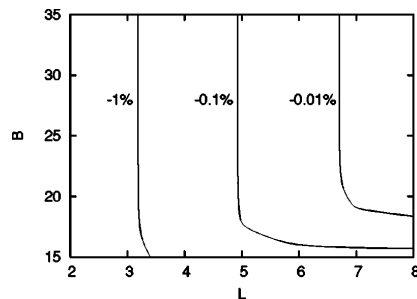


FIG. 10. Relative error of the hydrogen 3s orbital eigenvalue; unit of length $u=1.0$.

TABLE III. Parameters for HF computations.

Atom	α	$k_{\min}$	B	L
He	1.0	1	10	2,...,8
Li	1.0	1	20	2,...,8
Be	1.0	1	15	2,...,8
Ne	0.6	1	10	2,...,8
Na	0.7	1	20	2,...,7
Mg	0.7	1	20	2,...,7
Ar	0.7	2	25	2,...,7

$$\varepsilon_{n\ell} = -\frac{Z^2}{2n^2}. \quad (128)$$

We see that accuracy within 1% is achieved already at $L=4$. Expectation values of the kinetic energy and potential energy operators $\hat{T}$ and $\hat{V}$ for the hydrogen $1s$ orbital ($Z=1$) are shown in Fig. 4. The most accurate ($L=9$) numerical values are $\varepsilon_{1s} = -0.499\,996$, $\langle \hat{T} \rangle_{1s} = 0.499\,98$, and $\langle \hat{V} \rangle_{1s} = -0.999\,98$, the exact values for $Z=1$ being $-1/2$, $1/2$, and -1 , respectively. Other orbitals of the hydrogen atom ($2s$, $2p$, $3s$, $3p$, $3d$, and $4f$) were also calculated. We used a unit of length $u=1.0$ and minimum resolution level $k_{\min}=0$. The resulting orbital eigenvalues are shown in Fig. 5. Accuracy better than 1% is achieved at $L=4$ for all the computed orbitals. As the orbital quantum number ℓ increases the results get more accurate.

We also made a set of computations for hydrogen $1s$, $2p$, and $3s$ orbitals where both the number of resolution levels L and basis width B were varied. The hydrogen $1s$ orbital was computed with unit of length $u=0.6$, 1.0 , and 1.4 , and the other orbitals with unit of length $u=1.0$. We used $k_{\min}=0$ in these computations. The relative error of the hydrogen $1s$ eigenvalue (compared to the exact analytical result) is plotted as a contour plot in Figs. 6, 7 and 8, where the length units u are 0.6 , 1.0 , and 1.4 , respectively. Similar plots for $2p$

TABLE V. Results from Hartree-Fock calculations for lithium and sodium. Deviation from the accurate value [26] is given in parentheses so that negative deviation means that the computed value is less than the accurate value.

	Li	Na
E	-7.4321(7)	-161.3(6)
n_{iter}	17	27
ε_{1s}	-2.4775(3)	-40.2(3)
ε_{2s}	-0.196 309(14)	-2.78(2)
ε_{2p}		-1.521(-3)
ε_{3s}		-0.1817(5)
$\langle 1s 2s \rangle$	-5.7×10^{-4}	-5.9×10^{-8}
$\langle 1s 3s \rangle$		-1.4×10^{-6}
$\langle 2s 3s \rangle$		-2.8×10^{-4}

and $3s$ are presented in Figs. 9 and 10. The relative error is computed by $\Delta = (x - x_0)/x_0$ where x is the computed quantity and x_0 its exact value. For each orbital, the Schrödinger equation was solved using all combinations with $L = L_{\min}, L_{\min}+1, \dots, L_{\max}$ and $B = B_{\min}, B_{\min}+1, \dots, B_{\max}$ to cover the ranges of L and B .

Note that for fixed L the limiting value for the orbital eigenvalue as B tends to infinity is not the (physically) exact value but one with a L dependent shift. Therefore, the 0% contour appears in Figs. 7, 8, and 9.

C. Hartree-Fock results for many-electron atoms

We carried out HF calculations for helium, lithium, beryllium, neon, sodium, magnesium, and argon atoms. Lithium and sodium are open-shell and the others are closed-shell atoms. The relevant computation parameters are given in Table III. The basis sets were formed the same way as for the hydrogen atom. The same value of the weight parameter α_i defined by Eq. (78) is used for all orbitals, $\alpha_i = \alpha$. The unit of length was $u=1$ in all HF calculations. A matrix one-norm

TABLE IV. Results from Hartree-Fock calculations for helium, beryllium, neon, magnesium, and argon. Deviation from the accurate value [26] is given in parentheses so that negative deviation means that the computed value is less than the accurate value.

	He	Be	Ne	Mg	Ar
E	-2.861 57(11)	-14.571(3)	-128.45(10)	-198.8(9)	-525.8(11)
n_{iter}	21	23	31	27	25
ε_{1s}	0.917 93(3)	-4.7318(9)	-32.73(5)	-48.7(4)	-118.2(5)
ε_{2s}		-0.309 25(2)	-1.928(3)	-3.75(2)	-12.29(4)
ε_{2p}			-0.850(-4)	-2.287(-5)	-9.577(-6)
ε_{3s}				-0.2525(6)	-1.274(4)
ε_{3p}					-0.5916(-6)
$\langle 1s 2s \rangle$		-2.6×10^{-7}	-4.2×10^{-6}	-5.6×10^{-8}	-1.8×10^{-8}
$\langle 1s 3s \rangle$				-1.6×10^{-8}	-7.8×10^{-9}
$\langle 2s 3s \rangle$				-8.9×10^{-8}	-2.5×10^{-8}
$\langle 2p 3p \rangle$					-1.4×10^{-8}

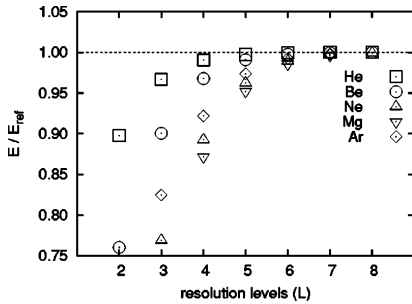


FIG. 11. Computed total energies for helium, beryllium, neon, magnesium, and argon. Ratio of computed and accurate [26] values is shown.

was used to compute the quantities z defined by Eq. (79). The value of the precision parameter z_0 was 10^{-10} in all HF computations.

The orbital eigenvalues and total energies from the most accurate computation for each atom are given in Tables IV and V. These values are compared with the values from standard HF calculations obtained from Ref. [26]. Total energies of atoms are plotted in Figs. 11 and 12. For helium, four resolution levels are needed to reach an accuracy of 1% with $k_{\min}=1$. For argon, six resolution levels are needed for this with $k_{\min}=2$. The HF calculations converged in 16 to 31 steps depending on the number of resolution levels L and weight parameter α .

The effect of neglecting nondiagonal Lagrange multipliers can be seen from the overlap integrals between orbitals. For the open-shell atoms (lithium and sodium) the largest overlap integral is of the order of magnitude 10^{-4} whereas for the closed-shell atoms all the overlap integrals are of the order of magnitude 10^{-6} or smaller.

VIII. CONCLUSIONS

We have demonstrated that interpolating wavelets can be successfully used to solve the atomic orbitals and the electronic structure of atoms. We are able to systematically increase the accuracy of the calculations by choosing the number of resolution levels and the number of basis functions in each level.

In this study we have concentrated on the basic formalism and developed it down to practical computations. Our study

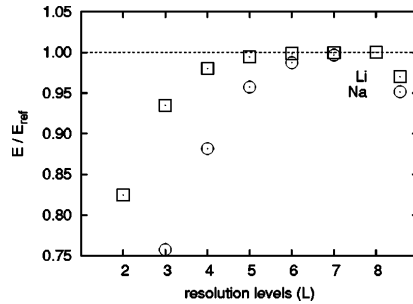


FIG. 12. Computed total energies for lithium and sodium. Ratio of computed and accurate [26] values is shown.

involves both development of algorithms, e.g., for conversion of matrices from nonstandard operator form to standard operator form, and testing with calculations. We have shown how to consider the singularity of the nuclear Coulomb potential and the centrifugal potential as well as the Slater integrals in evaluation of Hamiltonian and Fock matrix elements (see also Ref. [16]).

We have tested numerically the computation methods for the ground state of the hydrogen atom and hydrogenlike atoms, for excited states of hydrogen, and for some many-electron atoms. The numerical results converge to the accurate or reference values as the number of resolution levels increases. In principle, we should be able to make the error arising from the wavelet approximation arbitrarily small by enlarging the basis function set. Our numerical HF results support this. With a large number of resolution levels (about eight or more) the computation time grows considerably. Depending on the properties of the algorithms we can use basis sets with fewer resolution levels (possibly only one), higher minimum resolution, and more basis functions in each level. However, the possibility of using several resolution levels is one important benefit of wavelets. It might also be possible to optimize the computation by using convolutions in the computation of backward and forward wavelet transforms and products of operators with vectors instead of simply using matrix products as done in this study.

A noticeable feature in our development for the Hartree-Fock formalism is that all relevant operators, including those representing the two-electron integrals, can be evaluated analytically.

- [1] C. J. Tymczak and Xiao-Qian Wang, Phys. Rev. Lett. **78**, 3654 (1997).
- [2] P. Fischer and M. Defranceschi, SIAM (Soc. Ind. Appl. Math.) J. Numer. Anal. **35**, 1 (1998).
- [3] Siqing Wei and M. Y. Chou, Phys. Rev. Lett. **76**, 2650 (1996).
- [4] K. Yamaguchi and T. Mukoyama, J. Phys. B **29**, 4059 (1996).
- [5] K. Cho, T. A. Arias, J. D. Joannopoulos, and P. K. Lam, Phys. Rev. Lett. **71**, 1808 (1993).

- [6] P. Fischer and M. Defranceschi, Appl. Comput. Harmon. Anal. **1**, 232 (1994).
- [7] S. Goedecker and O. V. Ivanov, Solid State Commun. **105**, 665 (1998).
- [8] S. Goedecker, *Wavelets and Their Application for the Solution of Partial Differential Equations in Physics* (Presses Polytechniques et Universitaires Romandes, Lausanne, 1998).
- [9] I. Daubechies, Commun. Pure Appl. Math. **41**, 909 (1988).

- [10] I. Daubechies, *Ten Lectures on Wavelets*, CBMS-NSF Regional Conference Series in Applied Mathematics Vol. 61 (SIAM, Philadelphia, 1992).
- [11] K. Yamaguchi and T. Mukoyama, Nucl. Instrum. Methods Phys. Res. B **124**, 361 (1997).
- [12] R. A. Lippert, T. A. Arias, and A. Edelman, J. Comput. Phys. **140**, 278 (1998).
- [13] O. V. Vasilyev, S. Paolucci, and M. Sen, J. Comput. Phys. **120**, 33 (1995).
- [14] T. A. Arias, Rev. Mod. Phys. **71**, 267 (1999).
- [15] J. B. Mann, *Atomic Structure Calculations* (Los Alamos Scientific Laboratory of the University of California, Los Alamos, NM, 1967).
- [16] B. R. Johnson, J. L. Mackey, and J. L. Kinsey, J. Comput. Phys. **168**, 356 (2001).
- [17] G. Beylkin, R. Coifman, and V. Rokhlin, Commun. Pure Appl. Math. **44**, 141 (1991).
- [18] G. Beylkin, SIAM (Soc. Ind. Appl. Math.) J. Numer. Anal. **6**, 1716 (1992).
- [19] G. Beylkin and J. M. Keiser, J. Comput. Phys. **132**, 233 (1997).
- [20] P. W. Atkins and R. S. Friedman, *Molecular Quantum Mechanics* (Oxford University Press, Oxford, 1997).
- [21] V. Schmidt, *Electron Spectrometry of Atoms using Synchrotron Radiation* (Cambridge University Press, Cambridge, 1997).
- [22] R. D. Cowan, *The Theory of Atomic Structure and Spectra* (University of California Press, Berkeley, 1981).
- [23] I. N. Levine, *Quantum Chemistry* (Allyn and Bacon, Boston, 1983).
- [24] W. Dahmen and C. A. Micchelli, SIAM (Soc. Ind. Appl. Math.) J. Numer. Anal. **30**, 507 (1993).
- [25] S. Bertoluzza, C. Canuto, and K. Urban, Appl. Numer. Math. **34**, 13 (2000).
- [26] Ch. Froese Fischer, *The Hartree-Fock Method for Atoms—A Numerical Approach* (Wiley, New York, 1977).

PUBLICATION

II

Multiresolution Analysis for Compactly Supported Interpolating Tensor Product Wavelets

Tommi Höynälänmaa

International Journal of Wavelets, Multiresolution and Information Processing 13.2 (2015),
p. 1550010

DOI: 10.1142/S0219691315500101

Publication reprinted with the permission of the copyright holders.

Multiresolution analysis for compactly supported interpolating tensor product wavelets

Tommi Höynälänmaa

*Department of Physics, Tampere University of Technology
P. O. Box 692, FI-33101 Tampere, Finland*

Received 20 June 2014

Accepted 23 February 2015

Published 27 March 2015

We construct multidimensional interpolating tensor product multiresolution analyses (MRA's) of the function spaces $C_0(\mathbb{R}^n, K)$, $K = \mathbb{R}$ or $K = \mathbb{C}$, consisting of real or complex valued functions on $\mathbb{R}^n$ vanishing at infinity and the function spaces $C_u(\mathbb{R}^n, K)$ consisting of bounded and uniformly continuous functions on $\mathbb{R}^n$. We also construct an interpolating dual MRA for both of these spaces. The theory of the tensor products of Banach spaces is used. We generalize the Besov space norm equivalence from the one-dimensional case to our n -dimensional construction.

Keywords: Interpolating wavelets; multivariate wavelets; multiresolution analysis; tensor product; injective tensor norm; projective tensor norm; Besov space.

AMS Subject Classification: 46A32, 46B28, 15A69, 46E10

1. Introduction

Chui and Li⁶ have constructed a one-dimensional MRA of function space $C_u(\mathbb{R})$ (bounded and uniformly continuous complex valued functions on $\mathbb{R}$) for interpolating wavelets. Donoho¹⁷ has derived convergence results for interpolating wavelets on space $C_0(\mathbb{R})$. Goedecker's book²⁰ contains also some material about multidimensional interpolating wavelets. Goedecker²⁰ uses the term interpolating wavelets to mean Deslauriers–Dubuc wavelets whereas some other authors such as Chui and Li⁶ use the term to mean roughly wavelet families whose mother scaling function has the cardinal interpolation property $\varphi(k) = \delta_{k,0}$ for all $k \in \mathbb{Z}$ (one-dimensional case). We follow the latter convention in this paper. Chui and Li⁵ have also constructed a general framework for multivariate wavelets. However, the theory in that paper uses function space $L^2(\mathbb{R}^n)$ and so it is unsuitable for the approach in this paper. Dubuc and Deslauriers^{12,18} have investigated interpolation processes related to the Deslauriers–Dubuc fundamental functions. Han and Jia²³ have discussed

fundamental functions (see the paper for a definition) satisfying the cardinal interpolation property. Numerical values for the wavelet filters of the Deslauriers–Dubuc wavelets have been given in Refs. 20 and 30.

Theory for orthonormal wavelets has been developed e.g., by Daubechies,^{9,8} Meyer,³⁸ and Wojtaszczyk.⁴⁵ Kovačević and Sweldens³⁰ have investigated the use of digital filters for multidimensional biorthogonal wavelets. Lewis³⁶ has constructed a MRA of function space $L^2(\mathbb{R})$ for interpolating wavelets in one dimension. Lawton *et al.*³⁵ have presented conditions for the refinement mask of an orthonormal MRA. Ji and Shen²⁷ have given a condition for the refinement mask to be interpolatory and a condition for a dual refinement mask. Krivoshein and Skopina³¹ have presented convergence results for frame-like wavelets that are not frames. Karakaz'yan *et al.*²⁹ have described symmetric interpolatory masks generating dual compactly supported wavelet systems and they have also given formulas for dual refinement masks. Shui *et al.*⁴³ have shown how to construct M -band wavelets with all the following properties: compact support, orthogonality, linear-phase, regularity and interpolation. This kind of scaling functions exist only when $M \geq 4$. Dahlke *et al.*⁷ have developed a new method to construct higher-dimensional scaling functions. Their method is based on solutions to specific Lagrange interpolation problems by polynomials. Han²² has investigated symmetries of refinable functions. DeVore *et al.*¹³ have developed some theory for multidimensional orthonormal MRA of space $L^p(\mathbb{R}^d)$, $0 < p < \infty$, $d \in \mathbb{Z}_+$. He and Lai²⁵ have constructed nonseparable box spline wavelets on Sobolev spaces $H^s(\mathbb{R}^2)$. Wavelets have also been discussed in Ref. 24.

The theory about tensor products of Banach spaces has been presented e.g., in Ref. 41. We use the notation from Ref. 41 for Banach space tensor products in this paper. Schaefer's book⁴² contains some material about tensor products of topological vector spaces. Reference 37 contains also an introduction to tensor products of Banach spaces. Domański *et al.*^{15,16} have done some research on them. Michor³⁹ has represented tensor products of Banach spaces using category theory. Grothendieck²¹ gives a classical presentation for tensor products of locally convex spaces. Theory for tensor products of Banach spaces can also be found in book.¹¹ Kustermans and Vaes³² have developed some theory for space $C_0(G)$ where G is a compact or a locally compact group and for the tensor products of $C_0(G)$. Daws¹⁰ has presented some material on tensor products of Banach algebras. Glöckner¹⁹ has shown that the tensor products of topological vector spaces are not associative. Reinov⁴⁰ has investigated Banach spaces without the approximation property. Brodzki and Niblo⁴ have done some research on the rapid decay property of discrete groups and the metric approximation property.

An introduction to Besov spaces can be found e.g., in Ref. 3. An introduction to Besov spaces using the Fourier transform based definition of these spaces can be found in Ref. 44. DeVore and Popov¹⁴ have investigated the connection of Besov spaces with the dyadic spline approximation and interpolation of Besov spaces. Kyriazis and Petrushev³³ have given a method for the construction of unconditional

bases for Triebel–Lizorkin and Besov spaces. The relationship between orthonormal wavelets and Besov spaces has been discussed by Meyer.³⁸ Almeida¹ has investigated wavelet bases in (generalized) Besov spaces.

Section 2 introduces some definitions used in the rest of this paper. We give some general definitions needed by the MRA's in Sec. 3. A multivariate MRA of $C_u(\mathbb{R}^n, K)$, $K = \mathbb{R}$ or $K = \mathbb{C}$, is constructed in Sec. 4. A multivariate MRA of $C_0(\mathbb{R}^n, K)$, $K = \mathbb{R}$ or $K = \mathbb{C}$, is constructed in Sec. 5. The interpolating dual MRA is presented in Sec. 6. The Besov space norm equivalence from Donoho¹⁷ is generalized for the n -dimensional interpolating MRA's in Sec. 7. A longer version of this paper with more detailed proofs can be found at Ref. 26.

2. Preliminaries

2.1. General

The set of all positive real numbers is denoted by $\mathbb{R}_+$ and the extended real line by $\mathbb{R}_*$. The set of all positive integer numbers is denoted by $\mathbb{Z}_+$. We define $\mathbb{R}_0 := \{x \in \mathbb{R} : x \geq 0\}$ and $\mathbb{R}_{0*} := \{x \in \mathbb{R}_* : x \geq 0\}$. When A and B are arbitrary sets, f is a function from A into B , and $X \subset A$ the image of X under f is denoted by $f[X]$. The set-theoretic support of a function $f : X \rightarrow \mathbb{C}$ where X is a set is denoted by $\text{supp}_{\text{set}} f$. The topological support of a function $f : T \rightarrow \mathbb{C}$ where T is a topological space is denoted by $\text{supp } f$. When E is a metric space, $x \in E$, and $r \in \mathbb{R}_+$ the closed ball of radius r centred at x is denoted by $\overline{B}_E(x; r)$.

Definition 2.1. When $n \in \mathbb{Z}_+$ define

$$Z(n) := \{k \in \mathbb{Z}_+ : k \leq n\}.$$

We define the differences $\Delta_{\mathbf{h}}^m$ and $\Delta_{\mathbf{h}}$ as in Ref. 44 and Definition V.4.1 in Ref. 2.

Definition 2.2. Define

$$(\Delta_{\mathbf{h}}^1 f)(\mathbf{x}) := (\Delta_{\mathbf{h}} f)(\mathbf{x}) := f(\mathbf{x} + \mathbf{h}) - f(\mathbf{x})$$

for all $\mathbf{x} \in \mathbb{R}^n$, $\mathbf{h} \in \mathbb{R}^n$, and $f \in \mathbb{C}^{\mathbb{R}^n}$ and

$$\Delta_{\mathbf{h}}^m f := \Delta_{\mathbf{h}}(\Delta_{\mathbf{h}}^{m-1} f)$$

for all $m \in \mathbb{N} + 2$, $\mathbf{h} \in \mathbb{R}^n$, and $f \in \mathbb{C}^{\mathbb{R}^n}$.

Definition 2.3. Let $K = \mathbb{R}$ or $K = \mathbb{C}$ and $n \in \mathbb{Z}_+$. Let f be a function from $\mathbb{R}^n$ into K . Define

$$N_{\text{cover}}(f) := \max_{\mathbf{x} \in \mathbb{R}^n} \#\{\mathbf{k} \in \mathbb{Z}^n : f(\mathbf{x} - \mathbf{k}) \neq 0\}.$$

Definition 2.4. Let E and F be normed vector spaces. When f is a compactly supported function from E into F define

$$r_{\text{supp}}(f) := \inf\{r \in \mathbb{R}_0 : \text{supp}_{\text{set}} f \subset \overline{B}_E(0; r)\}.$$

Definition 2.5. Let $n \in \mathbb{Z}_+$. Define

$$I_{\text{trans}}(f, \mathbf{x}) := \{\mathbf{k} \in \mathbb{Z}^n : f(\mathbf{x} - \mathbf{k}) \neq 0\}$$

for all $f \in \mathbb{C}^{\mathbb{R}^n}$ and $\mathbf{x} \in \mathbb{R}^n$.

2.2. Sequences and Cartesian products

Definition 2.6. When $n \in \mathbb{Z}_+$ define

$$\mathbf{0}_n := (0)_{k \in Z(n)}.$$

Definition 2.7. When $n \in \mathbb{Z}_+$ define $J_+(n) := \{0, 1\}^n \setminus \{\mathbf{0}_n\}$.

Definition 2.8. Define $\check{\mathbf{e}}_k := (\delta_{j,k})_{j \in \mathbb{Z}}$ for all $k \in \mathbb{Z}$. When $n \in \mathbb{Z}_+$ define $\mathbf{e}_k^{[n]} := \mathbf{e}_k^{Z(n)}$ for all $k \in Z(n)$.

2.3. Vector spaces

Suppose that A and B are topological vector spaces. We define $\mathcal{L}(A, B)$ to be the set of all continuous linear functions from A into B .

The term *operator* shall mean a bounded linear function from a normed vector space into another one. The term *projection* shall mean a linear projection of a vector space onto a vector space. The topological dual of a Banach space A is denoted by A^* . Unless otherwise stated A^* is equipped with the norm topology.

When A and B are Banach spaces we use the notation $A \subset_1 B$ to mean that A is isometrically embedded in B , i.e. $A \subset B$ and the inclusion map is distance preserving. When A and B are topological vector spaces we define $A =_{\text{tvs}} B$ to be true if and only if A and B are equal topological vector spaces. When B is a Banach space we use the notation $A \subset_{\text{c.s.}} B$ to mean that A is a closed subspace of B . When E is a Banach space, $A \subset E$, and $B \subset E^*$ we define $B \perp A$ to be true if and only if $\langle \tilde{b}, a \rangle = 0$ for all $a \in A$ and $\tilde{b} \in B$.

When E is a normed vector space and $x \in E$ we may use the notation $\|x|E\|$ to mean the norm of x in E . When B is a normed vector space and we write $A :=_{\text{n.s.}} \{x \in B : P(x)\}$ we assume that $\|x|A\| := \|x|B\|$ for each $x \in A$.

When E is a Banach space and A and B open or closed subspaces of E the topological direct sum of A and B is denoted by $A \dot{+} B$.

Definition 2.9. Let E be a set and A be a vector space so that $A \subset E$. Suppose that $\|\cdot\|_A : E \rightarrow \mathbb{R}_{0*}$ is a norm on A . We say that the norm $\|\cdot\|_A$ characterizes A on E if and only if $\|x\|_A < \infty$ for all $x \in A$ and $\|y\|_A = \infty$ for all $y \in E \setminus A$.

2.4. Function spaces and sequence spaces

When $p \in [1, \infty]$, B is a Banach space, and I a denumerable set we denote the l^p space consisting of a subset of B^I by $l^p(I, B)$. As usual, $l^p(I) :=_{\text{n.s.}} l^p(I, \mathbb{C})$. When

$K = \mathbb{R}$ or $K = \mathbb{C}$, $n \in \mathbb{Z}_+$, and $p \in [1, \infty]$ we denote the L^p space consisting of a subset of the Borel functions from $\mathbb{R}^n$ into K by $L^p(\mathbb{R}^n, K)$. As usual, $L^p(\mathbb{R}^n) :=_{\text{n.s.}} L^p(\mathbb{R}^n, \mathbb{C})$. When X and Y are Borel spaces define $\text{bor}(X, Y)$ to be the set of all Borel functions from X into Y .

Let $K = \mathbb{R}$ or $K = \mathbb{C}$. When T is a topological space we denote the space of K -valued bounded and continuous functions on T by $C_b(T, K)$. When E is a metric space the space of K -valued bounded and uniformly continuous functions on E is denoted by $C_u(E, K)$. When T is a locally compact Hausdorff space the space of K -valued bounded and continuous functions vanishing at infinity^{34,17} is denoted by $C_0(T, K)$. The space of K -valued compactly supported and continuous functions on T is denoted by $C_{\text{com}}(T, K)$.

Definition 2.10. Let $K = \mathbb{R}$ or $K = \mathbb{C}$ and I be a denumerable set. Define

$$c_0(I, K) := \left\{ (a_\lambda)_{\lambda \in I} : (a_{\sigma(k)})_{k=0}^\infty \in c_0(\mathbb{N}, K) \text{ for some bijection } \sigma : \mathbb{N} \rightarrow I \right\}$$

$$\|\mathbf{a}\|_{c_0(I, K)} := \|\mathbf{a}\|_\infty, \quad \mathbf{a} \in c_0(I, K).$$

Banach space $c_0(I, K)$ is isometrically isomorphic to $c_0(\mathbb{N}, K)$.

Definition 2.11. Let $K = \mathbb{R}$ or $K = \mathbb{C}$ and $n \in \mathbb{Z}_+$. Let E be a closed subspace of $C_b(\mathbb{R}^n, K)$ for which the following condition is true:

$$\forall f \in C_b(\mathbb{R}^n, K), c \in \mathbb{R}_+, \mathbf{d} \in \mathbb{R}^n : f \in E \Leftrightarrow f(c \cdot -\mathbf{d}) \in E.$$

Let $a \in \mathbb{R}_+$, $\mathbf{b} \in \mathbb{R}^n$, and $\tilde{f} \in E^*$. The a -dilatation and $\mathbf{b}$ -translation of $\tilde{f}$, denoted by $\tilde{f}(a \cdot -\mathbf{b})$, is defined by⁶

$$\langle \tilde{f}(a \cdot -\mathbf{b}), f \rangle := \frac{1}{a^n} \left\langle \tilde{f}, f \left(\frac{\cdot + \mathbf{b}}{a} \right) \right\rangle$$

for all $f \in E$.

Definition 2.12. Let $f \in \mathbb{C}^{\mathbb{R}^n}$, $r_1 \in \mathbb{R}_+$, and $\tilde{f} \in C(\overline{B}_{\mathbb{R}^n}(0; r_1))^*$. Let $m \in \mathbb{N}$. We say that pair $(\tilde{f}, f)$ spans all the polynomials of degree at most m if and only if

$$\sum_{\mathbf{k} \in \mathbb{Z}^n} \langle \tilde{f}, p(\cdot + \mathbf{k})|_{\overline{B}_{\mathbb{R}^n}(0; r_1)} \rangle f(\mathbf{x} - \mathbf{k}) = p(\mathbf{x})$$

for all $\mathbf{x} \in \mathbb{R}^n$ and for all polynomials p of n variables that are of degree at most m .

We define the modulus of continuity in the standard way (see Definition V.4.2 in Ref. 2):

Definition 2.13. When $n \in \mathbb{Z}_+$, $m \in \mathbb{Z}_+$, and $p \in [1, \infty]$ define

$$\omega_p^m(f; t) := \sup \{ \|\Delta_{\mathbf{h}}^m f\|_{L^p(\mathbb{R}^n)} : \mathbf{h} \in \overline{B}_{\mathbb{R}^n}(0; t) \}$$

and

$$\omega(f; t) := \omega_\infty^1(f; t)$$

for all $f \in \text{bor}(\mathbb{R}^n, \mathbb{C})$ and $t \in \mathbb{R}_0$.

The Besov spaces on $\mathbb{R}^n$ are denoted by $B_{p,q}^s(\mathbb{R}^n)$. We have $\mathcal{Z}^s(\mathbb{R}^n) =_{\text{tvs}} B_{\infty,\infty}^s(\mathbb{R}^n)$ for all $s \in \mathbb{R}_+$ where $\mathcal{Z}^s(\mathbb{R}^n)$ are the Hölder–Zygmund spaces.⁴⁴ We also have $C^s(\mathbb{R}^n) =_{\text{tvs}} \mathcal{Z}^s(\mathbb{R}^n) =_{\text{tvs}} B_{\infty,\infty}^s(\mathbb{R}^n)$ when $s \in \mathbb{R}_+ \setminus \mathbb{Z}_+$ where $C^s(\mathbb{R}^n)$, $s \in \mathbb{R}_+ \setminus \mathbb{Z}_+$, are the Hölder spaces on $\mathbb{R}^n$.⁴⁴ When $m \in \mathbb{N}$ we denote the Banach space of functions with bounded and uniformly continuous partial derivatives up to m th degree equipped with the usual norm by $C^m(\mathbb{R}^n)$, see Ref. 44.

Definition 2.14. Let $n \in \mathbb{R}_+$, $s \in \mathbb{R}_+$, $p \in [1, \infty]$, and $q \in [1, \infty]$. Let $m \in \mathbb{Z}_+$ and $m > s$. Define

$$\|f\|_{B_{p,q}^s(\mathbb{R}^n);m}^{(c)} := \|f\|_{L^p(\mathbb{R}^n)} + \|t \in]0, 1[\mapsto t^{-s-\frac{1}{q}} \omega_p^m(f; t)\|_{L^q([0,1])}$$

for all $f \in \text{bor}(\mathbb{R}^n, \mathbb{C})$.

Norm $\|\cdot\|_{B_{p,q}^s(\mathbb{R}^n);m}^{(c)}$ is an equivalent norm on $B_{p,q}^s(\mathbb{R}^n)$ for the range of parameters given in Definition 2.14. Norm $\|\cdot\|_{B_{p,q}^s(\mathbb{R}^n);m}^{(c)}$ characterizes the Besov space $B_{p,q}^s(\mathbb{R}^n)$ on $\text{bor}(\mathbb{R}^n, \mathbb{C})$ for the given range of parameters. Note that $L^p(\mathbb{R}^n) \subset S'(\mathbb{R}^n)$ for all $n \in \mathbb{Z}_+$ and $p \in [1, \infty]$. See Definition V.4.3 in Ref. 2.

2.5. Tensor products

Definition 2.15. When $n \in \mathbb{Z}_+$ define

$$\check{\mathbf{e}}_{\mathbf{k}}^{\otimes} := \bigotimes_{l=1}^n \check{\mathbf{e}}_{\mathbf{k}[l]}.$$

for all $\mathbf{k} \in \mathbb{Z}^n$.

When $n \in \mathbb{Z}_+$, α is a uniform crossnorm, and $A_1, \dots, A_n$ are Banach spaces then the completed tensor product of several Banach spaces is defined by the recursive formula

$$A_1 \hat{\otimes}_{\alpha} \cdots \hat{\otimes}_{\alpha} A_n :=_{\text{n.s.}} (A_1 \hat{\otimes}_{\alpha} \cdots \hat{\otimes}_{\alpha} A_{n-1}) \hat{\otimes}_{\alpha} A_n.$$

The indexed completed tensor product is defined by

$$\bigotimes_{j=1}^n \hat{\otimes}_{\alpha} A_j :=_{\text{n.s.}} \left(\bigotimes_{j=1}^{n-1} \hat{\otimes}_{\alpha} A_j \right) \hat{\otimes}_{\alpha} A_n,$$

where $n > 1$. When $n = 1$ define

$$\bigotimes_{j=1}^1 \hat{\otimes}_{\alpha} A_j :=_{\text{n.s.}} A_1.$$

Uniform crossnorms do not generally respect subspaces. However, when X is a closed subspace of a Banach space E , Y is a closed subspace F , and α is a reasonable crossnorm on $E \otimes F$ it is possible to use the norm inherited from $E \otimes_{\alpha} F$ on vector

space $X \otimes Y$ (see Chap. 1 in Ref. 37). We give the following definition for this kind of construction.

Definition 2.16. Let E and F be Banach spaces and α a norm on $E \otimes F$. Let X be a closed subspace of E and Y a closed subspace of F . Define $X \otimes_{\alpha; E \hat{\otimes}_{\alpha} F} Y$ to be the normed vector space formed by using the norm inherited from $E \hat{\otimes}_{\alpha} F$ in the vector space $X \otimes Y$, i.e. $\|u\|_{X \otimes_{\alpha; E \hat{\otimes}_{\alpha} F} Y} := \alpha_{E, F}(u)$ for all $u \in X \otimes Y$. Define $X \hat{\otimes}_{\alpha; E \hat{\otimes}_{\alpha} F} Y$ to be the closure of $X \otimes_{\alpha; E \hat{\otimes}_{\alpha} F} Y$ in space $E \hat{\otimes}_{\alpha} F$. The notations $X \otimes_{\alpha; E \otimes F} Y$ and $X \hat{\otimes}_{\alpha; E \otimes F} Y$ may also be used for the aforementioned definitions.

Now $X \otimes_{\alpha; E \hat{\otimes}_{\alpha} F} Y$ is a normed subspace of $E \hat{\otimes}_{\alpha} F$ and $X \hat{\otimes}_{\alpha; E \hat{\otimes}_{\alpha} F} Y$ is a closed subspace of $E \hat{\otimes}_{\alpha} F$.

Definition 2.17. Let $n \in \mathbb{Z}_+$. Let $A_1, \dots, A_n$ and $B_1, \dots, B_n$ be Banach spaces so that A_1 is a closed subspace of B_1 and $B_k \otimes A_{k+1}$ is a linear subspace of B_{k+1} for $k \in Z(n-1)$. When $k \geq 2$ define

$$\bigotimes_{j=1}^k (B_j) A_j :=_{\text{n.s.}} \text{clos}_{B_k} T_k,$$

where

$$T_k :=_{\text{n.s.}} \left(\bigotimes_{j=1}^{k-1} (B_j) A_j \right) \otimes_{(B_k)} A_k.$$

When $k = 1$ define

$$\bigotimes_{j=1}^k (B_j) A_j :=_{\text{n.s.}} A_1.$$

When the assumptions of Definition 2.17 hold

$$\bigotimes_{j=1}^k (B_j) A_j$$

is a closed subspace of Banach space B_k for all $k \in Z(n)$.

Definition 2.18. Let $n \in \mathbb{Z}_+$. Let $A_1, \dots, A_n$, $B_1, \dots, B_n$, $E_1, \dots, E_n$, and $F_1, \dots, F_n$ be Banach spaces so that

- A_1 is a closed subspace of E_1 and $E_k \otimes A_{k+1}$ is a linear subspace of E_{k+1} for all $k = 1, \dots, n-1$.
- B_1 is a closed subspace of F_1 and $F_k \otimes B_{k+1}$ is a linear subspace of F_{k+1} for all $k = 1, \dots, n-1$.

Suppose that $P_k : A_k \rightarrow B_k$, $k = 1, \dots, n$ are operators. Let $S_1 := P_1$, $T_1 := S_1 = P_1$, and $S_k := T_{k-1} \otimes P_k$ for $k = 2, \dots, n$. When $k \in \{2, \dots, n\}$ and S_k is continuous let

$$T_k : \bigotimes_{l=1}^k \underset{(E_l)}{\hat{\otimes}} A_l \rightarrow \bigotimes_{l=1}^k \underset{(F_l)}{\hat{\otimes}} B_l,$$

be the unique continuous linear extension of S_k to

$$\bigotimes_{l=1}^k \underset{(E_l)}{\hat{\otimes}} A_l.$$

If $k \in \{2, \dots, n\}$ and S_k is not continuous let $T_k = 0$. When all of the functions S_k , T_k , $k = 1, \dots, n$ are operators define

$$\bigotimes_{k=1}^n \underset{(E_k, F_k)}{\hat{\otimes}} P_k = T_n.$$

If any of the functions S_k , T_k , $k = 1, \dots, n$ is not an operator then

$$\bigotimes_{k=1}^n \underset{(E_k, F_k)}{\hat{\otimes}} P_k$$

is undefined.

There is an isometric embedding

$$X^* \otimes_{\alpha^s} Y^* \subset_1 (X \otimes_{\alpha} Y)^* \quad (2.1)$$

for tensor norms α and Banach spaces X and Y ,⁴¹ see also Ref. 11. When $K = \mathbb{R}$ or $K = \mathbb{C}$, $n \in \mathbb{N} + 2$, and $X_1, \dots, X_n$ are closed subspaces of $C_b(\mathbb{R}, K)$ the tensor product $X_1 \hat{\otimes}_{\varepsilon} \dots \hat{\otimes}_{\varepsilon} X_n$ is a closed subspace of $C_b(\mathbb{R}^n, K)$.

3. General Definitions for a Compactly Supported Interpolating MRA

3.1. Mother scaling function

Definition 3.1. Let $K = \mathbb{R}$ or $K = \mathbb{C}$ and $n \in \mathbb{Z}_+$. A compactly supported interpolating mother scaling function is a function $\varphi \in C_{\text{com}}(\mathbb{R}^n, K)$ satisfying the following conditions:

(MSF.1)

$$\forall \mathbf{k} \in \mathbb{Z}^n : \varphi(\mathbf{k}) = \delta_{\mathbf{k},0}$$

(MSF.2)

$$\forall \mathbf{x} \in \mathbb{R}^n : \varphi(\mathbf{x}) = \sum_{\mathbf{k} \in \mathbb{Z}^n} \varphi\left(\frac{\mathbf{k}}{2}\right) \varphi(2\mathbf{x} - \mathbf{k}).$$

The Deslauriers–Dubuc fundamental functions satisfy these conditions.¹⁷

3.2. General definitions for the univariate MRA's

We shall denote the function space for which the MRA is defined by E in this section. We have either $E = C_u(\mathbb{R}, K)$ or $E = C_0(\mathbb{R}, K)$ where $K = \mathbb{R}$ or $K = \mathbb{C}$. We shall assume that $\varphi \in C_{\text{com}}(\mathbb{R}, K)$ is a compactly supported interpolating mother scaling function throughout this subsection.

Definition 3.2. Define function $\psi \in C_{\text{com}}(\mathbb{R}, K)$ by

$$\psi(x) := \varphi(2x - 1)$$

for all $x \in \mathbb{R}$. Function ψ is called the mother wavelet.

Definition 3.3. Define

$$\varphi_{j,k} := \varphi(2^j \cdot -k)$$

and

$$\psi_{j,k} := \psi(2^j \cdot -k)$$

for all $j \in \mathbb{Z}$ and $k \in \mathbb{Z}$.

Definition 3.4. Define

$$\zeta_s := \begin{cases} \varphi; & s = 0, \\ \psi; & s = 1, \end{cases}$$

where $s \in \{0, 1\}$.

Definition 3.5. When $k \in \mathbb{Z}$ define

$$\begin{aligned} h_k &:= \varphi\left(\frac{k}{2}\right), \\ g_k &:= \delta_{k,1}, \\ \tilde{h}_k &:= \delta_{k,0}, \\ \tilde{g}_k &:= (-1)^{k-1} h_{1-k}. \end{aligned}$$

Definition 3.6. Define $\tilde{\varphi} := \delta \in E^*$ and $\tilde{\psi} \in E^*$ by

$$\tilde{\psi} := 2 \sum_{k \in \mathbb{Z}} \tilde{g}_k \tilde{\varphi}(2 \cdot -k). \quad (3.1)$$

Define $\tilde{\varphi}_{j,k} := 2^j \tilde{\varphi}(2^j \cdot -k)$ and $\tilde{\psi}_{j,k} := 2^j \tilde{\psi}(2^j \cdot -k)$ where $j, k \in \mathbb{Z}$.

As φ is compactly supported only a finite number of numbers $h_k, k \in \mathbb{Z}$, and the other three filters defined by Definition 3.5 are nonzero. Consequently the series in Eq. (3.1) has a finite number of nonzero terms.

Definition 3.7. Define

$$\tilde{\zeta}_s := \begin{cases} \tilde{\varphi}; & s = 0, \\ \tilde{\psi}; & s = 1, \end{cases}$$

where $s \in \{0, 1\}$.

3.3. General definitions for multivariate MRA's

We will assume that $n \in \mathbb{Z}_+$ and either $K = \mathbb{R}$ or $K = \mathbb{C}$ throughout this subsection. We will also assume that $E =_{\text{n.s.}} C_u(\mathbb{R}, K)$ or $E =_{\text{n.s.}} C_0(\mathbb{R}, K)$. Furthermore, $\varphi \in C_{\text{com}}(\mathbb{R}, K)$ shall be a compactly supported interpolating mother scaling function throughout this subsection.

We set

$$F :=_{\text{n.s.}} \begin{cases} C_u(\mathbb{R}^n, K); & E = C_u(\mathbb{R}, K), \\ C_0(\mathbb{R}^n, K); & E = C_0(\mathbb{R}, K). \end{cases}$$

Definition 3.8. Define function $\varphi^{[n]} \in C_{\text{com}}(\mathbb{R}^n, K)$ by

$$\varphi^{[n]} := \bigotimes_{k=1}^n \varphi.$$

Function $\varphi^{[n]}$ is called an n -dimensional tensor product mother scaling function generated by φ . Define also $\varphi_{j,\mathbf{k}}^{[n]} := \varphi^{[n]}(2^j \cdot -\mathbf{k})$ where $j \in \mathbb{Z}$ and $\mathbf{k} \in \mathbb{Z}^n$.

Function $\varphi^{[n]}$ is a compactly supported interpolating mother scaling function on $\mathbb{R}^n$.

Definition 3.9. When $\mathbf{s} \in \{0, 1\}^n$ define function $\psi_{\mathbf{s}}^{[n]} \in C_{\text{com}}(\mathbb{R}^n, K)$ by

$$\psi_{\mathbf{s}}^{[n]} := \bigotimes_{k=1}^n \zeta_{\mathbf{s}[k]}$$

and $\psi_{\mathbf{s},j,\mathbf{k}}^{[n]} := \psi_{\mathbf{s}}^{[n]}(2^j \cdot -\mathbf{k})$.

The domain of the Dirac δ functional varies in this paper. That is, we may keep δ as an element of different dual spaces A^* . When $z_1, \dots, z_m \in \mathbb{R}$ we will identify $\delta(\cdot - z_1) \otimes \dots \otimes \delta(\cdot - z_m)$ with $\delta(\cdot - (z_1, \dots, z_m))$.

Definition 3.10. Define $\tilde{\varphi}^{[n]} \in F^*$ by

$$\tilde{\varphi}^{[n]} := \bigotimes_{l=1}^n \tilde{\varphi}$$

and $\tilde{\varphi}_{j,\mathbf{k}}^{[n]} \in F^*$ by $\tilde{\varphi}_{j,\mathbf{k}}^{[n]} := 2^j \tilde{\varphi}^{[n]}(2^j \cdot -\mathbf{k})$ where $j \in \mathbb{Z}$ and $\mathbf{k} \in \mathbb{Z}^n$. Define also $\tilde{\psi}_{\mathbf{s}}^{[n]} \in F^*$ by

$$\tilde{\psi}_{\mathbf{s}}^{[n]} := \bigotimes_{l=1}^n \tilde{\zeta}_{\mathbf{s}[l]},$$

where $\mathbf{s} \in \{0, 1\}^n$ and $\tilde{\psi}_{\mathbf{s},j,\mathbf{k}}^{[n]} \in F^*$ by $\tilde{\psi}_{\mathbf{s},j,\mathbf{k}}^{[n]} := 2^j \tilde{\psi}_{\mathbf{s}}^{[n]}(2^j \cdot -\mathbf{k})$ where $\mathbf{s} \in \{0, 1\}^n$, $j \in \mathbb{Z}$, and $\mathbf{k} \in \mathbb{Z}^n$.

Goedecker²⁰ gives formulas for wavelet filters, too.

Lemma 3.1. *Let $f \in \mathbb{C}$, $m \in \mathbb{N}$, $r_1 \in \mathbb{R}_+$, and $\tilde{f} \in C(\overline{B}_{\mathbb{R}}(0; r_1))^*$. Let*

$$f^{[n]} := \bigotimes_{i=0}^n f$$

and

$$\tilde{f}^{[n]} := \bigotimes_{i=0}^n \tilde{f}.$$

If $(\tilde{f}, f)$ spans all polynomials of degree at most m then $(\tilde{f}^{[n]}, f^{[n]})$ spans all polynomials of degree at most m .

Proof. Let

$$p(\mathbf{x}) := \prod_{i=1}^n p_i(\mathbf{x}[i]) = \prod_{i=1}^n (\mathbf{x}[i])^{\mathbf{a}[i]},$$

where $\mathbf{a}[i] \in Z_0(m)$, $i = 1, \dots, n$. Define $r_2 \in \mathbb{R}_+$ so that $(\overline{B}_{\mathbb{R}}(0; r_1))^n \subset \overline{B}_{\mathbb{R}^n}(0; r_2)$. Now

$$\begin{aligned} & \sum_{\mathbf{k} \in \mathbb{Z}^n} \langle \tilde{f}^{[n]}(\cdot - \mathbf{k}), p|_{\overline{B}_{\mathbb{R}^n}(\mathbf{k}; r_2)} \rangle f^{[n]}(\mathbf{x} - \mathbf{k}) \\ &= \sum_{k_1 \in \mathbb{Z}} \cdots \sum_{k_n \in \mathbb{Z}} \prod_{i=1}^n \langle \tilde{f}(\cdot - \mathbf{k}[i]), p_i|_{\overline{B}_{\mathbb{R}}(\mathbf{k}[i]; r_1)} \rangle f(\mathbf{x}[i] - \mathbf{k}[i]) \\ &= \prod_{i=1}^n \sum_{k \in \mathbb{Z}} \langle \tilde{f}(\cdot - k), p_i|_{\overline{B}_{\mathbb{R}}(k; r_1)} \rangle f(\mathbf{x}[i] - k) = \prod_{i=1}^n p_i(\mathbf{x}[i]) = p(\mathbf{x}) \end{aligned}$$

for all $\mathbf{x} \in \mathbb{R}^n$. □

In particular, if φ spans all polynomials of degree at most m then $\varphi^{[n]}$ spans all polynomials of n variables and of degree at most m .

4. Compactly Supported Interpolating MRA of $C_u(\mathbb{R}^n, K)$

We will assume that $n \in \mathbb{Z}_+$ and $K = \mathbb{R}$ or $K = \mathbb{C}$ throughout this section. We will also assume that $\varphi^{[n]} \in C_{\text{com}}(\mathbb{R}^n, K)$ is an n -dimensional tensor product mother scaling function in this section. Unless otherwise stated, we shall assume that the same values of n , K , and $\varphi^{[n]}$ are used throughout this section. Chui and Li⁶ have developed a MRA in the univariate case $C_u(\mathbb{R})$.

Definition 4.1. Define

$$V_{n,j}^{(u)} := \left\{ \mathbf{x} \in \mathbb{R}^n \mapsto \sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{a}[\mathbf{k}] \varphi^{[n]}(2^j \mathbf{x} - \mathbf{k}) : \mathbf{a} \in l^\infty(\mathbb{Z}^n, K) \right\} \quad (4.1)$$

$$\|f|V_{n,j}^{(u)}\| := \|f\|_\infty, \quad f \in V_{n,j}^{(u)}$$

for all $j \in \mathbb{Z}$.

Definition 4.2. Let spaces $V_{n,j}^{(u)}$, $j \in \mathbb{Z}$, be defined by Definition 4.1. We call $\{V_{n,j}^{(u)} : j \in \mathbb{Z}\}$ an interpolating tensor product MRA of $C_u(\mathbb{R}^n, K)$ generated by $\varphi^{[n]}$ provided that the following conditions are satisfied:

- (MRA1.1) $\forall j \in \mathbb{Z} : V_{n,j}^{(u)} \subset V_{n,j+1}^{(u)}$
- (MRA1.2) $\bigcup_{j \in \mathbb{Z}} V_{n,j}^{(u)} = C_u(\mathbb{R}^n, K)$
- (MRA1.3) $\bigcap_{j \in \mathbb{Z}} V_{n,j}^{(u)} = K$
- (MRA1.4) $\forall j \in \mathbb{Z}, f \in K^{\mathbb{R}^n} : f \in V_{n,j}^{(u)} \Leftrightarrow f(2 \cdot) \in V_{n,j+1}^{(u)}$
- (MRA1.5) $\forall j \in \mathbb{Z}, \mathbf{k} \in \mathbb{Z}^n, f \in K^{\mathbb{R}^n} : f \in V_{n,j}^{(u)} \Leftrightarrow f(\cdot - 2^{-j}\mathbf{k}) \in V_{n,j}^{(u)}$
- (MRA1.6) $\forall \mathbf{k} \in \mathbb{Z}^n : \varphi^{[n]}(\mathbf{k}) = \delta_{\mathbf{k},0}$.

Our requirements for the definition of interpolating multiresolution analysis are stricter and simpler than those in Ref. 6. Condition (MRA1.6) is replaced by a weaker condition for φ in Ref. 6 but it is possible to construct function φ_L that satisfies condition (MRA1.6) and generates the same subspaces $V_{1,j}^{(u)}$ as function φ .

Under the conditions given at the start of this section ($\varphi^{[n]}$ is an n -dimensional tensor product mother scaling function) the conditions (MRA1.1), (MRA1.4), (MRA1.5) and (MRA1.6) are true. We will show later that conditions (MRA1.2) and (MRA1.3) are true, too.

Spaces $V_{n,j}^{(u)}$, $j \in \mathbb{Z}$, are topologically isomorphic to $l^\infty(\mathbb{Z}^n, K)$. It has been proved in Ref. 28 that

$$\sum_{\mathbf{k} \in \mathbb{Z}^n} \varphi^{[n]}(\mathbf{y} - \mathbf{k}) = \widehat{\varphi^{[n]}}(0)$$

for all $\mathbf{y} \in \mathbb{R}^n$. It follows from the cardinal interpolation property (MSF.1) that

$$\sum_{\mathbf{k} \in \mathbb{Z}^n} \varphi^{[n]}(\mathbf{y} - \mathbf{k}) = 1 \tag{4.2}$$

for all $\mathbf{y} \in \mathbb{R}^n$.

Remark 4.1. The series in Eq. (4.1) converges (pointwise) for all $\mathbf{a} \in l^\infty(\mathbb{Z}^n, K)$ but the series $\sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{a}[\mathbf{k}] \varphi^{[n]}(2^j \cdot - \mathbf{k})$ need not converge in the norm topology of $C_u(\mathbb{R}^n, K)$. For example, consider sequence $\mathbf{a}[\mathbf{k}] = 1$, $\mathbf{k} \in \mathbb{Z}^n$. Now $\sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{a}[\mathbf{k}] \varphi^{[n]}(2^j \mathbf{x} - \mathbf{k}) = 1$ for all $\mathbf{x} \in \mathbb{R}^n$ but the series $\sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{a}[\mathbf{k}] \varphi^{[n]}(2^j \cdot - \mathbf{k})$ does not converge in the norm topology of $C_u(\mathbb{R}^n, K)$.

Theorem 4.1. *We have*

$$\bigcap_{j \in \mathbb{Z}} V_{n,j}^{(u)} = K.$$

Proof. The proof is similar to a part of the proof of [6, Theorem 3.2]. □

Definition 4.3. When $j \in \mathbb{Z}$ and $\mathbf{s} \in \{0, 1\}^n$ define

$$W_{n,\mathbf{s},j}^{(u)} := \left\{ \mathbf{x} \in \mathbb{R}^n \mapsto \sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{a}[\mathbf{k}] \psi_{\mathbf{s},j,\mathbf{k}}^{[n]}(\mathbf{x}) : \mathbf{a} \in l^\infty(\mathbb{Z}^n, K) \right\}$$

$$\|f\|_{W_{n,\mathbf{s},j}^{(u)}} := \|f\|_\infty, \quad f \in W_{n,\mathbf{s},j}^{(u)}.$$

Spaces $W_{n,\mathbf{s},j}^{(u)}$, $\mathbf{s} \in \{0, 1\}^n$, $j \in \mathbb{Z}$, are topologically isomorphic to $l^\infty(\mathbb{Z}^n, K)$.

Definition 4.4. When $\mathbf{s} \in \{0, 1\}^n$ and $j \in \mathbb{Z}$ define

$$(Q_{n,\mathbf{s},j}^{(u)} f)(\mathbf{x}) := \sum_{\mathbf{k} \in \mathbb{Z}^n} \langle \tilde{\psi}_{\mathbf{s},j,\mathbf{k}}^{[n]}, f \rangle \psi_{\mathbf{s},j,\mathbf{k}}^{[n]}(\mathbf{x})$$

for all $\mathbf{x} \in \mathbb{R}^n$ and $f \in C_u(\mathbb{R}^n, K)$. When $j \in \mathbb{Z}$ define $P_{n,j}^{(u)} := Q_{n,\mathbf{0}_n,j}^{(u)}$.

Operator $Q_{n,\mathbf{s},j}^{(u)}$ is a continuous projection of $C_u(\mathbb{R}^n, K)$ onto $W_{n,\mathbf{s},j}^{(u)}$ for each $\mathbf{s} \in \{0, 1\}^n$ and $j \in \mathbb{Z}$.

Definition 4.5. When $j \in \mathbb{Z}$ define

$$W_{n,j}^{(u)} :=_{\text{n.s.}} \sum_{\mathbf{s} \in J_+(n)} W_{n,\mathbf{s},j}^{(u)}$$

and

$$Q_{n,j}^{(u)} := \sum_{\mathbf{s} \in J_+(n)} Q_{n,\mathbf{s},j}^{(u)}.$$

Spaces $W_{n,j}^{(u)}$, $j \in \mathbb{Z}$, are topologically isomorphic to $l^\infty(J_+(n) \times \mathbb{Z}^n, K)$. When $j \in \mathbb{Z}$ we have

$$V_{n,j+1}^{(u)} =_{\text{n.s.}} V_{n,j}^{(u)} \dot{+} W_{n,j}^{(u)} =_{\text{n.s.}} V_{n,j}^{(u)} \dot{+} \sum_{\mathbf{s} \in J_+(n)} W_{n,\mathbf{s},j}^{(u)} =_{\text{n.s.}} \sum_{\mathbf{s} \in \{0,1\}^n} W_{n,\mathbf{s},j}^{(u)}. \quad (4.3)$$

Operator $Q_{n,j}^{(u)}$ is a continuous projection of $C_u(\mathbb{R}^n, K)$ onto $W_{n,j}^{(u)}$ for each $j \in \mathbb{Z}$.

We also have $Q_{n,j}^{(u)} = P_{n,j+1}^{(u)} - P_{n,j}^{(u)}$ for all $j \in \mathbb{Z}$.

Theorem 4.2. *There exist $c_1 \in \mathbb{R}_+$ and $c_2 \in \mathbb{R}_+$ so that*

$$\|f - P_{n,j}^{(u)} f\|_\infty \leq c_1 \omega(f; 2^{-j} c_2)$$

for all $f \in C_u(\mathbb{R}^n)$ and $j \in \mathbb{Z}$.

Proof. Let $f \in C_u(\mathbb{R}^n)$ and $j \in \mathbb{Z}$. Define $r_1 := r_{\text{supp}}(\varphi^{[n]})$. Let $\mathbf{x} \in \mathbb{R}^n$. Define $I := I_{\text{trans}}(\varphi^{[n]}, 2^j \mathbf{x})$. Now by Eq. (4.2) we have

$$\begin{aligned} (f - P_{n,j}^{(u)} f)(\mathbf{x}) &= \sum_{\mathbf{k} \in \mathbb{Z}^n} \left(f(\mathbf{x}) - f\left(\frac{\mathbf{k}}{2^j}\right) \right) \varphi^{[n]}(2^j \mathbf{x} - \mathbf{k}) \\ &= \sum_{\mathbf{k} \in I} \left(f(\mathbf{x}) - f\left(\frac{\mathbf{k}}{2^j}\right) \right) \varphi^{[n]}(2^j \mathbf{x} - \mathbf{k}). \end{aligned}$$

Let $\ell \in I$. Now $2^j \mathbf{x} - \ell \in \overline{B}_{\mathbb{R}^n}(0; r_1)$ from which it follows that $\mathbf{x} - 2^{-j} \ell \in \overline{B}_{\mathbb{R}^n}(0; 2^{-j} r_1)$. Hence

$$\left| f(\mathbf{x}) - f\left(\frac{\ell}{2^j}\right) \right| \leq \omega(f; 2^{-j} r_1). \quad (4.4)$$

Let $c_1 := N_{\text{cover}}(\varphi^{[n]}) \|\varphi^{[n]}\|_\infty$ and $c_2 := r_1 = r_{\text{supp}}(\varphi^{[n]})$. By Eq. (4.4) we have

$$|(f - P_{n,j}^{(u)} f)(\mathbf{x})| \leq c_1 \omega(f; 2^{-j} c_2). \quad \square$$

Theorem 4.3. *Let $f \in C_u(\mathbb{R}^n)$. Now*

$$\lim_{j \rightarrow \infty} \|f - P_{n,j}^{(u)} f\|_\infty = 0.$$

Proof. See also Theorem 3.2 in Ref. 6 and Theorem 2.4 in Ref. 17. Let $j \in \mathbb{Z}$. By Theorem 4.2 we have $\|f - P_{n,j}^{(u)} f\|_\infty \leq c_1 \omega(f; 2^{-j} c_2)$ where c_1 and c_2 do not depend on j or f . Since f is uniformly continuous

$$\lim_{t \rightarrow 0} \omega(f; t) = 0$$

and hence

$$\lim_{j \rightarrow \infty} \|f - P_{n,j}^{(u)} f\|_\infty = 0. \quad \square$$

Corollary 4.1.

$$\overline{\bigcup_{j \in \mathbb{Z}} V_{n,j}^{(u)}} = C_u(\mathbb{R}^n, K).$$

Theorem 4.4. *Let $t \in \mathbb{R}_+$. There exists a constant $c_1 \in \mathbb{R}_+$, which may depend on t , so that*

$$\forall f \in C_u(\mathbb{R}^n), \quad j \in \mathbb{Z} : \omega(P_{n,j}^{(u)} f; 2^{-j} t) \leq c_1 \omega(f; 2^{-j} \sqrt{n}).$$

Proof. The proof of case $n = 1$ is similar to the proof in Sec. 7.1 in Ref. 17. We will assume that $n \geq 2$ in the sequel. Define bijection $\sigma_c^{[n]} : \mathbb{N} \rightarrow \mathbb{Z}^n$ so that $\|\sigma_c^{[n]}(p+1) - \sigma_c^{[n]}(p)\|_\infty = 1$ for all $p \in \mathbb{N}$. It can be proved that this kind of bijection always exists.²⁶ Define

$$\begin{aligned} v_{j,l}(\mathbf{x}, \mathbf{h}) := & \sum_{p=0}^l (\varphi^{[n]}(2^j \mathbf{x} - \sigma_c^{[n]}(p) - \lfloor 2^j \mathbf{x} \rfloor + 2^j \mathbf{h}) \\ & - \varphi^{[n]}(2^j \mathbf{x} - \sigma_c^{[n]}(p) - \lfloor 2^j \mathbf{x} \rfloor)), \end{aligned}$$

where $j, l \in \mathbb{N}$, $\mathbf{x} \in \mathbb{R}^n$, and $\mathbf{h} \in \overline{B}_{\mathbb{R}^n}(0; 2^{-j} t)$. Using Eq. (4.2) it can be proved that there exists $c_1 \in \mathbb{R}_+$ so that

$$\sum_{l=0}^{\infty} |v_{j,l}(\mathbf{x}, \mathbf{h})| \leq c_1$$

for all $j \in \mathbb{N}$, $\mathbf{x} \in \mathbb{R}^n$, and $\mathbf{h} \in \overline{B}_{\mathbb{R}^n}(0; 2^{-j}t)$. Let $f \in C_u(\mathbb{R}^n)$, $j_1 \in \mathbb{Z}$, $\mathbf{x}_1 \in \mathbb{R}^n$, and $\mathbf{h}_1 \in \overline{B}_{\mathbb{R}^n}(0; 2^{-j_1}t)$. Let $\mathbf{a} := (f(2^{-j_1}\mathbf{k}))_{\mathbf{k} \in \mathbb{Z}^n}$. Now

$$\begin{aligned} z &:= (P_{n,j_1}^{(u)}f)(\mathbf{x}_1 + \mathbf{h}_1) - (P_{n,j_1}^{(u)}f)(\mathbf{x}_1) \\ &= \sum_{l=0}^{\infty} (\mathbf{a}[\sigma_c^{[n]}(l)] - \mathbf{a}[\sigma_c^{[n]}(l+1)])v_{j_1,l}(\mathbf{x}_1, \mathbf{h}_1) \end{aligned}$$

from which it follows that

$$|z| \leq \left(\sup_{l \in \mathbb{N}} |\mathbf{a}[\sigma_c^{[n]}(l)] - \mathbf{a}[\sigma_c^{[n]}(l+1)]| \right) \cdot \sum_{l=0}^{\infty} |v_{j_1,l}(\mathbf{x}_1, \mathbf{h}_1)| \leq \omega(f; 2^{-j}\sqrt{n}) \cdot c_1. \quad \square$$

Theorem 4.5. *Let $j_0 \in \mathbb{Z}$. Suppose that the mother scaling function φ is Lipschitz continuous and let $\varphi^{[n]}$ be the tensor product mother scaling function generated by φ . Then*

$$V_{n,j_0}^{(u)} \dot{+} \sum_{j=j_0}^{\infty} W_{n,j}^{(u)} \neq C_u(\mathbb{R}^n, K).$$

Proof. Let

$$A := V_{n,j_0}^{(u)} \dot{+} \sum_{j=j_0}^{\infty} W_{n,j}^{(u)}.$$

Define function $f \in C_u(\mathbb{R}, K)$ by

$$f(x) := \begin{cases} \sqrt{x}; & x \in [0, 1], \\ -x + 2; & x \in [1, 2], \\ 0; & x \leq 0 \vee x \geq 2 \end{cases}$$

and function $f^{[n]} \in C_u(\mathbb{R}^n, K)$ by

$$f^{[n]} := \bigotimes_{k=1}^n f.$$

Functions f and $f^{[n]}$ are not Lipschitz continuous. As φ is Lipschitz continuous all the functions $P_{n,j}^{(u)}g$ are Lipschitz continuous for each $g \in C_u(\mathbb{R}^n, K)$. A is a locally convex space with an inductive limit topology. It follows from Theorem 6.2 in Ref. 42 that the space A is complete.

Suppose that A would be equal to $C_u(\mathbb{R}^n, K)$ as a set. Then we would have $f^{[n]} \in A$. It follows from the definition of the locally convex direct sum that

$$f^{[n]} \in V_{n,j_0}^{(u)} \dot{+} \sum_{j=j_0}^{j_1} W_{n,j}^{(u)}$$

for some $j_1 \in \mathbb{Z}$, $j_1 \geq j_0$. Now $f^{[n]} = P_{n,j_1+1}^{(u)}f^{[n]}$. It follows that $f^{[n]}$ is Lipschitz continuous, which is a contradiction. Hence A is not equal to $C_u(\mathbb{R}^n, K)$ as a set. $\square$

The definition of locally convex direct sums from Ref. 42 is used here. An example of a Lipschitz continuous mother scaling function is a Deslauriers–Dubuc fundamental function with Hölder regularity greater than 1. By Eq. (4.3) and Corollary 4.1 we have

$$C_u(\mathbb{R}^n, K) =_{\text{n.s.}} \text{clos} \left(\bigcup_{l=j_0}^{\infty} \left(V_{n,j_0}^{(u)} + \sum_{j=j_0}^l W_{n,j}^{(u)} \right) \right)$$

for all $j_0 \in \mathbb{Z}$.

5. Compactly Supported Interpolating MRA of $C_0(\mathbb{R}^n, K)$

A MRA of space $C_0(\mathbb{R}^n, K)$ can be developed in the same way as the MRA of space $C_u(\mathbb{R}^n, K)$. Donoho¹⁷ has developed a MRA for the one-dimensional case $C_0(\mathbb{R})$. We will assume that $n \in \mathbb{Z}_+$ and $K = \mathbb{R}$ or $K = \mathbb{C}$ throughout this section. We will also assume that $\varphi^{[n]} \in C_{\text{com}}(\mathbb{R}^n, K)$ is an n -dimensional tensor product mother scaling function in this section. Unless otherwise stated, we shall assume that the same values of n , K , and $\varphi^{[n]}$ are used throughout this section. Note that many of the series that are pointwise convergent with $C_u(\mathbb{R}^n, K)$ converge in the norm in $C_0(\mathbb{R}^n, K)$. We are also able to represent many subspaces and operators related to the MRA of $C_0(\mathbb{R}^n, K)$ as tensor products of the corresponding one-dimensional cases.

Definition 5.1. Define

$$V_{n,j}^{(0)} := \left\{ \sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{a}[\mathbf{k}] \varphi^{[n]}(2^j \cdot -\mathbf{k}) : \mathbf{a} \in c_0(\mathbb{Z}^n, K) \right\} \quad (5.1)$$

$$\|f|_{V_{n,j}^{(0)}}\| := \|f\|_{\infty}, \quad f \in V_{n,j}^{(0)}$$

for each $j \in \mathbb{Z}$.

Definition 5.2. Let spaces $V_{n,j}^{(0)}$, $j \in \mathbb{Z}$, be defined by Definition 5.1. We call $\{V_{n,j}^{(0)} : j \in \mathbb{Z}\}$ an interpolating tensor product MRA of $C_0(\mathbb{R}^n, K)$ generated by $\varphi^{[n]}$ provided that the following conditions are satisfied:

$$\text{(MRA2.1)} \quad \forall j \in \mathbb{Z} : V_{n,j}^{(0)} \subset V_{n,j+1}^{(0)}$$

$$\text{(MRA2.2)} \quad \bigcup_{j \in \mathbb{Z}} V_{n,j}^{(0)} = C_0(\mathbb{R}^n, K)$$

$$\text{(MRA2.3)} \quad \bigcap_{j \in \mathbb{Z}} V_{n,j}^{(0)} = \{0\}$$

$$\text{(MRA2.4)} \quad \forall j \in \mathbb{Z}, f \in K^{\mathbb{R}^n} : f \in V_{n,j}^{(0)} \Leftrightarrow f(2 \cdot) \in V_{n,j+1}^{(0)}$$

$$\text{(MRA2.5)} \quad \forall j \in \mathbb{Z}, \mathbf{k} \in \mathbb{Z}^n, f \in K^{\mathbb{R}^n} : f \in V_{n,j}^{(0)} \Leftrightarrow f(\cdot - 2^{-j}\mathbf{k}) \in V_{n,j}^{(0)}$$

$$\text{(MRA2.6)} \quad \forall \mathbf{k} \in \mathbb{Z}^n : \varphi^{[n]}(\mathbf{k}) = \delta_{\mathbf{k},0}$$

Note that in this definition the intersection of spaces $V_{n,j}^{(0)}$ is $\{0\}$ instead of $\mathbb{C}$ (all complex valued constant functions on $\mathbb{R}^n$) as in Ref. 6 since here the MRA

is constructed for functions vanishing at infinity. Donoho¹⁷ does not require the mother scaling function φ to be compactly supported but φ has to be of rapid decay in his construction. He also includes requirements for the regularity and polynomial span of φ , which are needed for the norm equivalences to Besov and Triebel–Lizorkin spaces, into the definition of the MRA. Under the conditions given at the start of this section ($\varphi^{[n]}$ is an n -dimensional tensor product mother scaling function) the conditions (MRA2.1), (MRA2.2), (MRA2.3), (MRA2.4), (MRA2.5) and (MRA2.6) are true.

Definition 5.3. Let $j \in \mathbb{Z}$ and $\mathbf{s} \in \{0, 1\}^n$. Define

$$W_{n,\mathbf{s},j}^{(0)} := \left\{ \sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{a}[\mathbf{k}] \psi_{\mathbf{s},j,\mathbf{k}}^{[n]} : \mathbf{a} \in c_0(\mathbb{Z}^n, K) \right\}$$

$$\|f\|_{W_{n,\mathbf{s},j}^{(0)}} := \|f\|_{\infty}, \quad f \in W_{n,\mathbf{s},j}^{(0)}.$$

Definition 5.4. Let $j \in \mathbb{Z}$. Define operator $P_{n,j}^{(0)} : C_0(\mathbb{R}^n, K) \rightarrow V_{n,j}^{(0)}$ by

$$P_{n,j}^{(0)} f = \sum_{\mathbf{k} \in \mathbb{Z}^n} \langle \tilde{\varphi}_{j,\mathbf{k}}^{[n]}, f \rangle \varphi_{j,\mathbf{k}}^{[n]}$$

for all $f \in C_0(\mathbb{R}^n, K)$. Define operator $Q_{n,\mathbf{s},j}^{(0)} : C_0(\mathbb{R}^n, K) \rightarrow W_{n,\mathbf{s},j}^{(0)}$ by

$$Q_{n,\mathbf{s},j}^{(0)} f = \sum_{\mathbf{k} \in \mathbb{Z}^n} \langle \tilde{\psi}_{\mathbf{s},j,\mathbf{k}}^{[n]}, f \rangle \psi_{\mathbf{s},j,\mathbf{k}}^{[n]}$$

for all $f \in C_0(\mathbb{R}^n, K)$ and $\mathbf{s} \in \{0, 1\}^n$.

We now have

$$\begin{aligned} V_{n,j}^{(0)} &=_{\text{n.s.}} \bigotimes_{\varepsilon, k=1}^n V_{1,j}^{(0)}, & W_{n,\mathbf{s},j}^{(0)} &=_{\text{n.s.}} \bigotimes_{\varepsilon, k=1}^n W_{1,\mathbf{s}[k],j}^{(0)}, \\ P_{n,j}^{(0)} &= \bigotimes_{\varepsilon, k=1}^n P_{1,j}^{(0)}, & \text{and } Q_{n,\mathbf{s},j}^{(0)} &= \bigotimes_{\varepsilon, k=1}^n Q_{1,\mathbf{s}[k],j}^{(0)}. \end{aligned}$$

We give now a general result on the tensor products of the function space $C_0(\mathbb{R}, K)$ with itself.

Theorem 5.1. *We have*

$$\bigotimes_{\varepsilon, j=1}^n C_0(\mathbb{R}, K) =_{\text{n.s.}} C_0(\mathbb{R}^n, K).$$

Proof. Define

$$F^{[n]} :=_{\text{n.s.}} \bigotimes_{\varepsilon, j=1}^n C_0(\mathbb{R}, K).$$

We have $F^{[n]} \subset C_0(\mathbb{R}^n, K)$. Let φ be the Deslauriers–Dubuc fundamental function of some degree m and $\varphi^{[n]}$ the n -dimensional tensor product mother scaling function

generated by φ . Let spaces $V_{1,j}^{(0)}$, $j \in \mathbb{Z}$, belong to the interpolating multiresolution analysis generated by φ and spaces $V_{n,j}^{(0)}$, $j \in \mathbb{Z}$, be the corresponding tensor product spaces. Let $f \in C_0(\mathbb{R}^n, K)$. It follows from Theorem 4.3 that $P_{n,j}^{(0)} f \rightarrow f$ as $j \rightarrow \infty$. Now $P_{n,j}^{(0)} f \in V_{n,j}^{(0)} \subset F^{[n]}$ for all $j \in \mathbb{Z}$ from which it follows that $f \in \overline{F^{[n]}} = F^{[n]}$. Consequently $F^{[n]} =_{\text{n.s.}} C_0(\mathbb{R}^n, K)$. $\square$

For example, $C_0(\mathbb{R}) \hat{\otimes}_\varepsilon C_0(\mathbb{R}) =_{\text{n.s.}} C_0(\mathbb{R}^2)$. As in the case of $C_u(\mathbb{R}^n, K)$ we get

$$V_{n,j_0}^{(0)} \dot{+} \sum_{j=j_0}^{\infty} W_{n,j}^{(0)} \neq C_0(\mathbb{R}^n, K)$$

when the mother scaling function is Lipschitz continuous. We also have

$$C_0(\mathbb{R}^n, K) =_{\text{n.s.}} \text{clos} \left(\bigcup_{l=j_0}^{\infty} \left(V_{n,j_0}^{(0)} \dot{+} \sum_{j=j_0}^l W_{n,j}^{(0)} \right) \right)$$

for all $j_0 \in \mathbb{Z}$.

6. Interpolating Dual MRA

We shall have $K = \mathbb{R}$ or $K = \mathbb{C}$ and $n \in \mathbb{Z}_+$ throughout this section. We shall also have $E = C_u(\mathbb{R}^n, K)$ or $E = C_0(\mathbb{R}^n, K)$.

6.1. General

Definition 6.1. When $j \in \mathbb{Z}$ define

$$\tilde{V}_{n,j} :=_{\text{n.s.}} \left\{ \sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{d}[\mathbf{k}] \tilde{\varphi}_{j,\mathbf{k}}^{[n]} : \mathbf{d} \in l^1(\mathbb{Z}^n, K) \right\}$$

$$\|\tilde{f}| \tilde{V}_{n,j}\| := \|\tilde{f}| C_u(\mathbb{R}^n, K)^*\| = \|\tilde{f}| C_0(\mathbb{R}^n, K)^*\|, \quad \tilde{f} \in \tilde{V}_{n,j}.$$

We may identify Banach space $\tilde{V}_{n,j}$ for both $E = C_u(\mathbb{R}^n, K)$ and $E = C_0(\mathbb{R}^n, K)$ for each $j \in \mathbb{Z}$. It follows also that function $\tilde{\iota}_{n,j} : l^1(\mathbb{Z}^n, K) \rightarrow \tilde{V}_{n,j}$ defined by

$$\tilde{\iota}_{n,j}(\mathbf{d}) := \sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{d}[\mathbf{k}] \tilde{\varphi}_{j,\mathbf{k}}^{[n]}$$

for all $\mathbf{d} \in l^1(\mathbb{Z}^n, K)$ is an isometric isomorphism from $l^1(\mathbb{Z}^n, K)$ onto $\tilde{V}_{n,j}$. We have

$$\tilde{f} \in \tilde{V}_{n,j} \Leftrightarrow \tilde{f}(2 \cdot) \in \tilde{V}_{n,j+1}$$

and

$$\tilde{f} \in \tilde{V}_{n,j} \Leftrightarrow \tilde{f}(\cdot - 2^{-j} \mathbf{k}) \in \tilde{V}_{n,j}.$$

for all $\tilde{f} \in C_u(\mathbb{R}^n, K)^*$, $j \in \mathbb{Z}$, and $\mathbf{k} \in \mathbb{Z}^n$.

Definition 6.2. When $j \in \mathbb{Z}$ and $\mathbf{s} \in \{0, 1\}^n$ define

$$\tilde{W}_{n,\mathbf{s},j} :=_{\text{n.s.}} \left\{ \sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{d}[\mathbf{k}] \tilde{\psi}_{\mathbf{s},j,\mathbf{k}}^{[n]} : \mathbf{d} \in l^1(\mathbb{Z}^n, K) \right\},$$

$$\|\tilde{f}\|_{\tilde{W}_{n,\mathbf{s},j}} := \|\tilde{f}\|_{C_u(\mathbb{R}^n, K)^*} = \|\tilde{f}\|_{C_0(\mathbb{R}^n, K)^*}, \quad \tilde{f} \in \tilde{W}_{n,\mathbf{s},j}.$$

Spaces $\tilde{W}_{n,\mathbf{s},j}$, $\mathbf{s} \in \{0, 1\}^n$, $j \in \mathbb{Z}$, are topologically isomorphic to $l^1(\mathbb{Z}^n, K)$. Assume that $j \in \mathbb{Z}$, $\mathbf{d} \in l^1(J_+(n) \times \mathbb{Z}^n, K)$, and

$$\tilde{f} := \sum_{\mathbf{s} \in J_+(n)} \sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{d}[\mathbf{s}, \mathbf{k}] \tilde{\psi}_{\mathbf{s},j,\mathbf{k}}^{[n]}.$$

Now $\|\tilde{f}\|_{C_u(\mathbb{R}^n, K)^*} = \|\tilde{f}\|_{C_0(\mathbb{R}^n, K)^*}$. Consequently we may identify the Banach space $\tilde{W}_{n,\mathbf{s},j}$ for both $E = C_u(\mathbb{R}^n, K)$ and $E = C_0(\mathbb{R}^n, K)$ for each $\mathbf{s} \in \{0, 1\}^n$ and $j \in \mathbb{Z}$.

Definition 6.3. When $n \in \mathbb{Z}_+$ and $j \in \mathbb{Z}$ define

$$\tilde{P}_{n,j} \tilde{f} := \sum_{\mathbf{k} \in \mathbb{Z}^n} \langle \tilde{f}, \varphi_{j,\mathbf{k}}^{[n]} \rangle \tilde{\varphi}_{j,\mathbf{k}}^{[n]}$$

for all $\tilde{f} \in E^*$.

Definition 6.4. When $n \in \mathbb{Z}_+$, $\mathbf{s} \in \{0, 1\}^n$, and $j \in \mathbb{Z}$ define

$$\tilde{Q}_{n,\mathbf{s},j} \tilde{f} := \sum_{\mathbf{k} \in \mathbb{Z}^n} \langle \tilde{f}, \psi_{\mathbf{s},j,\mathbf{k}}^{[n]} \rangle \tilde{\psi}_{\mathbf{s},j,\mathbf{k}}^{[n]}$$

for all $\tilde{f} \in E^*$.

We have $\tilde{Q}_{n,\mathbf{0}_n,j} = \tilde{P}_{n,j}$ for all $j \in \mathbb{Z}$.

Lemma 6.1. (i) $\forall j \in \mathbb{Z}, \mathbf{s} \in \{0, 1\}^n, \mathbf{t} \in \{0, 1\}^n : \mathbf{s} \neq \mathbf{t} \Rightarrow \forall \tilde{f} \in \tilde{W}_{n,\mathbf{s},j} : \tilde{Q}_{n,\mathbf{t},j} \tilde{f} = 0$.

(ii) Operator $\tilde{Q}_{n,\mathbf{s},j}$ is a continuous projection of E^* onto $\tilde{W}_{n,\mathbf{s},j}$ for all $j \in \mathbb{Z}$ and $\mathbf{s} \in \{0, 1\}^n$.

(iii) $\tilde{Q}_{n,\mathbf{s},j} = \tilde{Q}_{n,\mathbf{s},j} \circ \tilde{P}_{n,j'}$ for all $j, j' \in \mathbb{Z}$, $j < j'$, and $\mathbf{s} \in \{0, 1\}^n$.

For example, when $n = 2$ and $\mathbf{t} = (0, 1)$ we have $\tilde{Q}_{n,\mathbf{t},j} \delta = 0$ for all $j \in \mathbb{Z}$. When $j \in \mathbb{Z}$, $\mathbf{s}, \mathbf{t} \in \{0, 1\}^n$, and $\mathbf{s} \neq \mathbf{t}$ we have $\tilde{W}_{n,\mathbf{s},j} \cap \tilde{W}_{n,\mathbf{t},j} = \{0\}$.

Definition 6.5. When $j \in \mathbb{Z}$ define

$$\tilde{W}_{n,j} :=_{\text{n.s.}} \sum_{\mathbf{s} \in J_+(n)} \tilde{W}_{n,\mathbf{s},j}.$$

Definition 6.6. When $j \in \mathbb{Z}$ define

$$\tilde{Q}_{n,j} := \sum_{\mathbf{s} \in J_+(n)} \tilde{Q}_{n,\mathbf{s},j}.$$

Assume that $j \in \mathbb{Z}$. Now operator $\tilde{Q}_{n,j}$ is a continuous projection of E^* onto $\tilde{W}_{n,j}$ and $\tilde{Q}_{n,j}\tilde{f} = 0$ for all $\tilde{f} \in \tilde{V}_{n,j}$. We also have $\tilde{Q}_{n,j} = \tilde{P}_{n,j+1} - \tilde{P}_{n,j}$ and $\tilde{V}_{n,j+1} =_{\text{n.s.}} \tilde{V}_{n,j} \dot{+} \tilde{W}_{n,j}$.

Theorem 6.1. (i) $\forall j \in \mathbb{Z}, \mathbf{s} \in \{0, 1\}^n, \mathbf{t} \in \{0, 1\}^n : \mathbf{s} \neq \mathbf{t} \Leftrightarrow \tilde{W}_{n,\mathbf{s},j} \perp W_{n,\mathbf{t},j}^{(u)}$,
(ii) $\forall j_1, j_2 \in \mathbb{Z} : j_1 \leq j_2 \Leftrightarrow \tilde{V}_{n,j_1} \perp W_{n,j_2}^{(u)}$,
(iii) $\forall j_1, j_2 \in \mathbb{Z} : j_1 \geq j_2 \Leftrightarrow \tilde{W}_{n,j_1} \perp V_{n,j_2}^{(u)}$,
(iv) $\forall j_1, j_2 \in \mathbb{Z} : j_1 \neq j_2 \Leftrightarrow \tilde{W}_{n,j_1} \perp W_{n,j_2}^{(u)}$.

Proof. Let $j \in \mathbb{Z}$, $\mathbf{s}, \mathbf{t} \in \{0, 1\}^n$, and $\mathbf{k}, \ell \in \mathbb{Z}^n$. Proposition (i) follows from $\langle \tilde{\psi}_{\mathbf{s},j,\ell}^{[n]}, \psi_{\mathbf{t},j,\mathbf{k}}^{[n]} \rangle = \delta_{\mathbf{s},\mathbf{t}} \delta_{\ell,\mathbf{k}}$. Suppose that $j_1, j_2 \in \mathbb{Z}$ and $j_1 \neq j_2$. If $j_1 > j_2$ then $W_{n,j_2}^{(u)} \subset V_{n,j_1}^{(u)}$ and $\tilde{W}_{n,j_1} \perp V_{n,j_1}^{(u)}$ and hence $\tilde{W}_{n,j_1} \perp W_{n,j_2}^{(u)}$. If $j_1 < j_2$ then $\tilde{W}_{n,j_1} \subset \tilde{V}_{n,j_2}$ and $\tilde{V}_{n,j_2} \perp W_{n,j_2}^{(u)}$ and hence $\tilde{W}_{n,j_1} \perp W_{n,j_2}^{(u)}$. So proposition (iv) is true. $\square$

Theorem 6.2. Let $\tilde{f} \in C_0(\mathbb{R}^n, K)^*$. Then $\tilde{P}_{n,j}\tilde{f} \rightarrow \tilde{f}$ in the weak-* topology of $C_0(\mathbb{R}^n, K)^*$ as $j \rightarrow \infty$.

Proof. Let $\tilde{f} \in C_0(\mathbb{R}^n, K)^*$. Suppose that $f \in C_0(\mathbb{R}^n, K)$. Then

$$\begin{aligned} \langle \tilde{P}_{n,j}\tilde{f}, P_{n,j}^{(0)}f \rangle &= \sum_{\mathbf{k} \in \mathbb{Z}^n} \langle \tilde{f}, \varphi_{j,\mathbf{k}}^{[n]} \rangle \langle \tilde{\varphi}_{j,\mathbf{k}}^{[n]}, P_{n,j}^{(0)}f \rangle \\ &= \left\langle \tilde{f}, \sum_{\mathbf{k} \in \mathbb{Z}^n} \langle \tilde{\varphi}_{j,\mathbf{k}}^{[n]}, f \rangle \varphi_{j,\mathbf{k}}^{[n]} \right\rangle \\ &= \langle \tilde{f}, P_{n,j}^{(0)}f \rangle. \end{aligned}$$

There exists $c \in \mathbb{R}_+$ so that $\|\tilde{P}_{n,j}\| \leq c$ for all $j \in \mathbb{Z}$. Consequently

$$\begin{aligned} |\langle \tilde{f}, f \rangle - \langle \tilde{P}_{n,j}\tilde{f}, f \rangle| &\leq |\langle \tilde{f}, f \rangle - \langle \tilde{f}, P_{n,j}^{(0)}f \rangle| \\ &\quad + |\langle \tilde{P}_{n,j}\tilde{f}, P_{n,j}^{(0)}f \rangle - \langle \tilde{P}_{n,j}\tilde{f}, f \rangle| \\ &= |\langle \tilde{f}, f - P_{n,j}^{(0)}f \rangle| + |\langle \tilde{P}_{n,j}\tilde{f}, P_{n,j}^{(0)}f - f \rangle| \\ &\leq \|\tilde{f}\| \|f - P_{n,j}^{(0)}f\| + c\|\tilde{f}\| \|f - P_{n,j}^{(0)}f\| \rightarrow 0, \end{aligned}$$

as $j \rightarrow \infty$. $\square$

For example, let

$$\tilde{f}(x) := \begin{cases} x + 1; & x \in [-1, 0[, \\ -x + 1; & x \in [0, 1[, \\ 0; & \text{otherwise} \end{cases}$$

and

$$f(x) := \begin{cases} -2x - 2; & x \in [-1, 0[, \\ 2x - 2; & x \in [0, 1[, \\ 0; & \text{otherwise} \end{cases}$$

for all $x \in \mathbb{R}$. Now

$$\langle \tilde{P}_{1,j} \tilde{f}, f \rangle \rightarrow \langle \tilde{f}, f \rangle = \int_{\mathbb{R}} \tilde{f}(x) f(x) dx = -\frac{4}{3}$$

as $j \rightarrow \infty$.

6.2. Tensor product representation of the dual MRA

It follows from Eq. (2.1) that $C_0(\mathbb{R}^n, K)^* \hat{\otimes}_{\varepsilon^s} C_0(\mathbb{R}, K)^*$ is a closed subspace of $C_0(\mathbb{R}^{n+1}, K)^*$.

Definition 6.7. Let $j \in \mathbb{Z}$. Define

$$\tilde{M}_{n,j} :=_{\text{n.s.}} \bigotimes_{k=1}^n \hat{\bigotimes}_{(C_0(\mathbb{R}^k, K)^*)} \tilde{V}_{1,j}.$$

Banach space $\tilde{M}_{n,j}$ is a closed subspace of $C_0(\mathbb{R}^n, K)^*$.

Definition 6.8. Define function

$$\xi^{[n]} : \bigotimes_{k=1}^n \pi l^1(\mathbb{Z}, K) \rightarrow l^1(\mathbb{Z}^n, K)$$

by

$$\xi^{[n]}(\check{\mathbf{e}}_{\mathbf{k}}^{\otimes}) := \check{\mathbf{e}}_{\mathbf{k}}, \quad \mathbf{k} \in \mathbb{Z}^n,$$

and extending by linearity and continuity onto whole $\hat{\bigotimes}_{k=1}^n \pi l^1(\mathbb{Z}, K)$.

Function $\xi^{[n]}$ is an isometric isomorphism from Banach space $\hat{\bigotimes}_{k=1}^n \pi l^1(\mathbb{Z}, K)$ onto Banach space $l^1(\mathbb{Z}^n, K)$.

Lemma 6.2. When $j \in \mathbb{Z}$

$$\bigotimes_{k=1}^n \pi \tilde{V}_{1,j} =_{\text{n.s.}} \tilde{V}_{n,j}.$$

Proof. Let

$$E :=_{\text{n.s.}} \bigotimes_{k=1}^n \pi \tilde{V}_{1,j}$$

and

$$F :=_{\text{n.s.}} \bigotimes_{k=1}^n \pi l^1(\mathbb{Z}, K).$$

Let

$$\alpha := \bigotimes_{k=1}^n \pi \tilde{l}_{1,j}$$

Function α is an isometric isomorphism from F onto E . Let $\beta := \alpha \circ (\xi^{[n]})^{-1}$. Now β is an isometric isomorphism from $l^1(\mathbb{Z}^n, K)$ onto E and $\beta(\check{\mathbf{e}}_{\mathbf{k}}) = \tilde{\varphi}_{j,\mathbf{k}}^{[n]} = \tilde{l}_{n,j}(\check{\mathbf{e}}_{\mathbf{k}})$ for all $\mathbf{k} \in \mathbb{Z}^n$. When $\mathbf{d} \in l^1(\mathbb{Z}^n, K)$ we have $\beta(\mathbf{d}) = \tilde{l}_{n,j}(\mathbf{d})$ and $\|\beta(\mathbf{d})\|_E = \|\tilde{l}_{n,j}(\mathbf{d})\|_{C_0(\mathbb{R}^n, K)^*}$. $\square$

Lemma 6.3. *When $j \in \mathbb{Z}$*

$$\tilde{V}_{n,j} =_{\text{n.s.}} \tilde{M}_{n,j} =_{\text{n.s.}} \bigotimes_{k=1}^n \pi \tilde{V}_{1,j} =_{\text{n.s.}} \bigotimes_{k=1}^n \varepsilon^s \tilde{V}_{1,j}.$$

Proof. Use induction by n , metric approximation property of l^1 , and Proposition 7.1 in Ref. 41. $\square$

Definition 6.9. Define

$$\tilde{N}_{n,\mathbf{s},j} :=_{\text{n.s.}} \bigotimes_{k=1}^n \tilde{W}_{1,\mathbf{s}[k],j},$$

where $j \in \mathbb{Z}$ and $\mathbf{s} \in \{0, 1\}^n$.

Definition 6.10. Let $j \in \mathbb{Z}$ and $\mathbf{s} \in \{0, 1\}^n$. Define operator $\tilde{R}_{n,\mathbf{s},j} : \tilde{V}_{n,j+1} \rightarrow \tilde{N}_{n,\mathbf{s},j}$ by

$$\tilde{R}_{n,\mathbf{s},j} = \bigotimes_{k=1}^n (\tilde{Q}_{1,\mathbf{s}[k],j} | \tilde{V}_{1,j+1}).$$

Assume that $j \in \mathbb{Z}$, and $\mathbf{s} \in \{0, 1\}^n$. Now

$$\tilde{R}_{n,\mathbf{s},j} \tilde{f} = \sum_{\mathbf{k} \in \mathbb{Z}^n} \langle \tilde{f}, \psi_{\mathbf{s},j,\mathbf{k}}^{[n]} \rangle \tilde{\psi}_{\mathbf{s},j,\mathbf{k}}^{[n]} \quad (6.1)$$

for all $\tilde{f} \in \tilde{V}_{n,j+1}$. The series in Eq. (6.1) converges absolutely for all $\tilde{f} \in \tilde{V}_{n,j+1}$. We also have $\tilde{W}_{n,\mathbf{s},j} =_{\text{n.s.}} \tilde{N}_{n,\mathbf{s},j}$ and $\tilde{Q}_{n,\mathbf{s},j} = \tilde{R}_{n,\mathbf{s},j} \circ \tilde{P}_{n,j+1}$.

7. Besov Space Norm Equivalence

7.1. Norm equivalence for the Besov spaces in the n -dimensional case

This derivation is based on the corresponding one-dimensional derivation in Ref. 17. The cases $p < 1$ or $q < 1$ yielding quasi-Banach spaces $B_{p,q}^\sigma$ are not discussed in

this paper. We assume that $n \in \mathbb{Z}_+$ throughout this section.

We give first some definitions similar to those in Ref. 38 related to orthonormal wavelets.

Definition 7.1. Let $\bar{\varphi} : \mathbb{R}^n \rightarrow K$ be a mother scaling function of an orthonormal wavelet family. When $j \in \mathbb{Z}$, $\mathbf{k} \in \mathbb{Z}^n$, and $f \in L^\infty(\mathbb{R}^n)$ define

$$\bar{\alpha}_{j,\mathbf{k}}(f) := 2^{nj} \int_{\mathbf{x} \in \mathbb{R}^n} \bar{\varphi}^*(2^j \mathbf{x} - \mathbf{k}) f(\mathbf{x}) d\tau.$$

The spaces $V_j(p)$ that are defined in Ref. 38 are denoted by $\bar{V}_j(p)$ in this document. Space $\bar{V}_j(p)$ is a closed subspace of $L^p(\mathbb{R}^n)$ for each $j \in \mathbb{Z}$ and $p \in [1, \infty]$ at least when the mother scaling function $\bar{\varphi}$ is continuous and compactly supported.

Definition 7.2. Let $\bar{\varphi} : \mathbb{R}^n \rightarrow \mathbb{C}$ be a scaling function of an orthonormal wavelet family. Let $p \in [1, \infty]$ and $j \in \mathbb{Z}$. Define operator $\bar{P}_j^{(p)} : L^p(\mathbb{R}^n) \rightarrow \bar{V}_j(p)$ by

$$(\bar{P}_j^{(p)} f)(\mathbf{x}) := \sum_{\mathbf{k} \in \mathbb{Z}^n} \bar{\alpha}_{j,\mathbf{k}}(f) \bar{\varphi}(2^j \mathbf{x} - \mathbf{k})$$

for all $f \in L^p(\mathbb{R}^n)$ and $\mathbf{x} \in \mathbb{R}^n$. Define also $\bar{Q}_j^{(p)} := \bar{P}_{j+1}^{(p)} - \bar{P}_j^{(p)}$.

When $\bar{\varphi}$ is a compactly supported and continuous function operator $\bar{P}_j^{(p)}$ is a continuous linear projection of $L^p(\mathbb{R}^n)$ onto $\bar{V}_j(p)$ for each $j \in \mathbb{Z}$ and $p \in [1, \infty]$.

Definition 7.3. Let $p \in [1, \infty]$, $q \in [1, \infty]$, and $\sigma \in \mathbb{R}_+$. Let $j_0 \in \mathbb{Z}$ and $\bar{r} \in \mathbb{Z}_+$, $\bar{r} > \sigma$. Let $\bar{\varphi} : \mathbb{R}^n \rightarrow \mathbb{C}$ be a mother scaling function of an $\bar{r}$ -regular orthonormal MRA of $L^2(\mathbb{R}^n)$ and $\bar{P}_j^{(p)}$ and $\bar{Q}_j^{(p)}$, $j \in \mathbb{Z}$, be the corresponding projection operators. When $f \in L^p(\mathbb{R}^n)$ define

$$\|f\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(o)} := \|\bar{P}_{j_0}^{(p)} f\|_{L^p(\mathbb{R}^n)} + \|\bar{\mathbf{h}}\|_{l^q(\mathbb{N} + j_0)},$$

where

$$\begin{aligned} \bar{h}_j &:= 2^{j\sigma} \|\bar{Q}_j^{(p)} f\|_{L^p(\mathbb{R}^n)}, \quad j \in \mathbb{N} + j_0 \\ \bar{\mathbf{h}} &:= (\bar{h}_j)_{j=j_0}^\infty. \end{aligned}$$

Norm $\|\cdot\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(o)}$ is an equivalent norm for the Besov space $B_{p,q}^\sigma(\mathbb{R}^n)$ and characterizes $B_{p,q}^\sigma(\mathbb{R}^n)$ on $\text{bor}(\mathbb{R}^n, \mathbb{C})$. This has been proved in Chap. 2.9, Proposition 4 in Ref. 38.

Definition 7.4. Let $p \in [1, \infty]$, $q \in [1, \infty]$, and $\sigma \in \mathbb{R}_+$. Let $j_0 \in \mathbb{Z}$. Let $P_{n,j}^{(u)}$ and $Q_{n,j}^{(u)}$, $j \in \mathbb{Z}$, be the projection operators belonging to a compactly supported

interpolating tensor product MRA of $C_u(\mathbb{R}^n)$. When $f \in C_u(\mathbb{R}^n)$ define

$$\|f\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(i)} := \|P_{n,j_0}^{(u)} f\|_{L^p(\mathbb{R}^n)} + \|\mathbf{h}\|_{l^q(\mathbb{N} + j_0)},$$

where

$$h_j := 2^{j\sigma} \|Q_{n,j}^{(u)} f\|_{L^p(\mathbb{R}^n)}, \quad j \in \mathbb{N} + j_0,$$

$$\mathbf{h} := (h_j)_{j=j_0}^\infty.$$

Definition 7.5. Let $p \in [1, \infty]$, $q \in [1, \infty]$, and $\sigma \in \mathbb{R}_+$. Let $j_0 \in \mathbb{Z}$. Let $\tilde{\varphi}_{j,\mathbf{k}}^{[n]}$ and $\tilde{\psi}_{\mathbf{s},j,\mathbf{k}}^{[n]}$, $j \in \mathbb{Z}$, $\mathbf{s} \in J_+(n)$, $\mathbf{k} \in \mathbb{Z}^n$, be the dual scaling functions and dual wavelets belonging to a compactly supported interpolating tensor product MRA of $C_u(\mathbb{R}^n)$. When $f \in C_u(\mathbb{R}^n)$ define

$$\begin{aligned} \|f\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(w)} &:= \|(\langle \tilde{\varphi}_{j_0,\mathbf{k}}^{[n]}, f \rangle)_{\mathbf{k} \in \mathbb{Z}^n}\|_p \\ &\quad + \|(2^{(\sigma - \frac{\sigma}{p})j} \|(\langle \tilde{\psi}_{\mathbf{s},j,\ell}^{[n]}, f \rangle)_{\mathbf{s} \in J_+(n), \ell \in \mathbb{Z}^n}\|_p)_{j=j_0}^\infty\|_q. \end{aligned}$$

Definition 7.6. When $j \in \mathbb{Z}$ and $p \in [1, \infty]$ define

$$V_{n,j}^{(u)}(p) := \left\{ \mathbf{x} \in \mathbb{R}^n \mapsto \sum_{\mathbf{k} \in \mathbb{Z}^n} \mathbf{a}[\mathbf{k}] \varphi_{j,\mathbf{k}}^{[n]}(\mathbf{x}) : \mathbf{a} \in l^p(\mathbb{Z}^n) \right\}$$

and $\|f|V_{n,j}^{(u)}(p)\| := \|f\|_{L^p(\mathbb{R}^n)}$ for all $f \in V_{n,j}^{(u)}(p)$.

Definition 7.7. Let $j \in \mathbb{Z}$ and $p \in [1, \infty]$. When $T \in \mathcal{L}(L^p(\mathbb{R}^n), L^p(\mathbb{R}^n))$ define

$$\|T\|_{V_{n,j}^{(u)}(p)} := \|(T|_{V_{n,j}^{(u)}(p)})|_{\mathcal{L}(V_{n,j}^{(u)}(p), L^p(\mathbb{R}^n))}\|.$$

Definition 7.8. Let $j \in \mathbb{Z}$ and $p \in [1, \infty]$. When $T \in \mathcal{L}(C_u(\mathbb{R}^n), C_u(\mathbb{R}^n))$ and $T[\bar{V}_j(p)] \subset L^p(\mathbb{R}^n)$ define

$$\|T\|_{\bar{V}_j(p)} := \|(T|_{\bar{V}_j(p)})|_{\mathcal{L}(\bar{V}_j(p), L^p(\mathbb{R}^n))}\|.$$

Definition 7.9. When $p \in [1, \infty]$ define

$$c_{\text{interp}}(p) := \begin{cases} \frac{p}{p-1}; & p \in]1, \infty[, \\ 1; & p = 1 \vee p = \infty. \end{cases}$$

Lemma 7.1. Suppose that $q \in [1, \infty]$ and $t \in \mathbb{R}_+$. Let $a(j, j') := 2^{-|j'-j|t}$ for all $j, j' \in \mathbb{N}$. Define

$$A\mathbf{b} := \left(\sum_{j'=0}^\infty a(j, j') b_{j'} \right)_{j \in \mathbb{N}}$$

for all $\mathbf{b} \in l^q(\mathbb{N})$. Then $A \in \mathcal{L}(l^q(\mathbb{N}), l^q(\mathbb{N}))$.

Proof. Cases $q = 1$ and $q = \infty$ can be proved by starting from the expression of $\mathbf{Ab}$ where $\mathbf{b} \in l^q(\mathbb{N})$. When $q \in]1, \infty[$ the proof is based on interpolation of Banach spaces, see Ref. 2. $\square$

Theorem 7.1. *Let $p \in [1, \infty]$, $q \in [1, \infty]$, $j_0 \in \mathbb{Z}$, $\sigma \in \mathbb{R}_+$, and $n/p < \sigma < r_0$. Let $\varphi^{[n]}$ be a scaling function of a compactly supported interpolating tensor product MRA of $C_u(\mathbb{R}^n)$ and $\bar{\varphi} : \mathbb{R}^n \rightarrow \mathbb{C}$ a compactly supported and continuous mother scaling function of a $(\lfloor \sigma \rfloor + 1)$ -regular orthonormal wavelet family. Suppose that $\varphi^{[n]} \in C^{r_0}(\mathbb{R}^n)$. Suppose also that $(\tilde{\varphi}^{[n]}, \varphi^{[n]})$ and $(2^{nj} \bar{\varphi}^*, \bar{\varphi})$ span all polynomials of degree at most $\lceil \sigma \rceil - 1$. Let B be the normed space $B_{p,q}^\sigma(\mathbb{R}^n) \cap C_u(\mathbb{R}^n)$ equipped with some Besov space norm. Then $\|\cdot\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(i)}$ and $\|\cdot\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(o)}$ are equivalent norms on the vector space B and norm $\|\cdot\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(i)}$ characterizes B on $C_u(\mathbb{R}^n)$.*

Proof. Let $\bar{r}_0 := \lfloor \sigma \rfloor + 1$. We prove first that $\|f\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(i)} \leq c \|f\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(o)}$ for all $f \in B$ and for some $c \in \mathbb{R}_+$. Define q' by

$$\frac{1}{q'} + \frac{1}{q} = 1.$$

There exists $c_1 \in \mathbb{R}_+$ so that

$$\|P_{n,j}^{(u)}\|_{\bar{V}_{j'}(p)} \leq c_1 \cdot 2^{n(j'-j)/p} \quad (7.1)$$

for all $j, j' \in \mathbb{Z}$, $j' \geq j$. There exists $c_2 \in \mathbb{R}_+$ so that

$$\|I - P_{n,j}^{(u)}\|_{\bar{V}_{j'}(p)} \leq c_2 \cdot c_{\text{interp}}(p) \cdot 2^{(j'-j)\bar{r}_0} \quad (7.2)$$

for all $j, j' \in \mathbb{Z}$, $j' \leq j$. These two results can be proved by Banach space interpolation between cases $p = 1$ and $p = \infty$. Let $f \in B$. We have

$$\begin{aligned} \|P_{n,j_0}^{(u)} f\|_p &= \left\| P_{n,j_0}^{(u)} \left(\bar{P}_{j_0}^{(p)} f + \sum_{j=j_0}^{\infty} \bar{Q}_j^{(p)} f \right) \right\|_p \\ &\leq \|P_{n,j_0}^{(u)}\|_{\bar{V}_{j_0}(p)} \|\bar{P}_{j_0}^{(p)} f\|_p + \sum_{j=j_0}^{\infty} \|P_{n,j_0}^{(u)}\|_{\bar{V}_{j+1}(p)} \|\bar{Q}_j^{(p)} f\|_p \\ &\leq c_3 \|\bar{P}_{j_0}^{(p)} f\|_p + c_3 \cdot 2^{(n-nj_0)/p} \sum_{j=j_0}^{\infty} 2^{-j(\sigma-\frac{n}{p})} \bar{\mathbf{h}}[j], \end{aligned}$$

where $\bar{\mathbf{h}} := (2^{j\sigma} \|\bar{Q}_j^{(p)} f\|_p)_{j=j_0}^{\infty}$. Let

$$c_4 := c_3 \cdot 2^{(n-nj_0)/p} \cdot \|(2^{-j'(\sigma-\frac{n}{p})})_{j'=j_0}^{\infty}\|_{q'}.$$

Now

$$\|P_{n,j_0}^{(u)} f\|_p \leq c_3 \|\bar{P}_{j_0}^{(p)} f\|_p + c_4 \|\bar{\mathbf{h}}\|_q \leq \max\{c_3, c_4\} \cdot \|f\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(o)},$$

where c_3 and c_4 do not depend on f . We have

$$\begin{aligned} \|Q_{n,j}^{(u)} f\|_p &= \left\| Q_{n,j}^{(u)} \left(\bar{P}_{j_0}^{(p)} f + \sum_{j'=j_0}^{\infty} \bar{Q}_{j'}^{(p)} f \right) \right\|_p \\ &\leq \|Q_{n,j}^{(u)}\|_{\bar{V}_{j_0}(p)} \|\bar{P}_{j_0}^{(p)} f\|_p + \sum_{j'=j_0}^{\infty} \|Q_{n,j}^{(u)}\|_{\bar{V}_{j'+1}(p)} \|\bar{Q}_{j'}^{(p)} f\|_p \end{aligned}$$

for all $j \in \mathbb{Z}$, $j \geq j_0$. It follows from Eq. (7.2) that

$$2^{j\sigma} \|Q_{n,j}^{(u)}\|_{\bar{V}_{j_0}(p)} \|\bar{P}_{j_0}^{(p)} f\|_p \leq c_5 \cdot 2^{-j(\bar{r}_0 - \sigma)} \|\bar{P}_{j_0}^{(p)} f\|_p$$

for all $j \in \mathbb{Z}$, $j \geq j_0$, where c_5 is independent of f . Consequently

$$\begin{aligned} \|(2^{j\sigma} \|Q_{n,j}^{(u)}\|_{\bar{V}_{j_0}(p)} \|\bar{P}_{j_0}^{(p)} f\|_p)_{j=j_0}^{\infty}\|_q &\leq c_5 \|(2^{-j(\bar{r}_0 - \sigma)})_{j=j_0}^{\infty}\|_q \|\bar{P}_{j_0}^{(p)} f\|_p \\ &= c_6 \|\bar{P}_{j_0}^{(p)} f\|_p \leq c_6 \|f\|_{B_{p,q}^{(o)}(\mathbb{R}^n); j_0}. \end{aligned} \quad (7.3)$$

When $j' < j$ it follows from Eq. (7.2) that

$$2^{j\sigma} \|Q_{n,j}^{(u)}\|_{\bar{V}_{j'+1}(p)} \|\bar{Q}_{j'}^{(p)} f\|_p \leq c_7 \cdot 2^{-|j'-j|(\bar{r}_0 - \sigma)} \bar{\mathbf{h}}[j']. \quad (7.4)$$

When $j' \geq j$ it follows from Eq. (7.1) that

$$2^{j\sigma} \|Q_{n,j}^{(u)}\|_{\bar{V}_{j'+1}(p)} \|\bar{Q}_{j'}^{(p)} f\|_p \leq c_8 \cdot 2^{-|j'-j|(\sigma - \frac{n}{p})} \bar{\mathbf{h}}[j']. \quad (7.5)$$

Let

$$w := \min \left\{ \sigma - \frac{n}{p}, \bar{r}_0 - \sigma \right\}$$

and $c_9 := \max\{c_7, c_8\}$. Now by Eqs. (7.4) and (7.5)

$$\begin{aligned} a &:= \left\| \left(2^{j\sigma} \sum_{j'=j_0}^{\infty} \|Q_{n,j}^{(u)}\|_{\bar{V}_{j'+1}(p)} \|\bar{Q}_{j'}^{(p)} f\|_p \right)_{j=j_0}^{\infty} \right\|_q \\ &\leq c_9 \left\| \left(\sum_{j'=j_0}^{\infty} 2^{-|j'-j|w} \bar{\mathbf{h}}[j'] \right)_{j=j_0}^{\infty} \right\|_q. \end{aligned}$$

It follows from Lemma 7.1 that

$$a \leq c_{10} \|\bar{\mathbf{h}}\|_q \leq c_{10} \|f\|_{B_{p,q}^{(o)}(\mathbb{R}^n); j_0}, \quad (7.6)$$

where c_{10} depends only on w and j_0 . By Equations (7.3) and (7.6) we have $\|f\|_{B_{p,q}^{(i)}(\mathbb{R}^n); j_0} \leq c_{10} \|f\|_{B_{p,q}^{(o)}(\mathbb{R}^n); j_0}$.

We prove then that $\|g\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(o)} \leq c\|g\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(i)}$ for all $g \in B$ and for some $c \in \mathbb{R}_+$. Now

$$\begin{aligned} \|P_{n,j_0}^{(u)}g\|_p + \sum_{j=j_0}^{\infty} \|Q_{n,j}^{(u)}g\|_p &= \|P_{n,j_0}^{(u)}g\|_p + \sum_{j=j_0}^{\infty} \|2^{-j\sigma} \cdot 2^{j\sigma} Q_{n,j}^{(u)}g\|_p \\ &\leq \|P_{n,j_0}^{(u)}g\|_p + \|(2^{j\sigma} \|Q_{n,j}^{(u)}g\|_p)_{j=j_0}^{\infty}\|_q \sum_{j=j_0}^{\infty} 2^{-j\sigma} \\ &\leq c_{11}\|g\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(i)} \leq c_{12}\|g\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(o)} \in \mathbb{R}_0, \end{aligned}$$

where c_{11} and c_{12} do not depend on g . Consequently

$$P_{n,j_0}^{(u)}g + \sum_{j=j_0}^m Q_{n,j}^{(u)}g \rightarrow g$$

in $L^p(\mathbb{R}^n)$ as $m \rightarrow \infty$. We have

$$\begin{aligned} \|\bar{P}_{j_0}^{(p)}g\|_p &= \left\| \bar{P}_{j_0}^{(p)} \left(P_{n,j_0}^{(u)}g + \sum_{j=j_0}^{\infty} Q_{n,j}^{(u)}g \right) \right\|_p \\ &\leq \|\bar{P}_{j_0}^{(p)}\| \|P_{n,j_0}^{(u)}g\|_p + \sum_{j'=j_0}^{\infty} \|\bar{P}_{j_0}^{(p)}\| \|Q_{n,j'}^{(u)}g\|_p \\ &\leq c_{13}\|P_{n,j_0}^{(u)}g\|_p + c_{13} \sum_{j=j_0}^{\infty} 2^{-j\sigma} \mathbf{h}[j] \\ &\leq c_{13}\|P_{n,j_0}^{(u)}g\|_p + c_{13}\|(2^{-j\sigma})_{j=j_0}^{\infty}\|_{q'} \|\mathbf{h}\|_q \\ &\leq c_{14}\|g\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(i)}, \end{aligned}$$

where $\mathbf{h} := (2^{j\sigma} \|Q_{n,j}^{(u)}g\|_p)_{j=j_0}^{\infty}$. There exists $c_{15} \in \mathbb{R}_+$ so that

$$\|I - \bar{P}_j^{(p)}\|_{V_{n,j'}^{(u)}(p)} \leq c_{15} \cdot c_{\text{interp}}(p) \cdot 2^{(j'-j)\sigma} \quad (7.7)$$

for all $j, j' \in \mathbb{Z}$, $j' \leq j$. This can be proved by Banach space interpolation between cases $p = 1$ and $p = \infty$. Furthermore,

$$\begin{aligned} \|\bar{Q}_j^{(p)}g\|_p &= \left\| \bar{Q}_j^{(p)} \left(P_{n,j_0}^{(u)}g + \sum_{j'=j_0}^{\infty} Q_{n,j'}^{(u)}g \right) \right\|_p \\ &\leq \|\bar{Q}_j^{(p)}\| \|P_{n,j_0}^{(u)}g\|_p + \sum_{j'=j_0}^{\infty} \|\bar{Q}_j^{(p)}\| \|Q_{n,j'}^{(u)}g\|_p. \end{aligned}$$

It follows from Eq. (7.7) that

$$2^{j\sigma} \|\bar{Q}_j^{(p)}\| \|P_{n,j_0}^{(u)} g\|_p \leq c_{16} \cdot 2^{-j(r_0-\sigma)} \|P_{n,j_0}^{(u)} g\|_p$$

for all $j \geq j_0$ where c_{16} is independent of g . Consequently

$$\begin{aligned} \|(2^{j\sigma} \|\bar{Q}_j^{(p)}\| \|P_{n,j_0}^{(u)} g\|_p)_{j=j_0}^\infty\|_q &\leq c_{16} \|(2^{-j(r_0-\sigma)})_{j=j_0}^\infty\|_q \|P_{n,j_0}^{(u)} g\|_p \\ &= c_{17} \|P_{n,j_0}^{(u)} g\|_p \leq c_{17} \|g\|_{B_{p,q}^{\sigma,(\mathbb{R}^n);j_0}}^{(i)}. \end{aligned} \quad (7.8)$$

When $j' < j$ it follows from Eq. (7.7) that

$$2^{j\sigma} \|\bar{Q}_j^{(p)}\| \|Q_{n,j'}^{(u)} g\|_p \leq c_{18} \cdot 2^{-|j'-j|(r_0-\sigma)} \mathbf{h}[j']. \quad (7.9)$$

When $j' \geq j$ it follows from uniform boundedness of the projection operators that

$$2^{j\sigma} \|\bar{Q}_j^{(p)}\| \|Q_{n,j'}^{(u)} g\|_p \leq c_{19} \cdot 2^{-|j'-j|\sigma} \mathbf{h}[j']. \quad (7.10)$$

Let

$$z := \min\{\sigma, r_0 - \sigma\}.$$

Now by Eqs. (7.9) and (7.10) we have

$$\begin{aligned} b &:= \left\| \left(\sum_{j'=j_0}^\infty 2^{j\sigma} \|\bar{Q}_j^{(p)}\| \|Q_{n,j'}^{(u)} g\|_p \right)_{j=j_0}^\infty \right\|_q \\ &\leq c_{20} \left\| \left(\sum_{j'=j_0}^\infty 2^{-|j'-j|z} \mathbf{h}[j'] \right)_{j=j_0}^\infty \right\|_q. \end{aligned}$$

It follows from Lemma 7.1 that

$$b \leq c_{21} \|\mathbf{h}\|_q \leq c_{21} \|f\|_{B_{p,q}^{\sigma,(\mathbb{R}^n);j_0}}^{(i)}, \quad (7.11)$$

where c_{21} depends only on z and j_0 . By Eqs. (7.8) and (7.11) we have $\|g\|_{B_{p,q}^{\sigma,(\mathbb{R}^n);j_0}}^{(o)} \leq c_{22} \|g\|_{B_{p,q}^{\sigma,(\mathbb{R}^n);j_0}}^{(i)}$.

Suppose then that $\|g\|_{B_{p,q}^{\sigma,(\mathbb{R}^n);j_0}}^{(o)} = \infty$. Let

$$A\mathbf{b} := \left(\sum_{j'=j_0}^\infty 2^{-|j'-j|z} \mathbf{b}[j'] \right)_{j=j_0}^\infty, \quad \mathbf{b} \in \mathbb{C}^{\mathbb{N}+j_0}.$$

Now

$$\infty = \|(2^{j\sigma} \|\bar{Q}_j^{(p)}\| \|g\|_p)_{j=j_0}^\infty\|_q \leq c_{17} \|P_{n,j_0}^{(u)} g\|_p + c_{20} \|A\mathbf{h}\|_q.$$

By the continuity of $A|_{l^q(\mathbb{N}+j_0)}$ we must have $\|\mathbf{h}\|_q = \infty$. Consequently $\|g\|_{B_{p,q}^{\sigma,(\mathbb{R}^n);j_0}}^{(i)} = \infty$. $\square$

It is possible to construct an orthonormal compactly supported Daubechies wavelet family with arbitrary high regularity $\bar{r} \in \mathbb{R}_+$ and polynomial span (number of vanishing moments) $\bar{d} \in \mathbb{N}$.⁸ Consequently, when $j_0 \in \mathbb{Z}$, $\sigma \in \mathbb{R}_+$, $p \in [1, \infty]$, $q \in [1, \infty]$, $n/p < \sigma < r_0$, $\varphi^{[n]} \in C^{r_0}(\mathbb{R}^n)$, and $(\tilde{\varphi}^{[n]}, \varphi^{[n]})$ spans all polynomials of degree at most $\lceil \sigma \rceil - 1$ function $\varphi^{[n]}$ defines an equivalent norm $\|\cdot\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(i)}$ on Banach space B .

Theorem 7.2. *Let $p \in [1, \infty]$, $q \in [1, \infty]$, $\sigma \in \mathbb{R}_+$, $j_0 \in \mathbb{Z}$, $r_0 \in \mathbb{R}_+$, and $n/p < \sigma < r_0$. Let $\varphi^{[n]}$ be a scaling function of a compactly supported interpolating tensor product MRA of $C_u(\mathbb{R}^n)$ and suppose that $\varphi^{[n]} \in C^{r_0}(\mathbb{R}^n)$. Let B be the normed space $B_{p,q}^\sigma(\mathbb{R}^n) \cap C_u(\mathbb{R}^n)$ equipped with some Besov space norm. Then $\|\cdot\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(i)}$ and $\|\cdot\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(w)}$ are equivalent to the norm of B and they characterize B on $C_u(\mathbb{R}^n)$.*

Proof. Define

$$\mathbf{a}_j(f) := (\langle \tilde{\psi}_{\mathbf{s},j,\mathbf{k}}^{[n]}, f \rangle)_{\mathbf{s} \in J_+(n), \mathbf{k} \in \mathbb{Z}^n},$$

where $f \in B$ and $j \in \mathbb{Z}$. By applying Banach space interpolation to cases $p = 1$ and $p = \infty$ we get

$$\begin{aligned} c_1 \cdot 2^{-\frac{nj_0}{p}} \|(\langle \tilde{\varphi}_{j_0,\mathbf{k}}^{[n]}, f \rangle)_{\mathbf{k} \in \mathbb{Z}^n}\|_p &\leq \|P_{n,j_0}^{(u)} f\| \\ &\leq c_2 \cdot 2^{-\frac{nj_0}{p}} \|(\langle \tilde{\varphi}_{j_0,\mathbf{k}}^{[n]}, f \rangle)_{\mathbf{k} \in \mathbb{Z}^n}\|_p \end{aligned} \quad (7.12)$$

and

$$c_3 \cdot 2^{-\frac{nj}{p}} \|\mathbf{a}_j(f)\|_p \leq \|Q_{n,j}^{(u)} f\|_p \leq c_4 \cdot 2^{-\frac{nj}{p}} \|\mathbf{a}_j(f)\|_p$$

for all $j \in \mathbb{N} + j_0$ and $f \in B$. Consequently

$$\begin{aligned} c_3 \|(2^{j(\sigma - \frac{n}{p})} \|\mathbf{a}_j(f)\|_p)_{j=j_0}^\infty\|_q &\leq \|(2^{j\sigma} \|Q_{n,j}^{(u)} f\|_p)_{j=j_0}^\infty\|_q \\ &\leq c_4 \|(2^{j(\sigma - \frac{n}{p})} \|\mathbf{a}_j(f)\|_p)_{j=j_0}^\infty\|_q \end{aligned} \quad (7.13)$$

for all $f \in B$.

Let $c_5 := \min\{c_1 \cdot 2^{-nj_0/p}, c_3\}$ and $c_6 := \max\{c_2 \cdot 2^{-nj_0/p}, c_4\}$. It follows from Eqs. (7.12) and (7.13) that

$$c_5 \|f\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(w)} \leq \|f\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(i)} \leq c_6 \|f\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(w)}$$

for all $f \in B$. □

It is possible to construct Deslauriers–Dubuc wavelet families with arbitrary high regularity $r \in \mathbb{R}_+$ (i.e. $\varphi^{[n]} \in C^r(\mathbb{R}^n)$) and polynomial span $d \in \mathbb{N}$.¹⁷ As a direct consequence of Theorems 7.1 and 7.2 norms $\|\cdot\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(w)}$ and $\|\cdot\|_{B_{p,q}^\sigma(\mathbb{R}^n);j_0}^{(i)}$ are equivalent to the restriction of some norm of Besov space $B_{p,q}^\sigma(\mathbb{R}^n)$ onto the vector space $B_{p,q}^\sigma(\mathbb{R}^n) \cap C_u(\mathbb{R}^n)$ and these norms characterize $B_{p,q}^\sigma(\mathbb{R}^n) \cap C_u(\mathbb{R}^n)$ on $C_u(\mathbb{R}^n)$.

7.2. Consequences of the Besov space norm equivalence

In particular, the Besov space norm equivalence holds for Hölder spaces $C^\sigma(\mathbb{R}^n)$ for $\sigma \in \mathbb{R}_+ \setminus \mathbb{Z}$. When $n \in \mathbb{Z}_+$, $\sigma \in \mathbb{R}_+$, and $q \in [1, \infty]$ we have $B_{\infty,q}^\sigma(\mathbb{R}^n) \subset C_u(\mathbb{R}^n)$ (see Proposition 2.3.2/2(i) and Eq. (2.3.5/1) in Ref. 44).

Definition 7.10. When $n \in \mathbb{Z}_+$ and $j_0 \in \mathbb{Z}$ define

$$\Omega(n, j_0) := \{(\mathbf{0}_n, j_0, \mathbf{k}) : \mathbf{k} \in \mathbb{Z}^n\} \cup \bigcup_{j=j_0}^{\infty} \bigcup_{\mathbf{s} \in J_+(n)} \{(\mathbf{s}, j, \mathbf{k}) : \mathbf{k} \in \mathbb{Z}^n\}.$$

As the Banach space $B_{\infty,\infty}^\sigma(\mathbb{R}^n) =_{\text{tvs}} \mathcal{Z}^\sigma(\mathbb{R}^n)$ is isomorphic to l^∞ (see Sec. 2.5.5, p. 87 in Ref. 44) the set $\{\psi_\alpha : \alpha \in \Omega(n, j_0)\}$ cannot be a Schauder basis of $B_{\infty,\infty}^\sigma(\mathbb{R}^n)$ with any summing order.

Remark 7.1. Suppose that $n \in \mathbb{Z}_+$, $j_0 \in \mathbb{Z}$, $\sigma \in \mathbb{R}_+$, and $\varphi^{[n]} \in C^r(\mathbb{R}^n)$ where $r \in \mathbb{R}_+$, $r > \sigma$. There exists $r_1 \in \mathbb{Z}_+$ so that $\text{supp } \varphi^{[n]} \in \overline{B}_{\mathbb{R}^n}(0; r_1)$. Consider

$$f := \sum_{k=0}^{\infty} 2^{-(j_0+k)\sigma} \psi_{\mathbf{e}_1^{[n]}, j_0+k, \eta(k)}^{[n]},$$

where

$$c := 2r_1 + \lceil 2^{j_0} \rceil (2\lceil \sigma \rceil + 1),$$

$$\eta(k) := c \cdot 2^k k \mathbf{e}_1^{[n]}$$

for all $k \in \mathbb{Z}$, $k \geq j_0$, and the series converges in $C_0(\mathbb{R}^n)$. Let $m := \lceil r \rceil$ and

$$g_k := 2^{-(j_0+k)\sigma} \psi_{\mathbf{e}_1^{[n]}, j_0+k, \eta(k)}^{[n]}$$

for all $k \in \mathbb{N}$. As $\psi_{\mathbf{e}_1^{[n]}}^{[n]} \in B_{\infty,\infty}^\sigma(\mathbb{R}^n)$ it follows that there exists $c_1 \in \mathbb{R}_+$ so that

$$\omega_\infty^m(g_k; t) \leq c_1 t^\sigma \tag{7.14}$$

for all $k \in \mathbb{N}$ and $t \in]0, 1[$. Define $S_{j,\ell}(y) := \overline{B}_{\mathbb{R}^n}(2^{-j}\ell; 2^{-j}r_1 + y)$, where $j \in \mathbb{Z}$, $\ell \in \mathbb{Z}^n$, and $y \in \mathbb{R}_0$. Suppose that $t_1 \in]0, 1[$. We have

$$\text{supp}_{\text{set}} \Delta_{\mathbf{h}}^m g_k \subset S_{j_0+k, \eta(k)}(m) \tag{7.15}$$

for all $\mathbf{h} \in \overline{B}_{\mathbb{R}^n}(0; t_1)$ and $k \in \mathbb{N}$. Furthermore,

$$S_{j_0+k, \eta(k)}(m) \cap S_{j_0+l, \eta(l)}(m) = \emptyset \tag{7.16}$$

for all $k, l \in \mathbb{N}$ and $k \neq l$. Using Eqs. (7.15) and (7.16) we obtain

$$\omega_\infty^m(f; t_1) \leq \sup\{\omega_\infty^m(g_k; t_1) : k \in \mathbb{N}\}. \tag{7.17}$$

We have $f \in L^\infty(\mathbb{R}^n)$ and by Eqs. (7.14) and (7.17) $\omega_\infty^m(f; t_1) \leq c_2 t_1^\sigma$. Thus $f \in B_{\infty,\infty}^\sigma(\mathbb{R}^n)$.

Suppose that

$$f = \sum_{k=0}^{\infty} \mathbf{d}[\iota(k)] \psi_{\iota(k)}$$

for some sequence $\mathbf{d} \in \mathbb{C}^{\Omega(n, j_0)}$ where the series converges in $B_{\infty, \infty}^{\sigma}(\mathbb{R}^n)$. Define

$$\xi_b := \sum_{k=0}^b \mathbf{d}[\iota(k)] \psi_{\iota(k)}$$

where $b \in \mathbb{N}$. Let $b_1 \in \mathbb{N}$. Define

$$j_1 := \max\{j(\iota(k)) \in \mathbb{Z} : k \in Z_0(b_1)\} + 1.$$

There exists $k_1 \in \mathbb{N}$ so that $\iota(k_1) = \alpha(j_1 - j_0)$. Now $j_1 \neq j(\iota(k))$ for all $k \in Z_0(b_1)$ and consequently $\iota(k_1) \neq \iota(k)$ for all $k \in Z_0(b_1)$. It follows that $k_1 > b_1$. Let $k_2 := j_1 - j_0$. Now

$$\iota(k_1) = (\mathbf{e}_1^{[n]}, j_1, c \cdot 2^{k_2} k_2 \mathbf{e}_1^{[n]}).$$

We have

$$|\langle \tilde{\psi}_{\iota(k_1)}, f - \xi_{b_1} \rangle| \leq \|(\langle \tilde{\psi}_{\mathbf{s}, j_1, \mathbf{k}}^{[n]}, f - \xi_{b_1} \rangle)_{\mathbf{s} \in J_+(n), \mathbf{k} \in \mathbb{Z}^n}\|_{\infty}$$

and $|\langle \tilde{\psi}_{\iota(k_1)}^{[n]}, f - \xi_{b_1} \rangle| = 2^{-(j_0 + k_2)\sigma}$. Hence

$$\begin{aligned} 1 &\leq 2^{(j_0 + k_2)\sigma} \|(\langle \tilde{\psi}_{\mathbf{s}, j_1, \mathbf{k}}^{[n]}, f - \xi_{b_1} \rangle)_{\mathbf{s} \in J_+(n), \mathbf{k} \in \mathbb{Z}^n}\|_{\infty} \\ &\leq \| (2^{j\sigma} \|(\langle \tilde{\psi}_{\mathbf{s}, j, \mathbf{k}}^{[n]}, f - \xi_{b_1} \rangle)_{\mathbf{s} \in J_+(n), \mathbf{k} \in \mathbb{Z}^n}\|_{\infty})_{j=j_0}^{\infty} \|_{\infty} \\ &\leq \|f - \xi_{b_1}\|_{B_{\infty, \infty}^{\sigma}(\mathbb{R}^n); j_0}^{(w)}. \end{aligned}$$

Thus $\xi_b \not\rightarrow f$ in Banach space $B_{\infty, \infty}^{\sigma}(\mathbb{R}^n)$ as $b \rightarrow \infty$.

Theorem 7.3. *Let $n \in \mathbb{Z}_+$, $\sigma \in \mathbb{R}_+$, $q \in [1, \infty[$, and $j_0 \in \mathbb{Z}$. Let $\varphi^{[n]}$ be a mother scaling function of a compactly supported tensor product MRA of $C_0(\mathbb{R}^n)$. Suppose that $\varphi^{[n]} \in C^r(\mathbb{R}^n)$ for some $r \in \mathbb{R}_+$, $r > \sigma$. Then $\{\psi_{\alpha} : \alpha \in \Omega(n, j_0)\}$ is an unconditional basis of Banach space $B_{\infty, q}^{\sigma}(\mathbb{R}^n) \cap C_0(\mathbb{R}^n)$ equipped with a norm of $B_{\infty, q}^{\sigma}(\mathbb{R}^n)$ and the coefficient functional corresponding to basis vector ψ_{α} is $\tilde{\psi}_{\alpha}$ for each $\alpha \in \Omega(n, j_0)$.*

Proof. Let

$$S_j(m) := \{(\mathbf{0}_n, j, \mathbf{k}) : \mathbf{k} \in \mathbb{Z}^n, \|\mathbf{k}\|_2 \leq m\}, \quad j \in \mathbb{Z}, \quad m \in \mathbb{N},$$

$$D_{\mathbf{s}, j}(m) := \{(\mathbf{s}, j, \mathbf{k}) : \mathbf{k} \in \mathbb{Z}^n, \|\mathbf{k}\|_2 \leq m\}, \quad \mathbf{s} \in \{0, 1\}^n, \quad j \in \mathbb{Z}, \quad m \in \mathbb{N},$$

$$D_j(m) := \bigcup_{\mathbf{s} \in J_+(n)} D_{\mathbf{s}, j}(m), \quad j \in \mathbb{Z}, \quad m \in \mathbb{N}.$$

Let

$$m_1 := \min\{m \in \mathbb{N} : \forall \mathbf{k} \in \mathbb{Z}^n : (\|\mathbf{k}\|_\infty > m \Rightarrow \forall \mathbf{s} \in \{0, 1\}^n : \tilde{g}_{\mathbf{s}, \mathbf{k}}^{[n]} = 0)\},$$

$$m_2 := \lceil m_1 \sqrt{n} \rceil,$$

$$A(k) := S_{j_0}(2^{j_0}k) \cup \bigcup_{l=j_0}^{j_0+k-1} D_l(m_2 + 2^{j_0+k}k), \quad k \in \mathbb{Z}_+.$$

Define $\mathbf{s}(\mathbf{a}) = \mathbf{s}'$, $j(\mathbf{a}) = j'$, and $\mathbf{k}(\mathbf{a}) = \mathbf{k}'$ for all $\mathbf{a} = (\mathbf{s}', j', \mathbf{k}')$, $\mathbf{s}' \in \{0, 1\}^n$, $j' \in \mathbb{Z}$, and $\mathbf{k}' \in \mathbb{Z}^n$. Let $f \in B_{\infty, q}^\sigma(\mathbb{R}^n) \cap C_0(\mathbb{R}^n)$. Let $\eta : \mathbb{N} \rightarrow \Omega(n, j_0)$ be a bijection. Let $\beta_\alpha := \langle \tilde{\psi}_\alpha, f \rangle$ for all $\alpha \in \Omega(n, j_0)$. Define

$$\beta_\alpha^{(m)} := \begin{cases} \langle \tilde{\psi}_\alpha, f \rangle; & \alpha \notin \eta[Z_0(m)], \\ 0; & \text{otherwise} \end{cases}$$

for all $m \in \mathbb{N}$ and $\alpha \in \Omega(n, j_0)$. Define

$$\xi_m := \sum_{\alpha \in \Omega(n, j_0)} \beta_\alpha^{(m)} \psi_\alpha$$

for all $m \in \mathbb{N}$. There exists $c_1 \in \mathbb{R}_+$ so that

$$|\langle \tilde{\psi}_\alpha, f \rangle| \leq c_1 \|f\|_\infty \quad (7.18)$$

for all $f \in C_0(\mathbb{R}^n)$ and $\alpha \in \Omega(n, j_0)$.

Let $h \in \mathbb{R}_+$. Choose $j_1 \in \mathbb{Z}$, $j_1 > \max\{j_0, 0\}$ so that

$$\|(2^{j_1 \sigma} \|(\langle \tilde{\psi}_{\mathbf{s}, j, \mathbf{k}}^{[n]}, f)_{\mathbf{s} \in J_+(n), \mathbf{k} \in \mathbb{Z}^n}\|_\infty)_{j=j_1}^\infty\|_q < \frac{h}{4}. \quad (7.19)$$

Choose $r_1 \in \mathbb{R}_+$ so that

$$\sup\{|f(\mathbf{x})| : \mathbf{x} \in \mathbb{R}^n, \|\mathbf{x}\| \geq r_1\} < \frac{h}{2^{n+2+j_1 \sigma}(j_1 - j_0)c_1} \quad (7.20)$$

and let $m_3 := \max\{j_1 - j_0, \lceil r_1 \rceil\}$.

Choose $m_4 \in \mathbb{Z}_+$ so that $A(m_3) \subset \eta[Z_0(m_4)]$. Let $l \in \mathbb{N}$, $l > m_4$. If $\mathbf{s}(\eta(l)) = \mathbf{0}_n$ we have

$$\|(\beta_{\mathbf{0}_n, j_0, \mathbf{k}}^{(m_4)})_{\mathbf{k} \in \mathbb{Z}^n}\|_\infty < \frac{h}{4}. \quad (7.21)$$

If $\mathbf{s}(\eta(l)) \neq \mathbf{0}_n$ we have

$$\|(2^{j \sigma} \|(\beta_{\mathbf{s}, j, \mathbf{k}}^{(m_4)})_{\mathbf{s} \in J_+(n), \mathbf{k} \in \mathbb{Z}^n}\|_\infty)_{j=j_0}^{j_1-1} l^q (j_0 + \mathbb{N})\| < \frac{1}{4} h. \quad (7.22)$$

Thus by Eqs. (7.21) and (7.22), we get

$$\|(2^{j \sigma} \|(\beta_{\mathbf{s}, j, \mathbf{k}}^{(m_4)})_{\mathbf{s} \in J_+(n), \mathbf{k} \in \mathbb{Z}^n}\|_\infty)_{j=j_0}^\infty l^q (j_0 + \mathbb{N})\| < \frac{h}{2}. \quad (7.23)$$

By Eqs. (7.21) and (7.23) we have $\|\xi_{m_4}\|_{B_{\infty, q}^\sigma(\mathbb{R}^n); j_0}^{(w)} < h$. It follows that

$$s_m := \sum_{l=0}^m \beta_{\eta(l)} \psi_{\eta(l)} \rightarrow g$$

as $m \rightarrow \infty$ where the series converges in Banach space $B_{\infty,q}^\sigma(\mathbb{R}^n)$. We also have $s_m \rightarrow g$ as $m \rightarrow \infty$ in Banach space $C_0(\mathbb{R}^n)$. If we had $g \neq f$ we would have $\langle \tilde{\psi}_\gamma, f - g \rangle = \langle \tilde{\psi}_\gamma, f \rangle - \langle \tilde{\psi}_\gamma, g \rangle \neq 0$ for some $\gamma \in \Omega(n, j_0)$. Now $\langle \tilde{\psi}_\gamma, g \rangle = \beta_\gamma = \langle \tilde{\psi}_\gamma, f \rangle$, which is a contradiction. Hence $f = g$. $\square$

Theorem 7.4. *Let $n \in \mathbb{Z}_+$ and $j_0 \in \mathbb{Z}$. Let $\sigma \in \mathbb{R}_+$, $p \in [1, \infty]$, and $q \in [1, \infty]$. Let $\varphi^{[n]}$ be a mother scaling function of a compactly supported tensor product MRA of $C_u(\mathbb{R}^n)$. Suppose that $\varphi^{[n]} \in C^r(\mathbb{R}^n)$ for some $r \in \mathbb{R}_+$, $r > \sigma$. Let $f \in B_{p,q}^\sigma(\mathbb{R}^n)$. Then*

$$f(\mathbf{x}) = \sum_{\alpha \in \Omega(n, j_0)} \langle \tilde{\psi}_\alpha, f \rangle \psi_\alpha(\mathbf{x})$$

for all $\mathbf{x} \in \mathbb{R}^n$ and the series above converges absolutely for each $\mathbf{x} \in \mathbb{R}^n$.

Proof. Let

$$a := \|(2^{(\sigma - \frac{n}{p})j} \|(\langle \tilde{\psi}_{\mathbf{s}, j, \mathbf{k}}^{[n]}, f \rangle)_{\mathbf{s} \in J_+(n), \mathbf{k} \in \mathbb{Z}^n}\|_p)_{j=j_0}^\infty\|_q.$$

Now

$$|\langle \tilde{\psi}_{\mathbf{s}, j, \mathbf{k}}^{[n]}, f \rangle| \leq 2^{-(\sigma - \frac{n}{p})j} a \quad (7.24)$$

for all $\mathbf{s} \in J_+(n)$, $j \in \mathbb{N} + j_0$, and $\mathbf{k} \in \mathbb{Z}^n$. Let

$$A_0(\mathbf{x}) := \{(\mathbf{0}_n, j_0, \mathbf{k}) : \mathbf{x} \in \text{supp } \varphi_{j_0, \mathbf{k}}^{[n]}, \mathbf{k} \in \mathbb{Z}^n\}$$

for each $\mathbf{x} \in \mathbb{R}^n$ and

$$A_k(\mathbf{x}) := \{(\mathbf{s}, j_0 + k - 1, \mathbf{k}) : \mathbf{x} \in \text{supp } \psi_{\mathbf{s}, j_0 + k - 1, \mathbf{k}}^{[n]}, \mathbf{s} \in J_+(n), \mathbf{k} \in \mathbb{Z}^n\}$$

for each $\mathbf{x} \in \mathbb{R}^n$ and $k \in \mathbb{Z}_+$. Let $\eta : \mathbb{N} \rightarrow \Omega(n, j_0)$ be a bijection and define

$$\beta_\alpha^{(m)} := \begin{cases} \langle \tilde{\psi}_\alpha, f \rangle; & \alpha \notin \eta[Z_0(m)], \\ 0; & \alpha \in \eta[Z_0(m)] \end{cases} \quad (7.25)$$

for each $m \in \mathbb{N}$ and $\alpha \in \Omega(n, j_0)$. Let

$$g_m(\mathbf{x}) := \sum_{k=0}^m \langle \tilde{\psi}_{\eta(k)}, f \rangle \psi_{\eta(k)}(\mathbf{x})$$

for all $\mathbf{x} \in \mathbb{R}^n$ and $m \in \mathbb{N}$. It follows from Theorem 4.3 that

$$f(\mathbf{x}) = \sum_{k=0}^{\infty} \sum_{\alpha \in A_k(\mathbf{x})} \langle \tilde{\psi}_\alpha, f \rangle \psi_\alpha(\mathbf{x})$$

for all $\mathbf{x} \in \mathbb{R}^n$. Define $c_1 := \max\{\|\psi_{\mathbf{s}}^{[n]}\|_\infty : \mathbf{s} \in \{0, 1\}^n\}$. Let $\mathbf{y} \in \mathbb{R}^n$ and $h \in \mathbb{R}_+$. Define $m_1 := \max\{\#A_k(\mathbf{x}) : \mathbf{x} \in \mathbb{R}^n\}$. Let

$$j_1 := \max \left\{ j_0 + 1, \left\lceil \left(\sigma - \frac{n}{p} \right)^{-1} \log_2 \frac{c_1 m_1 a}{(1 - 2^{-(\sigma - \frac{n}{p})h})} \right\rceil \right\}.$$

Choose $m_2 \in \mathbb{N}$ so that $A_k(\mathbf{y}) \subset \eta[Z_0(m_2)]$ for all $k \in Z_0(j_1 - j_0)$. Suppose that $m \in \mathbb{N}$, $m > m_2$, and $\alpha_0 \in A_{j_0+k}$ for some $k_0 \in Z_0(j_1 - j_0)$. By Eqs. (7.24) and

(7.25) we have

$$\begin{aligned} |f(\mathbf{y}) - g_m(\mathbf{y})| &\leq c_1 \sum_{k=0}^{\infty} \sum_{\alpha \in A_k(\mathbf{y})} |\beta_{\alpha}^{(m)}| = c_1 \sum_{k=j_1-j_0+1}^{\infty} \sum_{\alpha \in A_k(\mathbf{y})} |\beta_{\alpha}^{(m)}| \\ &\leq c_1 m_1 a \cdot 2^{-j_1(\sigma - \frac{n}{p})} \frac{1}{1 - 2^{-(\sigma - \frac{n}{p})}} < h. \end{aligned}$$

Thus $g_m(\mathbf{x}) \rightarrow f(\mathbf{x})$ as $m \rightarrow \infty$ for all $\mathbf{x} \in \mathbb{R}^n$. □

Acknowledgements

The author thanks to Prof. Tapio T. Rantala for support.

References

1. A. Almeida, Wavelet bases in generalized Besov spaces, *J. Math. Anal. Appl.* **304** (2005) 198–211.
2. C. Bennett and R. Sharpley, *Interpolation of Operators* (Academic Press, London, 1988).
3. P. Brenner, *Besov Spaces and Applications to Difference Methods for Initial Value Problems* (Springer, Berlin, 1975).
4. J. Brodzki and G. A. Niblo, Rapid decay and the metric approximation property, preprint (2004), arXiv:math.GR/0403423v2.
5. C. K. Chui and C. Li, A general framework of multivariate wavelets with duals, *Appl. Comput. Harmon. Anal.* **1** (1994) 368–390.
6. C. K. Chui and C. Li, Dyadic affine decompositions and functional wavelet transforms, *SIAM J. Math. Anal.* **27**(3) (1996) 865–890.
7. S. Dahlke, K. Gröchenig and P. Maass, A new approach to interpolating scaling functions: Scaling functions, *Appl. Anal.* **72**(3–4) (1999) 485–500.
8. I. Daubechies, Orthonormal bases of compactly supported wavelets, *Commun. Pure Appl. Math.* **XLI** (1988) 909–996.
9. I. Daubechies, *Ten Lectures on Wavelets* (SIAM, 1992).
10. M. Daws, Dual Banach algebras: Representations and injectivity, preprint (2006), arXiv:math.FA/0604372v1.
11. A. Defant and K. Floret, *Tensor Norms and Operator Ideals* (North-Holland, Amsterdam, 1993).
12. G. Deslauriers and S. Dubuc, Symmetric iterative interpolation processes, *Constr. Approx.* **5**(1) (1989) 49–68.
13. R. A. DeVore, B. Jawerth and B. J. Lucier, Image compression through wavelet transform coding, *IEEE Trans. Inform. Theory* **38**(2) (1992) 719–746.
14. R. A. DeVore and V. A. Popov, Interpolation of Besov spaces, *Trans. Amer. Math. Soc.* **305**(1) (1988) 397–414.
15. P. Domański and M. Lindström, Grothendieck spaces and duals of injective tensor products, *Bull. London Math. Soc.* **28** (1996) 617–626.
16. P. Domański, M. Lindström and G. Schlüchtermann, Grothendieck operators on tensor products, *Proc. Amer. Math. Soc.* **125**(8) (1997) 2285–2291.
17. D. L. Donoho, Interpolating wavelet transforms, tech. report, Department of Statistics, Stanford University (1992).

18. S. Dubuc, Interpolation through an iterative scheme, *J. Math. Anal. Appl.* **114** (1986) 185–204.
19. H. Glöckner, Tensor products in the category of topological vector spaces are not associative, preprint (2004), arXiv:math.FA/0307041v2.
20. S. Goedecker, *Wavelets and Their Application for the Solution of Partial Differential Equations in Physics* (Presses Polytechniques et Universitaires Romandes, Lausanne, 1998).
21. A. Grothendieck, Produits tensoriels topologiques et espaces nucléaires, *Mem. Amer. Math. Soc.* **16** (1955).
22. B. Han, Symmetry property and construction of wavelets with a general dilatation matrix, *Linear Algebra Appl.* **353** (2002) 207–225.
23. B. Han and R.-Q. Jia, Optimal interpolatory subdivision schemes in multidimensional spaces, *SIAM J. Numer. Anal.* **36**(1) (1998) 105–124.
24. W. Härdle, G. Kerkycharian, D. Picard and A. Tsybakov, Wavelets, Approximation, and Statistical Applications, <http://www.quantlet.com/mdstat/scripts/wav/html/>.
25. W. He and M. Lai, Bivariate box spline wavelets in Sobolev spaces, *SPIE's Int. Symp. on Optical Science, Engineering, and Instrumentation* (International Society for Optics and Photonics, 1998), pp. 56–66.
26. T. Höynälänmaa, Multiresolution analysis for compactly supported interpolating tensor product Wavelets (long version), preprint (2010), arXiv:1005.3371 [math.FA].
27. H. Ji and Z. Shen, Compactly supported (bi)orthogonal wavelets generated by interpolatory refinable functions, *Adv. Comput. Math.* **11**(1) (1999) 81–104.
28. R. Q. Jia and C. A. Micchelli, Using the refinement equations for the construction of pre-wavelets II: Powers of two, *Curves Surfaces* (1991) 209–246.
29. S. Karakaz'yan, M. Skopina and M. Tchobanou, Symmetric multivariate wavelets, *Int. J. Wavelets, Multiresolut. Inf. Process.* **7**(3) (2008) 1–28.
30. J. Kovačević and W. Sweldens, Wavelet families of increasing order in arbitrary dimensions, *IEEE Trans. Image Process.* **9**(3) (2000) 480–496.
31. A. Krivoshein and M. Skopina, Approximation by frame-like wavelet systems, *Appl. Comput. Harmon. Anal.* **31**(3) (2011) 410–428.
32. J. Kustermans and S. Vaes, The operator algebra approach to quantum groups, *Proc. Natl. Acad. Sci. USA* **97**(2) (2000) 547.
33. G. Kyriazis and P. Petrushev, New bases for Triebel-Lizorkin and Besov spaces, *Trans. Amer. Math. Soc.* **354**(2) (2002) 749–776.
34. H. E. Lacey, *The Isometric Theory of Classical Banach Spaces* (Springer-Verlag, 1974).
35. W. Lawton, S. L. Lee and Z. Shen, Stability and orthonormality of multivariate refinable functions, *SIAM J. Math. Anal.* **28**(4) (1997) 999–1014.
36. R. M. Lewis, Cardinal interpolating multiresolutions, *J. Approx. Theory* **76** (1994) 177–202.
37. W. A. Light and E. W. Cheney, *Approximation Theory in Tensor Product Spaces* (Springer-Verlag, 1985).
38. Y. Meyer, *Wavelets and Operators* (Cambridge University Press, 1992).
39. P. W. Michor, *Functors and Categories of Banach Spaces* (Springer-Verlag, 1978).
40. O. I. Reinov, On Banach spaces without the approximation property, preprint (2002), arXiv:math.FA/0203146v1.
41. R. A. Ryan, *Introduction to Tensor Products of Banach Spaces* (Springer, New York, 2002).
42. H. H. Schaefer, *Topological Vector Spaces* (The Macmillan Company, New York, 1966).

- 43. P.-L. Shui, Z. Bao and X.-D. Zhang, *M*-band Compactly supported orthogonal symmetric interpolating scaling functions, *IEEE Trans. Signal Process.* **49**(8) (2001) 1704–1713.
- 44. H. Triebel, *Theory of Function Spaces* (Birkhäuser-Verlag, Basel, 1983).
- 45. P. Wojtaszczyk, *A Mathematical Introduction to Wavelets* (Cambridge University Press, 1997).

PUBLICATION

III

Electronic Structure Calculations with the Exact Pseudopotential and Interpolating Wavelet Basis

Tommi Höynälänmaa and Tapio T. Rantala

Atoms 11 (2023)

DOI: <https://doi.org/10.3390/atoms11010009>

**Publication is licensed under a Creative Commons Attribution 4.0
International License CC-BY.**

Article

Electronic Structure Calculations with the Exact Pseudopotential and Interpolating Wavelet Basis

Tommi Höynälänmaa *  and Tapio T. Rantala * 

Computational Physics, Tampere University, P.O. Box 692, FI-33014 Tampere, Finland

* Correspondence: tommi.hoynalanmaa@tuni.fi (T.H.); tapio.rantala@tuni.fi (T.T.R.)

Abstract: Electronic structure calculations are mostly carried out with Coulomb potential singularity adapted basis sets such as STO or contracted GTO. With another basis or for heavy elements, the pseudopotentials may appear as a practical alternative. Here, we introduce the exact pseudopotential (EPP) to remove the Coulomb singularity and test it for orbitals of small atoms with the interpolating wavelet basis set. We apply EPP to the Galerkin method with a basis set consisting of Deslauriers–Dubuc scaling functions on the half-infinite real interval. We demonstrate the EPP–Galerkin method by computing the hydrogen atom 1s, 2s, and 2p orbitals and helium atom configurations He 1s², He 1s2s ¹S, and He 1s2s ³S. We compare the method to the ordinary interpolating wavelet Galerkin method (OIW–Galerkin), handling the singularity at the nucleus by excluding the scaling function located at the origin from the basis. We also compare the performance of our approach to that of finite-difference approach, which is another practical method for spherical atoms. We find the accuracy of the EPP–Galerkin method to be better than both of the above-mentioned methods.

Keywords: interpolating wavelet; electronic structure; Schrödinger equation; Hartree–Fock

MSC: 81V45



Citation: Höynälänmaa, T.; Rantala, T.T. Electronic Structure Calculations with the Exact Pseudopotential and Interpolating Wavelet Basis. *Atoms* **2023**, *11*, 9. <https://doi.org/10.3390/atoms11010009>

Received: 10 November 2022

Revised: 7 December 2022

Accepted: 28 December 2022

Published: 1 January 2023



Copyright: © 2023 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<https://creativecommons.org/licenses/by/4.0/>).

1. Introduction

The Coulomb singularity in the hamiltonian may appear as a challenge in electronic structure calculations. Singularity-adapted Slater type-atomic orbitals (STO) basis is the usual solution to this, and Gaussian-type contracted basis functions (GTO) have turned out to be useful with sufficient accuracy. The latter one is more popular due to other practical advantages.

Pseudopotentials removing the singularity are another possible solution to this problem. In this case, the core electrons do not play an essential role in the problem at hand or valence electrons are expanded in plane waves, like with heavy elements or periodic crystalline systems. In those cases, the pseudopotentials typically replace the nuclei and a number of core electrons with their charge distribution, and possibly, some other core properties.

One-dimensional interpolating wavelets have been used for atomic computations, for example, in Ref. [1]. Fischer and Defranceschi [2] have also solved hydrogen-like atoms with wavelets. In Ref. [1], we used ordinary Deslauriers–Dubuc interpolating wavelets [3–5] defined on the whole real axis, so including the negative real axis in the computations. We handled the singularity at the origin by excluding the scaling function at the origin from the basis. We used the nonstandard operator form for the various operators needed in the computations. We computed the Schrödinger equation of hydrogenlike atoms (ions) and Hartree–Fock equations of some light many-electron atoms (helium, lithium, beryllium, neon, sodium, magnesium, and argon). In this article, we repeat similar computations for hydrogen and helium atoms, but using a different method to handle the singularity of the potential and only one resolution level. We handle the singularity by computing the Schrödinger and Hartree–Fock equations for a range of variables $r \in [a, \infty]$, which does

not contain the origin. Here, r is the position coordinate. The range $r \in [0, a]$ is neglected for hydrogen, and for helium, its contribution to the Slater integrals is computed using the hydrogenic orbitals.

Arias [6] 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 $\mathbb{R}$ was conducted in Ref. [4]. One-dimensional interpolating multiresolution analysis in space $C_0(\mathbb{R})$ consisting of continuous functions in $\mathbb{R}$ and vanishing at infinity was constructed in [5]. Both of these constructions are based on Deslauriers–Dubuc functions [3]. Donoho [5] constructs wavelets on a finite real interval, too. We compute the eigenenergies of hydrogen atom 1s, 2s, and 2p orbitals and helium atom configurations He 1s², He 1s2s ¹S, and He 1s2s ³S with the EPP method Exact Pseudopotential Method (EPP) using both the Galerkin method with interpolating wavelets and the finite difference method.

We denote the pointwise product of functions f and g by $f \star g$. We use atomic units throughout this article ($e = m_e = \hbar = 4\pi\epsilon_0 = 1$) and denote the atomic unit of energy by Ha (Hartree).

2. Interpolating Wavelets on Half-Infinite Interval

2.1. Interpolating Wavelets

Interpolating wavelets are a biorthogonal wavelet family. Since the dual scaling functions and dual wavelets of these functions are finite sums of Dirac delta functions, the matrix elements involving interpolating wavelets usually require evaluating some functions in a finite set of points. An interpolating wavelet family is defined by a mother scaling function φ , mother wavelet ψ , and four finite filters h_j , g_j , $\tilde{h}_j$, and $\tilde{g}_j$ where $j = -m, \dots, m$. The functions φ , ψ , $\tilde{\varphi}$, and $\tilde{\psi}$ satisfy equations

$$\varphi(x) = \sum_{j=-m}^m h_j \varphi(2x - j), \quad (1)$$

$$\psi(x) = \sum_{j=-m}^m g_j \varphi(2x - j), \quad (2)$$

$$\tilde{\varphi}(x) = \sum_{j=-m}^m \tilde{h}_j \tilde{\varphi}(2x - j), \quad (3)$$

and

$$\tilde{\psi}(x) = \sum_{j=-m}^m \tilde{g}_j \tilde{\varphi}(2x - j). \quad (4)$$

The two-index basis functions and dual basis functions are

$$\varphi_{j,k}(x) = \varphi(2^j x - k), \quad (5)$$

$$\psi_{j,k}(x) = \psi(2^j x - k), \quad (6)$$

$$\tilde{\varphi}_{j,k}(x) = 2^j \tilde{\varphi}(2^j x - k), \quad (7)$$

and

$$\tilde{\psi}_{j,k}(x) = 2^j \tilde{\psi}(2^j x - k). \quad (8)$$

A wavelet basis consists of scaling functions $\varphi_{j_0,k}$, $k \in \mathbb{Z}$, and wavelets $\psi_{j,k}$, $j \geq j_0$, $k \in \mathbb{Z}$, where $j_0 \in \mathbb{Z}$ is the minimum resolution level. The expansion of an arbitrary (regular enough) function $f: \mathbb{R} \rightarrow \mathbb{R}$ in the wavelet basis is

$$f(x) = \sum_{k \in \mathbb{Z}} s_k \varphi_{j_0,k}(x) + \sum_{j \geq j_0} \sum_{k \in \mathbb{Z}} d_{j,k} \psi_{j,k}(x). \quad (9)$$

2.2. The Basis Set

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 φ to be a Deslauriers–Dubuc scaling function of some order D and $\varphi_{j,k}(x) := \varphi(2^j x - k)$ for $j, k \in \mathbb{Z}$.

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 define

$$\tilde{\beta}_{j,k} := \pi_j^\#(2^{-j}k) \quad (10)$$

for $k < 0$ and

$$\tilde{\beta}_{j,k} := \beta_{j,k} \quad (11)$$

for $k \geq 0$. Now, f can be extrapolated onto the whole real line by

$$\tilde{f} = \sum_{k=-\infty}^{\infty} \tilde{\beta}_{j,k} \varphi_{j,k}. \quad (12)$$

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

$$\tilde{\beta}_{j,k} = \sum_{k'=0}^D e_{k,k'}^\# \beta_{j,k'} \quad (13)$$

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

$$\tilde{\beta}_{j,k} = e_{k,l}^\# \quad (14)$$

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

$$\text{supp } \varphi_{j,k} \subset 2^{-j}[k - D, k + D] \quad (15)$$

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

$$\varphi_{j,k}^\# := \varphi_{j,k} + \sum_{l < 0} e_{l,k}^\# \varphi_{j,l} \quad (16)$$

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

$$\langle \tilde{\varphi}_{j,k}, \varphi_{j,l}^\# \rangle = \delta_{k,l} \quad (17)$$

for $k \geq 0$ and $0 \leq l \leq D$.

We define a wavelet expansion of function f by

$$\tilde{f} := \sum_{k=0}^D \beta_{j,k} \varphi_{j,k}^\# + \sum_{k=D+1}^{\infty} \beta_{j,k} \varphi_{j,k}. \quad (18)$$

When we use a finite basis of size W , we have

$$\tilde{f} := \sum_{k=0}^D \beta_{j,k} \varphi_{j,k}^\# + \sum_{k=D+1}^{W-1} \beta_{j,k} \varphi_{j,k}. \quad (19)$$

We must have $W > 2D$ so that functions $\varphi_{j,k}^\#(x)$, $0 \leq k \leq D$, vanish for $x \geq 2^{-j}W$. This kind of truncation of the basis requires that the function f approximately vanishes for $x > 2^{-j}W$.

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

$$\langle \tilde{\varphi}_{j,k}, A\varphi_{j,l}^\# \rangle = \langle \tilde{\varphi}_{j,k}, A\varphi_{j,l} \rangle + \sum_{\alpha < 0} e_{\alpha,l}^\# \langle \tilde{\varphi}_{j,k}, A\varphi_{j,\alpha} \rangle. \quad (20)$$

Let $v(f)$ denote the coefficient vector $(\beta_{j,k})_{k=0}^{W-1}$ defined by Equation (19) and define

$$M(f) := \left(f(2^{-j}k) \delta_{k,k'} \right)_{k,k'=0}^{W-1, W-1} \quad (21)$$

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

3. Schrödinger Equations of Hydrogen-like Atoms and Helium Atoms in the EPP-Wavelet Basis

3.1. General

Suppose that we have a system consisting of a positively charged nucleus at the origin and N electrons. In the EPP method, we choose a small radius r_0 so that inside the sphere with radius r_0 , the wavefunctions of the system are approximated by hydrogenic wavefunctions, and the actual computations are performed only for values $r \geq r_0$. Actually, we define a basis set for the half-infinite interval $[0, \infty]$ and make a change of the variables $s = r - r_0$. For Hartree–Fock calculations, the Slater integrals are computed by

$$\begin{aligned} \tilde{y}_{ab}^0(s) &= \frac{Q_{ab}}{s+r_0} + \frac{1}{s+r_0} \int_0^s \bar{P}_a(s') \bar{P}_b(s') ds' \\ &+ \int_s^\infty \frac{1}{s'+r_0} \bar{P}_a(s') \bar{P}_b(s') ds' \end{aligned} \quad (22)$$

where $s \geq 0$ and Q_{ab} is a system-dependent quantity that approximates the contribution of the EPP core region to the Slater integral.

3.2. Hydrogen-like Atoms

The Schrödinger equation of the hydrogen atom and Hartree–Fock equations of atoms [7] and their representation in the interpolating wavelet basis [1] denote our starting point. With a change in variables $s := r - r_0$, the Schrödinger equation of a hydrogen-like atom in interval $r \geq r_0$ takes the form

$$\left(-\frac{1}{2} \frac{d^2}{ds^2} - \frac{Z}{s+r_0} + \frac{l(l+1)}{2(s+r_0)^2} \right) \bar{P}(s) = E \bar{P}(s), \quad s \geq 0 \quad (23)$$

where Z is the charge of the nucleus, l is the angular momentum quantum number, and $\bar{P}(s) = P(r_0 + s)$ for $s \geq 0$.

We define the second derivative filter by

$$a_k := \langle \tilde{\varphi}, D^2 \varphi(\cdot - k) \rangle. \quad (24)$$

Matrix elements of the Laplacian operator L are computed by

$$L_{k,l} := \langle \tilde{\varphi}_{j,k}, L\varphi_{j,l}^\# \rangle = 2^{2j} \left(a_{l-k} + \sum_{\alpha=-D}^{-1} e_{\alpha,l}^\# a_{\alpha-k} \right) \quad (25)$$

for $0 \leq l \leq D$ and

$$L_{k,l} := \langle \tilde{\varphi}_{j,k}, L\varphi_{j,l} \rangle = 2^{2j} a_{l-k} \quad (26)$$

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

$$\hat{V}_{k,k} = V(2^{-j}k) \quad (27)$$

where

$$V(y) = -\frac{Z}{y+a} \quad (28)$$

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

3.3. Hartree–Fock Equations for Helium Atom

Define the Slater integrals as

$$y_{ab}^0(r) = \int_{r'=0}^{\infty} P_a(r')\gamma(r, r')P_b(r')dr' \quad (29)$$

where a and b denote the atomic orbitals and

$$\gamma(r, r') = \frac{1}{\max\{r, r'\}}. \quad (30)$$

We use symbol y instead of Y to avoid confusion with spherical harmonics. By carrying out a similar change in 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

$$\left(-\frac{1}{2}\frac{d^2}{ds^2} - \frac{2}{s+r_0} + y_{1s1s}^0(s+r_0)\right)\bar{P}_{1s}(s) = \epsilon_{1s}\bar{P}_{1s}(s), \quad s \geq 0. \quad (31)$$

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

$$\left(-\frac{1}{2}\frac{d^2}{ds^2} - \frac{2}{s+r_0} + y_{2s2s}^0(s+r_0)\right)\bar{P}_{1s}(s) = \epsilon_{1s}\bar{P}_{1s}(s) \quad (32)$$

$$\left(-\frac{1}{2}\frac{d^2}{ds^2} - \frac{2}{s+r_0} + y_{1s1s}^0(s+r_0)\right)\bar{P}_{2s}(s) = \epsilon_{2s}\bar{P}_{2s}(s) \quad (33)$$

and for helium $1s2s$ ^3S configuration

$$\begin{aligned} \left(-\frac{1}{2}\frac{d^2}{ds^2} - \frac{2}{s+r_0} + y_{2s2s}^0(s+r_0)\right)\bar{P}_{1s}(s) &= \epsilon_{1s}\bar{P}_{1s}(s) + \\ & y_{1s2s}^0(s+r_0)\bar{P}_{2s}(s) \end{aligned} \quad (34)$$

$$\begin{aligned} \left(-\frac{1}{2}\frac{d^2}{ds^2} - \frac{2}{s+r_0} + y_{1s1s}^0(s+r_0)\right)\bar{P}_{2s}(s) &= \epsilon_{2s}\bar{P}_{2s}(s) + \\ & y_{2s1s}^0(s+r_0)\bar{P}_{1s}(s) \end{aligned} \quad (35)$$

3.4. EPP of Helium Atom

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

$$(\hat{U}_0 f)(s) = \int_0^s f(s')ds' \quad (36)$$

and

$$(\hat{U}_\infty f)(s) = \int_s^\infty f(s')ds'. \quad (37)$$

Define $P_{1s,H}(r')$ and $P_{2s,H}(r')$ to be the hydrogenic orbitals of the helium atom. Then, we have

$$\langle \tilde{\varphi}_{j,k} \hat{U}_0 \varphi_{j,l} \rangle = 2^{-j} (\Phi(|k| - l) - \Phi - l) \quad (38)$$

and

$$\langle \tilde{\varphi}_{j,k} \hat{U}_\infty \varphi_{j,l} \rangle = 2^{-j} (1 - \Phi(|k| - l)) \quad (39)$$

where

$$\Phi(x) = \int_{-\infty}^x \varphi(y) dy. \quad (40)$$

The Slater integrals in the shifted variables are obtained from Equation (22) where we set

$$Q_{ab} := \frac{\bar{P}_a(0)}{\bar{P}_{a,H}(r_0)} \frac{\bar{P}_b(0)}{\bar{P}_{b,H}(r_0)} \int_0^{r_0} P_{a,H}(r') P_{b,H}(r') dr' \quad (41)$$

for the helium ground state, and

$$Q_{ab} := \int_0^{r_0} P_{a,H}(r') P_{b,H}(r') dr' \quad (42)$$

for the excited states of helium. Define

$$q(s) := \frac{1}{s + r_0} \quad (43)$$

and

$$S_0 := M(q)U_0 + U_\infty M(q). \quad (44)$$

Now,

$$v(\tilde{y}_{ab}^0) = Q_{ab}v(q) + S_0(v(\bar{P}_a \star \bar{P}_b)) \quad (45)$$

where U_0 and U_∞ are the matrices of operators $\hat{U}_0$ and $\hat{U}_\infty$ in the basis set constructed in Section 2. We define $\mathbf{v}_a = v(\bar{P}_a)$ and $\mathbf{v}_b = v(\bar{P}_b)$. The matrix of the exchange integral operator

$$(\hat{K}_a \bar{P}_a)(s) := \tilde{y}_{ab}^0(s) \bar{P}_b(s) \quad (46)$$

is computed by

$$K_a := W_a + M(\mathbf{v}_b)S_0M(\mathbf{v}_b). \quad (47)$$

The term $W_a \mathbf{v}_a$ approximates the first term in Equation (22) as a linear function of $\mathbf{v}_a$. For 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

$$\frac{Q_{ab}}{s + r_0} \bar{P}_b(s) \approx \frac{1}{s + r_0} \bar{P}_a(0) \left(\int_{s'=-r_0}^0 \left(1 + \frac{s'}{r_0} \right) P_{b,H}(s' + r_0) ds' \right) \bar{P}_b(s). \quad (48)$$

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 find the hydrogenic Slater integrals

$$y_{1s1s,H}^0(r) = \frac{1}{r} - e^{-2Zr} \left(\frac{1}{r} + Z \right) \quad (49)$$

$$y_{2s2s,H}^0(r) = \frac{1}{r} + e^{-Zr} \left(-\frac{Z^3}{8} r^2 - \frac{1}{4} Z^2 r - \frac{3Z}{4} - \frac{1}{r} \right) \quad (50)$$

$$y_{1s2s,H}^0(r) = \frac{1}{27\sqrt{2}} (12Z^2 r + 8Z) e^{-3Zr/2} \quad (51)$$

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

$$\begin{aligned} \langle P_a | y_{ab}^0 | P_b \rangle &\approx \left(\frac{\bar{P}_a(0)}{P_{a,H}(r_0)} \right)^2 \left(\frac{\bar{P}_b(0)}{P_{b,H}(r_0)} \right)^2 \\ &\quad \cdot \int_{r'=0}^{r_0} P_{a,H}(r') y_{ab,H}^0(r') P_{b,H}(r') dr' \\ &\quad + \int_{s=0}^{\infty} \bar{P}_a(s) \bar{y}_{ab}^0(s) \bar{P}_b(s) ds \end{aligned} \quad (52)$$

for the helium ground state and

$$\begin{aligned} \langle P_a | y_{ab}^0 | P_b \rangle &\approx \int_{r'=0}^{r_0} P_{a,H}(r') y_{ab,H}^0(r') P_{b,H}(r') dr' \\ &\quad + \int_{s=0}^{\infty} \bar{P}_a(s) \bar{y}_{ab}^0(s) \bar{P}_b(s) ds \end{aligned} \quad (53)$$

for the excited states of helium.

3.5. Total Energy of Helium Atom

The total energy of the ground state of the helium atom is

$$E(\text{He } 1s^2) = 2\varepsilon_{1s} - \langle P_{1s} | y_{1s1s}^0 | P_{1s} \rangle. \quad (54)$$

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

$$\begin{aligned} E(\text{He } 1s2s \ ^1S) &= \varepsilon_{1s} + \varepsilon_{2s} \\ &\quad - \frac{1}{2} \langle P_{1s} | y_{2s2s}^0 | P_{1s} \rangle - \frac{1}{2} \langle P_{2s} | y_{1s1s}^0 | P_{2s} \rangle \end{aligned} \quad (55)$$

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

$$\begin{aligned} E(\text{He } 1s2s \ ^3S) &= \varepsilon_{1s} + \varepsilon_{2s} \\ &\quad - \frac{1}{2} \langle P_{1s} | y_{2s2s}^0 | P_{1s} \rangle - \frac{1}{2} \langle P_{2s} | y_{1s1s}^0 | P_{2s} \rangle \\ &\quad + \langle P_{1s} | y_{1s2s}^0 | P_{2s} \rangle. \end{aligned} \quad (56)$$

4. Combination of EPP with Finite Difference Method

The Schrödinger and Hartree–Fock equations are converted to matrix equations using the biorthogonality relations of interpolating wavelets [1]. We compare these computations with the Finite Difference Method, which is a straightforward method for solving differential equations. The spatial and time domains are discretized, and the derivative at a point is computed with a stencil applied to the nearby points. This way the differential equation is converted to a matrix equation. The Laplacian operator is approximated by

$$u''(x) \approx \frac{u(x-h) - 2u(x) + u(x+h)}{h^2} \quad (57)$$

where h is the discretization step size.

We discretize the Schrödinger Equation (23) at points $p_j = jh$, $j = 0, \dots, J+1$, where J is the number of actual computation points and $h \in \mathbb{R}_+$ is the grid spacing. We define the discretized potential by $v_j = \bar{V}(s_j)$. The boundary condition at the end of the interval is set by $p_{J+1} = 0$. We have

$$-\frac{p_{j+1} + (-2 - 2h^2 v_j) p_j + p_{j-1}}{2h^2} = E p_j \quad (58)$$

for $j = 2, \dots, J$. We handle case $j = 1$ by extrapolating p_0 linearly from p_1 and p_2 . We obtain $p_0 = 2p_1 - p_2$ from which it follows that $p_2 + (-2 - 2h^2v_j)p_1 + p_0 = -2h^2v_1p_1$. Hence, the difference equation for $j = 1$ is

$$v_1p_1 = Ep_1. \quad (59)$$

In order to discretize the exchange operator $\hat{K}_a$ we need to discretize the integral operators

$$(\hat{I}_g(f))(s) = \int_0^s g(s')f(s')ds' \quad (60)$$

and

$$(\hat{I}_g^{\text{compl}}(f))(s) = \int_s^\infty g(s')f(s')ds'. \quad (61)$$

We define

$$(I(g))_{j,k} := \begin{cases} hg_k; & k < j \\ 0; & k \geq j \end{cases} \quad (62)$$

and

$$(I^{\text{compl}}(g))_{j,k} := \begin{cases} hg_k; & k \geq j \\ 0; & k < j \end{cases} \quad (63)$$

where $g_k = g(s_k)$. When f is a real function, we define $w(f) := (f(s_k))_{k=1}^J$. Now, the matrix of the exchange integral operator is computed by

$$K_a := W_a + K_a^0 \quad (64)$$

where W_a is computed as in the case of wavelets,

$$K_a^0 := \text{diag}(w(f_1))I(\bar{P}_b) + I^{\text{compl}}(f_1 \star \bar{P}_b), \quad (65)$$

and

$$f_1(s) := \frac{1}{s + r_0}, \quad s \geq 0. \quad (66)$$

5. Results

We demonstrate the EPP method by performing computations where the EPP radius r_0 and the basis size W are varied. We actually select a length scale $u = R/W$ and conduct a change of variables $s = us'$ in Equations (23) and (31)–(35). The length scale u specifies how many atomic units of length a length unit in our own coordinate system is. Here, R is the size of the computation domain. For hydrogen 1s, we have $R = 15$ a.u., for hydrogen 2s and 2p $R = 25$ a.u., for He 1s² $R = 15$ a.u., and for He 1s2s ¹S and ³S $R = 20$ a.u.. We also set $j = 0$ for the basis set (see Section 2), and hence u is equal to the grid spacing h_{EPP} . The relative errors of the quantities are given as

$$\varepsilon = \left| \frac{x_{\text{computed}} - x_{\text{exact}}}{x_{\text{exact}}} \right|. \quad (67)$$

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 $P_H(r_0)$.

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 ¹S are given in Figure 9 and the results for He 1s2s ³S in Figure 10. As expected, the energy results are best for large values of W and small values of r_0 . Using 200 basis functions for the helium ground state and computing the atom energies for $r_0 = 10^k$, $k = -10, \dots, -1$ shows that atom energies are equal up to seven decimal places for $r_0 \leq 10^{-6}$. Similar

computation for the hydrogen 1s orbital shows that the H 1s energy is equal to -0.5 Ha up to seven decimal places for $r_0 \leq 0.01$. For hydrogen 2s and 2p, the corresponding limit is $r_0 \leq 0.01$, too.

We also found that when the number of basis functions is sufficiently large for a given system, there is an approximate threshold value so that reducing r_0 below it does not make the accuracy of the computed energy better. When the number of basis functions is sufficiently large and r_0 is sufficiently small, the hydrogenic orbitals are approximately continuous at r_0 .

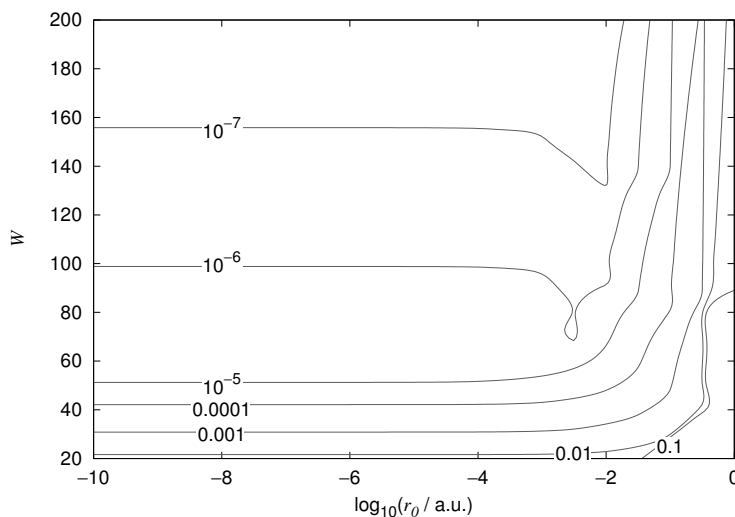


Figure 1. Hydrogen 1s orbital eigenenergy relative error. The r_0 is the EPP radius in atomic units and W is the basis size.

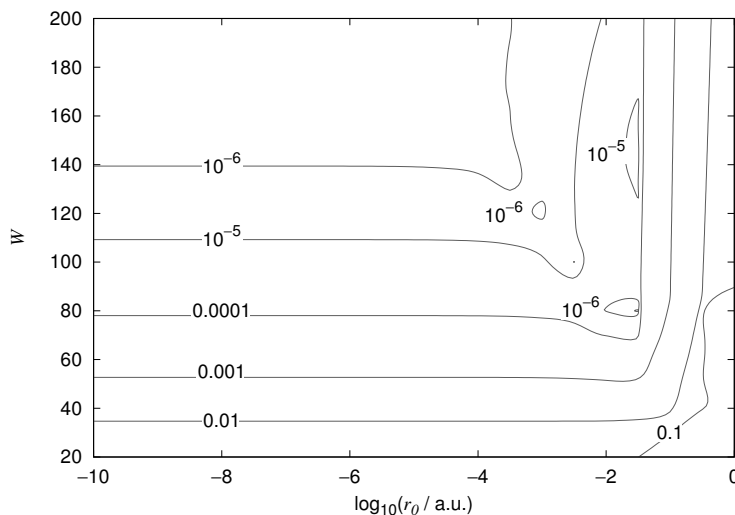


Figure 2. Relative error of the wavefunction value at the core radius for the hydrogen 1s orbital. Notations as in Figure 1.

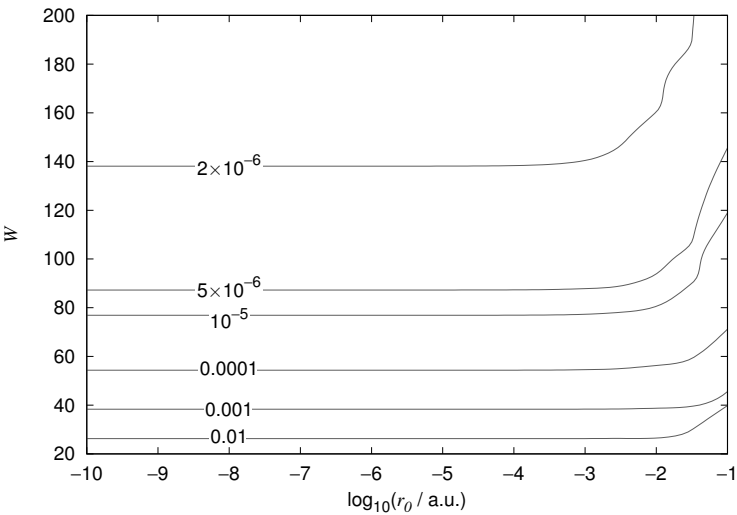


Figure 3. Hydrogen 2s orbital eigenenergy relative error. Notations as in Figure 1.

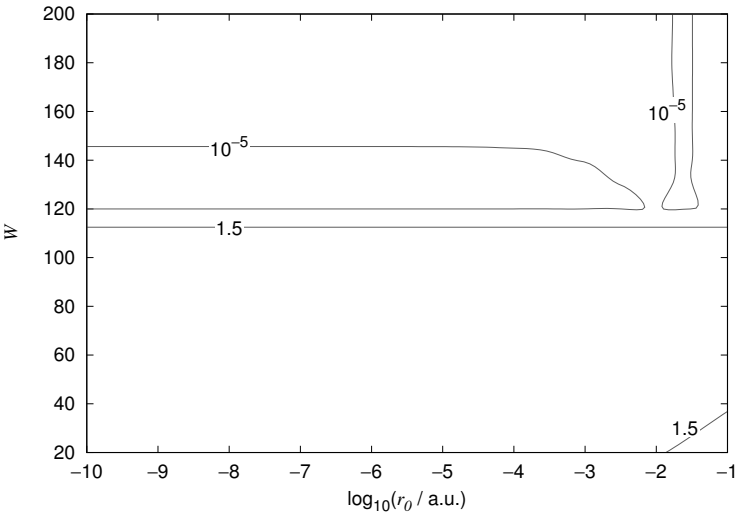


Figure 4. Relative error of the wavefunction value at the core radius for the hydrogen 2s orbital. Notations as in Figure 1.

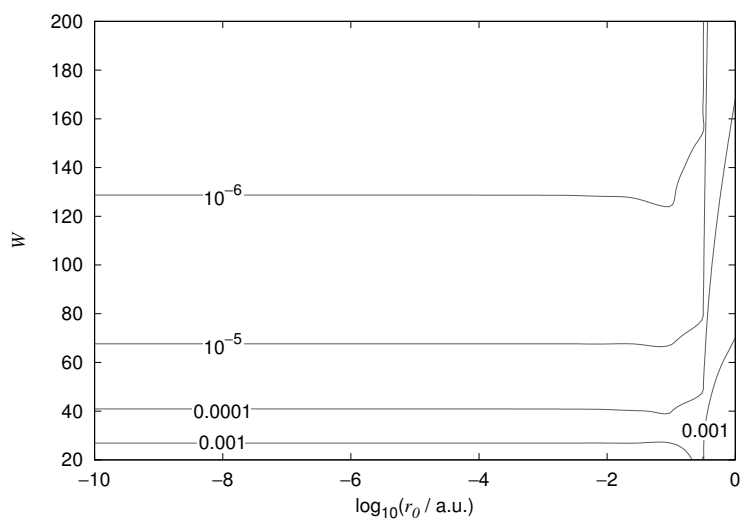


Figure 5. Hydrogen 2p orbital eigenenergy relative error. Notations as in Figure 1.

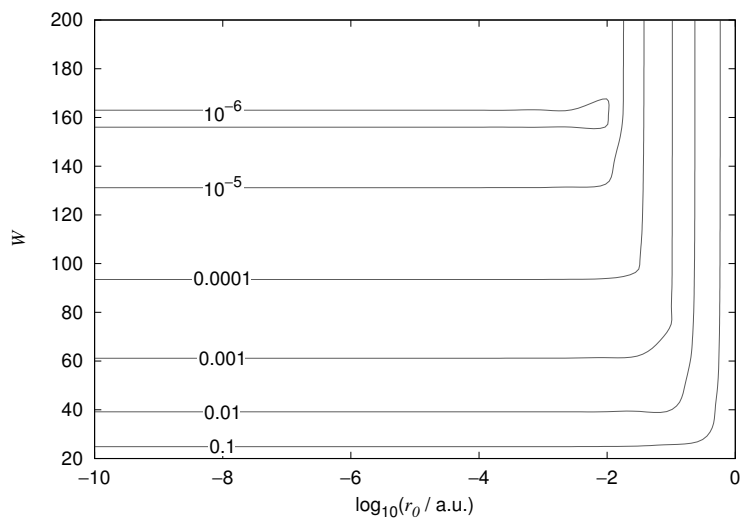


Figure 6. Relative error of the wavefunction value at the core radius for the hydrogen 2p orbital. Notations as in Figure 1.

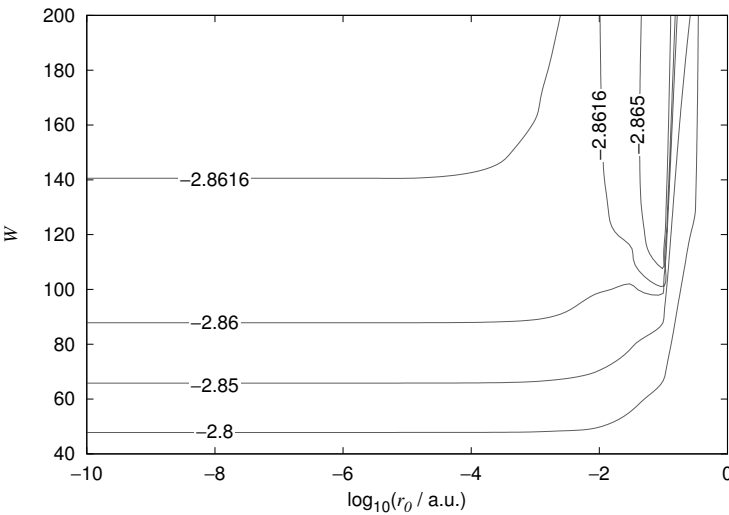


Figure 7. The ground state energy of helium atom. The HF limit is given in Table 1. Notations as in Figure 1.

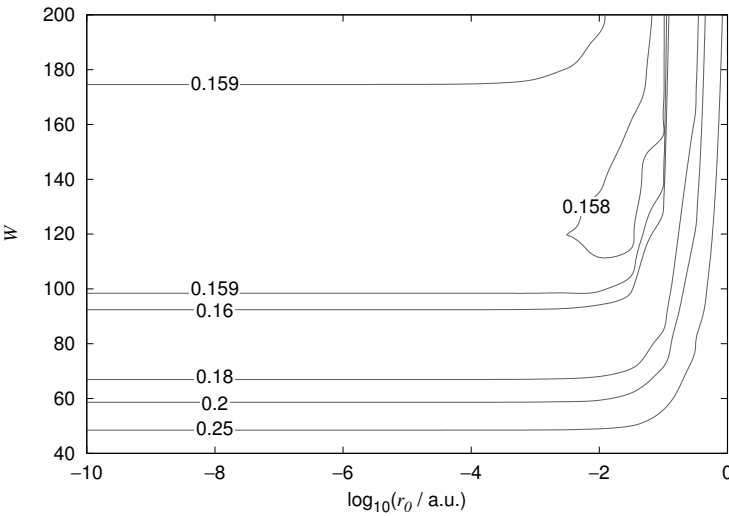


Figure 8. Relative error of the wavefunction value at the core radius for the 1s orbital of the ground state of the helium atom. Notations as in Figure 1.

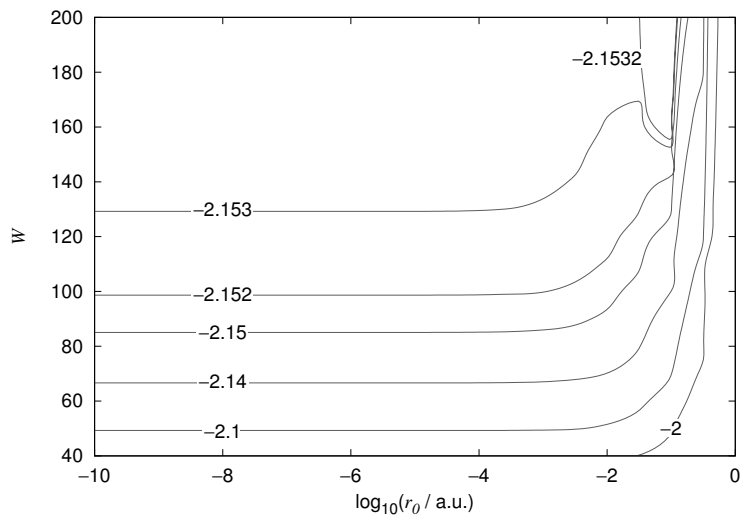


Figure 9. Helium 1s2s ^1S total energy. The HF limit is given in Table 1. Notations as in Figure 1.

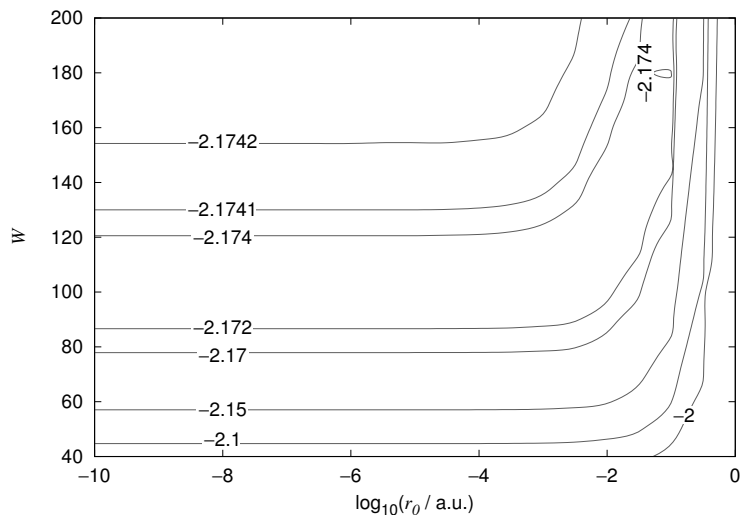


Figure 10. Helium 1s2s ^3S total energy. The HF limit is given in Table 1. Notations as in Figure 1.

The most accurate computations are in the upper left corners of the figures. The orbitals of He 1s2s, except He 1s2s ^3S 1s, are not continuous at all at r_0 , and no continuity plots are presented for them. The computation results and exact results are given in Table 1. For the EPP–Galerkin method the best energies (largest basis and smallest r_0) of the computed systems are presented. The OIW–Galerkin results with same number of basis functions and grid spacing the same order of magnitude as for the most accurate EPP results are given, too. The accuracies of both of the methods depend on the grid spacing. The EPP–Galerkin method gives better results with the same number of basis functions and larger grid spacing. The results of the Finite Difference Method are also given. Note that for He 1s2s systems, the OIW–Galerkin method with a basis set of 601 functions and finest grid

point distance 2^{-9} a.u. gives $E_{\text{He } 1s2s \ ^1S} = -2.153$ Ha and $E_{\text{He } 1s2s \ ^3S} = -2.174$ Ha, which are approximately the same as the results of the EPP–Galerkin method.

Table 1. Hartree–Fock total energies of H and He occupation configurations. E_{ref} are chosen reference values. E_{EPP} is the energy given by the EPP–Galerkin-method, h_{EPP} is the grid spacing in the EPP–Galerkin method, E_{OIW} is the energy given by the OIW–Galerkin method, E_{FDM} is the energy given by the Finite Difference Method, and N_{FDM} is the number of grid points in the Finite Difference Method. For EPP, the most accurate results are given. For OIW computations, the number of basis functions is 201 and the finest grid spacing is 0.00625 a.u..

System	E_{ref}/Ha	E_{EPP}/Ha	$h_{\text{EPP}}/\text{a.u.}$	E_{OIW}/Ha	E_{FDM}/Ha	N_{FDM}
H 1s	$-0.5 \text{ * }^\dagger$	−0.500000	0.075	−0.50	−0.49803	1001
H 2s	$-0.125 \text{ * }^\dagger$	−0.125000	0.125	−0.125	−0.124741	2001
H 2p	$-0.125 \text{ * }^\dagger$	−0.125000	0.125	−0.124998	−0.124995	2001
He 1s ²	$-2.8616800 \text{ }^\dagger$ [8] -2.903724 * [9]	−2.8617	0.075	−2.834868	−2.839	1001
He 1s2s ¹ S	-2.147 ° [10] -2.145974 * [9]	−2.1532	0.1	−2.133579	−2.132	1001
He 1s2s ³ S	-2.171 ° [10] -2.175229 * [9]	−2.1742	0.1	−2.154536	−2.155	1001

*: exact energy; [†]: HF limit; [°]: HF result.

Some of the computations using the diagonalization of the Hamiltonian operator yield an unphysical state for the minimum eigenvalue. For 1s and 2s orbitals, this eigenvalue seems to be about $-Z/r_0$ (in atomic units) and the corresponding eigenvector $v(\vec{P}) = (-\delta_{k,0})_{k \geq 0}$. For the hydrogen 2p orbital, the unphysical eigenvector does not appear. The unphysical state remains the same during the HF iteration of He 1s², He 1s2s ¹S, and He 1s2s ³S. The physical admissibility of the wavefunctions $P_{nl}(r)$ was characterized by the condition

$$\lim_{r \rightarrow 0} P_{nl}(r) = 0. \quad (68)$$

We checked this condition by extrapolating solutions $P_{nl}(r)$ polynomially at $r = 0$. Actually, we extrapolate polynomially $\tilde{P}(s)$ at $s = -r_0$ using some points s near 0. Note that Fischer and Defranceschi [2] also find unphysical states in wavelet computations of hydrogen-like atoms. Their iteration scheme yields an unphysical result that is actually the mathematical ground state corresponding to the pseudopotential.

6. Discussion

The EPP–Galerkin method gives seven correct decimal places for the hydrogenic 1s orbital, six correct decimal places for the hydrogenic 2s and 2p orbitals, and four correct decimal places for He 1s². For He 1s2s ¹S and ³S, we obtain energies close to the HF limit. The OIW–Galerkin method with the finest grid spacing 0.0625 a.u. gives energies with two to five correct decimal places. The grid size of OIW–Galerkin calculations is smaller compared to the EPP–Galerkin calculations. The Finite Difference Method yields rather inaccurate results even though the grid spacing is considerably smaller compared to the EPP–Galerkin calculations.

To our surprise, the EPP Hartree–Fock total energy of the He excited state configuration 1s2s ¹S is lower than the exact energy including correlations. This has been observed earlier in Ref. [10], and Cohen and Kelly [11] have shown that the reason is the nonorthogonality of this particular state and the ground state 1s² ¹S. Thus, the kind of "orbital relaxation" of the excited HF state 1s2s ¹S lowers the total energy by mixing a little of the ground state with the excited state wave function. In the present case, the EPP overlap integral of these two states is 0.0274, and there are obvious ways to work out the pure excited states, but this is out of the scope of this study.

We were able to obtain results near the Hartree–Fock limit by using a large enough basis and small enough parameter r_0 . It turns out that the EPP–Galerkin method yields better methods than the OIW–Galerkin method and considerably better results than the Finite Difference Method.

Author Contributions: Conceptualization, T.T.R. and T.H.; methodology, T.H. and T.T.R.; software, T.H.; validation, T.H. and T.T.R.; formal analysis, T.H.; investigation, T.H.; data curation, T.H.; writing—original draft preparation, T.H.; writing—review and editing, T.T.R.; visualization, T.H.; supervision, T.T.R. All authors have read and agreed to the published version of the manuscript.

Funding: APC from Tampere University.

Institutional Review Board Statement: Not applicable.

Data Availability Statement: Not applicable.

Conflicts of Interest: The authors declare no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript:

EPP	Exact Pseudopotential Method
OIW	Ordinary Interpolating Wavelet Method
FDM	Finite Difference Method
HF	Hartree–Fock

References

1. Höynälänmaa, T.; Rantala, T.T.; Ruotsalainen, K. Solution of atomic orbitals in an interpolating wavelet basis. *Phys. Rev. E* **2004**, *70*, 066701. [CrossRef] [PubMed]
2. Fischer, P.; Defranceschi, M. Numerical Solution of the Schrödinger Equation in a Wavelet Basis for Hydrogen-like Atoms. *SIAM J. Numer. Anal.* **1998**, *35*, 1–12. [CrossRef]
3. Deslauriers, G.; Dubuc, S. Symmetric Iterative Interpolation Processes. *Constr. Approx.* **1989**, *5*, 49–68. [CrossRef]
4. Chui, C.K.; Li, C. Dyadic affine decompositions and functional wavelet transforms. *SIAM J. Math. Anal.* **1996**, *27*, 865–890. [CrossRef]
5. Donoho, D. *Interpolating Wavelet Transforms*; Department of Statistics, Stanford University: Stanford, CA, USA, 1992.
6. Arias, T.A. Multiresolution analysis of electronic structure: Semicardinal and wavelet bases. *Rev. Mod. Phys.* **1999**, *71*, 267–311. [CrossRef]
7. Cowan, R.D. *The Theory of Atomic Structure and Spectra*; University of California Press: Berkeley, CA, USA, 1981.
8. Froese-Fischer, C. *The Hartree–Fock Method for Atoms—A Numerical Approach*; John Wiley & Sons: New York, NY, USA, 1977. [CrossRef]
9. Drake, G.W. *Atomic, Molecular, and Optical Physics Handbook*; AIP Press: New York, NY, USA, 1996.
10. Tang, T.L. Hartree-Fock Method for Helium Excited State. Available online: <https://nukephysik101.wordpress.com> (accessed on 22 October 2017).
11. Cohen, M.; Kelly, P.S. Hartree–Fock Wavefunctions for Excited States: The 1^1S State of Helium. *Can. J. Phys.* **1965**, *43*, 1867–1881. [CrossRef]

Disclaimer/Publisher’s Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.

PUBLICATION

IV

Electronic structure calculations with interpolating tensor product wavelet basis

Tommi Höynälänmaa and Tapio T. Rantala

Physical Review E 108 (2023), p. 025307

DOI: <https://doi.org/10.1103/PhysRevE.108.025307>

**Reprinted with permission from Tommi Höynälänmaa and Tapio T. Rantala,
Physical Review E, 108, 025307, 2023. Copyright (2023) by the American
Physical Society.**

Electronic structure calculations with interpolating tensor product wavelet basisTommi Höynälänmaa[✉] and Tapio T. Rantala[†]*Computational Physics, P. O. Box 692, FI-33014 Tampere University, Finland*

(Received 21 March 2023; accepted 4 August 2023; published 22 August 2023)

We introduce a basis set consisting of three-dimensional Deslauriers-Dubuc wavelets and solve numerically the Schrödinger equations of H and He atoms and molecules H_2 , H_2^+ , and LiH with Hartree-Fock and density functional theory (DFT) methods. We also compute the $2s$ and $2p$ excited states of hydrogen. The Coulomb singularity at the nucleus is handled by using a pseudopotential. The eigenvalue problem is solved with Arnoldi and Lanczos methods, Poisson equation with generalized minimal residual method and conjugate gradient on the normal equations methods, and matrix elements are computed using the biorthogonality relations of the interpolating wavelets. Performance is compared with those of CCCBDB and BIGDFT.

DOI: 10.1103/PhysRevE.108.025307

I. INTRODUCTION

Standard approaches to assess properties of atoms, molecules and models of nanostructures in quantum chemistry are Hartree-Fock (HF) and density functional theory (DFT). Both of these invoke numerical solutions of the Schrödinger differential equation of the many-body system of electrons. Thus, controlled approximations are inevitable and practical numerical algorithms are necessary.

The vast majority of the algorithms are based on finding the solutions or orbitals as series expansion of basis functions, the basis set. A finite basis set leads to the Roothaan-Hall equations, a generalized matrix eigenvalue problem. Gaussian-type basis functions are the most popular due to their advantageous analytical features. Here, we introduce a different type basis set, wavelet functions, point out their advantages and drawbacks, and consider a few test cases and compare their performance with conventional approaches.

Wavelets and related scaling functions are functions generated by translations and dilatations of the so-called mother wavelet and mother scaling function. Interpolating wavelets use a mother scaling function satisfying the cardinal interpolating property $\varphi(k) = \delta_{k,0}$ where k is an integer. Orthonormal wavelets form an orthonormal basis in function space $L^2(\mathbb{R})$. Both of these wavelet types can be generalized to multivariate functions.

Studies of wavelets have been active, and new ones with various properties have been found during the past tens of years [1,2]. One-dimensional interpolating wavelets in function space $C_u(\mathbb{R})$ consisting of bounded and uniformly continuous functions on $\mathbb{R}$ are defined in Ref. [2]. One-dimensional interpolating wavelets in function space $C_0(\mathbb{R})$ consisting of functions on $\mathbb{R}$ vanishing at infinity are defined in Ref. [3]. Deslauriers-Dubuc wavelets have also been discussed in Refs. [4,5]. Compactly supported interpolating

wavelets have been generalized to multiple dimensions in Refs. [6,7]. Fukuda, Kinoshita, and Suzuki [8] have studied unconditional convergence of wavelet expansions. They have shown that uniformly convergent wavelet expansions even for continuous functions do not always converge unconditionally in $L^\infty(\mathbb{R})$. Pathak [9] has investigated translation and convolution associated with discrete wavelet transform.

Arias [10] and Engeness and Arias [11] have 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. Lippert *et al.* [12] introduce a Lagrangian based formalism for the multiresolution analysis (MRA) of electronic structure. Arias [10] uses a carbon atom and a N_2 molecule as examples. Engeness and Arias [11] use both calcium and aluminum atoms and molecules O_2 and H_2O as examples.

Fischer and Defranceschi use Daubechies wavelets [1] for computation of hydrogenlike atoms [13]. They have developed an iterative method based on nonstandard operator form of the Schrödinger operator. Their work shows that this method is well suited for computations of hydrogenlike atoms. Fischer and Defranceschi have presented Hartree-Fock equations in an orthonormal wavelet basis [14]. They have also analyzed the Hartree-Fock method with a continuous wavelet transform [15] and demonstrated it using the hydrogenic Schrödinger equation with an iterative solution scheme.

Wei and Chou [16] have used orthonormal wavelets in self-consistent electronic structure calculations within the local-density approximation and demonstrated their method with H_2 and O_2 molecules. Tymczak and Wang [17] have used orthonormal Daubechies wavelets for quantum molecular dynamic simulations and developed a wavelet selection scheme for computations. They used a hydrogen atom and a H_2 molecule as examples. Their method shows systematic convergence with increasing grid size. Yamaguchi and Mukoyama [18] have carried out electronic structure calculations with the Hartree-Fock method and Meyer wavelets.

[✉]Corresponding author: tommy.hoynalanmaa@tuni.fi[†]tapio.rantala@tuni.fi

Our earlier contribution [19] is use of one-dimensional interpolating wavelets to solve the Hartree-Fock equations in the central field approximation for orbitals of several test case atoms. We were able to derive analytic formulas for all the relevant matrix elements of Hamiltonian and Fock operators. We also developed the exact pseudopotential method [20] for one-dimensional calculations of atoms and applied it to the hydrogen and helium ground states and for some excited states.

Iyengar and Frisch [21] have studied relationship between Gaussian basis sets and wavelets. They use a time-dependent basis function set: Gaussian functions centered at nuclei of the system. When the nuclei move the basis functions move, too. Gaussian functions are an example of *multiwavelets* [21–23] for which the J th level scaling space is decomposed into N -scaling spaces via

$$\dots \mathbf{V}_{J-1}^{(N)} \subset \mathbf{V}_J^{(1)} \subset \mathbf{V}_J^{(2)} \subset \dots \subset \mathbf{V}_J^{(N)} \subset \mathbf{V}_{J+1}^{(1)} \dots \quad (1)$$

Comparative studies of wavelets and Gaussian functions are presented, e.g., in Refs. [24,25]. Harrison *et al.* [26] use multiwavelets for quantum chemistry computations. Yanai *et al.* [27] present a numerical algorithm to evaluate Hartree-Fock exchange in the self-consistent field method. Yanai *et al.* [28,29] develop a method to do time-dependent Hartree-Fock and density functional theory computation with multiwavelets. Jensen *et al.* [30] perform multiwavelet computations of total energies with generalized gradient approximation-Perdew-Burke-Ernzerhof (PBE) and hybrid-PBE0 density functionals for 211 molecules. Jensen *et al.* [31] compute some magnetic properties with multiwavelets.

Han *et al.* [32] have developed an all-electron density-functional program using the Mexican hat wavelets. They analyze H_2 , CO, and H_2O molecules and $1s$ core-ionized C*O and CO* molecules. Their method shows very good performance over the plane-wave-based methods. Genovese *et al.* [33] and Mohr *et al.* [34] have composed a software package BIGDFT that implements the DFT method for quantum physical systems using three-dimensional Daubechies wavelets as a basis function set.

In three-dimensional space, the number of basis functions may grow relatively large to give sufficient accuracy. Therefore, we do not construct the Hamiltonian matrix explicitly. Instead, we use iterative algorithms in solving the Roothaan-Hall equation, though correspondingly, the computation gets slower in self-consistent iteration of Hartree-Fock or DFT orbitals for many electron systems.

In this paper, we demonstrate evaluation of electronic structure with three-dimensional interpolating tensor product wavelets and use of dual multiresolution analysis in computation of the matrix elements of the various operators. We make calculations for the hydrogen and helium atoms, the hydrogen molecule ion, the hydrogen molecule, and the lithium hydride molecule. Self-consistent iteration, Hartree-Fock, and DFT methods are used for many electron systems. Pseudopotentials are used for two different purposes to handle the Coulomb singularity at nuclei and also as the frozen core. We use the data from BIGDFT as the reference for our calculations with the interpolating tensor product Deslauriers-Dubuc wavelet basis function set.

An advantage of the interpolating wavelets compared to the orthonormal wavelets is that computing a wavelet expansion of the function does not require numerical evaluation of integrals since the dual wavelets are weighted sums of δ functions. In case the interpolating wavelets are compactly supported, these sums are finite, too. We have to choose the wavelet family so that its Hölder regularity is, at least, 2 in order to enable the evaluation of the Laplacian operator. BIGDFT uses Daubechies orthonormal wavelets for the computation of atomic orbitals and scalar products and interpolating wavelets for charge density, function products, and the Poisson solver. We use a rectangular computation grid, whereas, BIGDFT uses a spherical one.

From now on, we use atomic units throughout this article ($e = m_e = \hbar = 4\pi\epsilon_0 = 1$). Thus, units for energy and length, “Hartree” and “Bohr” are used and abbreviated as (Ha) and (B). Notations for wavelet basis functions and filters is similar to that in Ref. [6] and computation of matrix elements is similar to that in Ref. [7].

II. SOLVING THE SCHRÖDINGER EQUATIONS

A. General

Consider a system with n electrons and m nuclei with atomic numbers Z_i and locations $\mathbf{R}_i$. Within the Born-Oppenheimer approximation, dynamics of electrons and nuclei are independent, and then, the wave function separates to two factors, correspondingly. Here, we consider the electronic part, the orbitals, only, and keep the nuclear conformation $\{\mathbf{R}_i\}$ fixed.

With the fixed nuclear conformation, the Coulomb potential for dynamics of electrons is

$$V_N(\mathbf{r}) = - \sum_{i=1}^m \frac{Z_i}{|\mathbf{r} - \mathbf{R}_i|}, \quad (2)$$

and the internuclear repulsion energy,

$$E_R = \sum_{i=1}^{m-1} \sum_{j>i}^m \frac{Z_i Z_j}{|\mathbf{R}_i - \mathbf{R}_j|}. \quad (3)$$

For an atom, we have $E_R = 0$.

Let us denote the orbitals by ϕ as symbols φ and ψ are used for scaling functions and wavelets.

If the spacing between grid points is a (usually negative) power of 2, we can handle this by choosing $j_{\min}$ in Eqs. (25) and (26) properly. Otherwise, we have to make a change in variables $\mathbf{r} = a\mathbf{r}'$ in the Schrödinger equation. Here, one unit in the computation grid corresponds to a Bohrs.

B. Single-electron system

The Schrödinger equation of a single-electron system is

$$(-\frac{1}{2}\nabla^2 + V_N)\phi = \varepsilon\phi, \quad (4)$$

where ε is the orbital energy and the total energy including nuclear repulsion is

$$E_{\text{total}} = \varepsilon + E_R. \quad (5)$$

The wave equation of a single-electron system is solved by the implicitly restarted Arnoldi method [35,36]. The Arnoldi method is able to find also other than the lowest eigenvalue.

C. Hartree-Fock method

The HF equation for an n electron system is

$$\left(-\frac{1}{2}\nabla^2 + V_N + V_H + V_x^i\right)\phi_i = \varepsilon_i\phi_i, \quad (6)$$

where the Hartree potential is given by

$$V_H(\mathbf{r}) = \int_{\mathbb{R}^3} \rho(\mathbf{r}') \frac{1}{|\mathbf{r} - \mathbf{r}'|} d^3\mathbf{r}', \quad (7)$$

and the charge density by

$$\rho(\mathbf{r}) = \sum_{i=1}^n |\phi_i(\mathbf{r})|^2. \quad (8)$$

The exchange potentials V_x^i , $i = 1, \dots, n$, are defined in Ref. [37], Sec. 2.2 but not needed in our paper. For a two-electron system with both electrons occupying the same orbital as the singlet state HF equation can be written as

$$\left(-\frac{1}{2}\nabla^2 + V_N + \frac{1}{2}V_H\right)\phi_1 = \varepsilon_1\phi_1. \quad (9)$$

The Hartree potential is computed by solving the Poisson equation,

$$\nabla^2 V_H = -4\pi\rho, \quad (10)$$

numerically.

In this case where there are more than one resolution level in an interpolating wavelet basis, the matrix L of the Laplacian operator is not generally Hermitian, so we cannot solve Eq. (10) directly with the conjugate gradient method. The non-Hermiticity arises because our matrix elements are not computed as ordinary inner products between functions. In this case, we use one of the following two methods:

(1) conjugate gradient on the normal equations (CGNR): solve

$$L^T L V_H = -4\pi L^T \rho, \quad (11)$$

with the conjugate gradient method.

(2) Generalized minimal residual method (GMRES) [38].

When the basis set consists of a single resolution level, we may use the ordinary conjugate gradient method to solve (10).

The total energy of a two electron system is

$$E_{\text{total}} = 2\varepsilon_1 - \frac{1}{4} \int_{\mathbb{R}^3} \rho(\mathbf{r}) V_H(\mathbf{r}) d^3\mathbf{r} + E_R. \quad (12)$$

In this paper, we consider restricted Hartree-Fock approach, only.

D. Density functional theory and local density approximation

Suppose that we have a system with M electronic orbitals whose total wave functions are Ψ . The Kohn-Sham equation [37,39,40] for the electronic structure is

$$\left(-\frac{1}{2}\nabla^2 + V_N + V_H + V_{xc}[\rho]\right)\phi_i = E_i\phi_i, \quad (13)$$

where the charge density is

$$\rho(\mathbf{r}_1) = \sum_{s_1=\pm 1/2} M \int |\Psi(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_M)|^2 d\mathbf{x}_2 \cdots d\mathbf{x}_M, \quad (14)$$

and the Hartree potential,

$$V_H(\mathbf{r}) = \int_{\mathbb{R}^3} \rho(\mathbf{r}') \frac{1}{|\mathbf{r} - \mathbf{r}'|} d^3\mathbf{r}', \quad (15)$$

and $V_{xc}[\rho]$ is the *exchange-correlation potential*. We have

$$V_{xc}[\rho] = V_x[\rho] + V_c[\rho], \quad (16)$$

where $V_x[\rho]$ is the *exchange potential* and $V_c[\rho]$ is the *correlation potential*. In this article, we set $V_c[\rho] = 0$. The exchange-correlation energy is defined by

$$E_{xc}[\rho] = E_x[\rho] + E_c[\rho], \quad (17)$$

where $E_x[\rho]$ is the *exchange energy* and $E_c[\rho]$ is the *correlation energy*. In this article, we ignore the correlation energy.

Within the local density approximation (LDA), we define

$$E_x[\rho] = \int \rho(\mathbf{r}) \varepsilon_x[\rho](\mathbf{r}) d^3\mathbf{r}, \quad (18)$$

where $\varepsilon_x[\rho](\mathbf{r})$ is the exchange energy per particle of a uniform electron gas at a density of ρ . It follows from the Kohn-Sham theorem [37], Sec. 3.1 that the exchange potential is

$$V_x[\rho] = \frac{\delta E_x[\rho]}{\delta \rho}. \quad (19)$$

We have

$$E_x[\rho] = -\frac{3}{4} \left(\frac{3}{\pi}\right)^{1/3} \int [\rho(\mathbf{r})]^{4/3} d^3\mathbf{r}, \quad (20)$$

and

$$V_x[\rho](\mathbf{r}) = -\left(\frac{3}{\pi}\rho(\mathbf{r})\right)^{1/3}. \quad (21)$$

The total energy of the system is

$$E_{\text{KS}} = \sum_{i=1}^n E_i - \frac{1}{2} \int \rho(\mathbf{r}) V_H(\mathbf{r}) d^3\mathbf{r} + E_{xc}[\rho] - \int \rho(\mathbf{r}) V_{xc}[\rho](\mathbf{r}) d^3\mathbf{r}. \quad (22)$$

The Kohn-Sham equations are solved by a similar self-consistent iteration as the HF equations.

III. THREE-DIMENSIONAL WAVELET BASIS SET

A. The basis set

Let $j_{\min}$ and $j_{\max}$ be the minimum and maximum resolution levels of the point grid. Let

$$Z_j = \left\{ \frac{k}{2^j} \mid k \in \mathbb{Z} \right\}, \quad (23)$$

and

$$V_j = Z_j^3, \quad (24)$$

where $j \in \mathbb{Z}$. Define sets Q_j by

$$Q_{j_{\min}} = V_{j_{\min}}, \quad (25)$$

$$Q_j = V_j \setminus V_{j-1} \quad \text{for } j > j_{\min}. \quad (26)$$

The point grid G will be some finite subset of $V_{j_{\max}}$. We define

$$G_j := G \cap Q_j \quad (27)$$

for $j \geq j_{\min}$. The functions $\varphi_{j,k}$ and $\psi_{j,k}$ are scaling functions and wavelets belonging to an interpolating wavelet family. Functions $\tilde{\varphi}_{j,k}$ and $\tilde{\psi}_{j,k}$ are dual basis functions of interpolating wavelets.

Define

$$\psi_{s,j,k} := \begin{cases} \varphi_{j,k}, & \text{if } s = 0, \\ \psi_{j,k}, & \text{if } s = 1, \end{cases} \quad (28)$$

$$\tilde{\psi}_{s,j,k} := \begin{cases} \tilde{\varphi}_{j,k}, & \text{if } s = 0, \\ \tilde{\psi}_{j,k}, & \text{if } s = 1, \end{cases} \quad (29)$$

and

$$\eta_{j,k} := \begin{cases} \varphi_{j_{\min},k}, & \text{if } j = j_{\min}, \\ \varphi_{j-1,k/2}, & \text{if } j > j_{\min} \text{ and } k \text{ even}, \\ \psi_{j-1,(k-1)/2}, & \text{if } j > j_{\min} \text{ and } k \text{ odd}, \end{cases} \quad (30)$$

$$\tilde{\eta}_{j,k} := \begin{cases} \tilde{\varphi}_{j_{\min},k}, & \text{if } j = j_{\min}, \\ \tilde{\varphi}_{j-1,k/2}, & \text{if } j > j_{\min} \text{ and } k \text{ even}, \\ \tilde{\psi}_{j-1,(k-1)/2}, & \text{if } j > j_{\min} \text{ and } k \text{ odd}. \end{cases} \quad (31)$$

When $\alpha \in Q_j$ and $j \geq j_{\min}$ define

$$\zeta_\alpha := \eta_{j,\mathbf{k}[1]} \otimes \eta_{j,\mathbf{k}[2]} \otimes \eta_{j,\mathbf{k}[3]}, \quad (32)$$

and

$$\tilde{\zeta}_\alpha := \tilde{\eta}_{j,\mathbf{k}[1]} \otimes \tilde{\eta}_{j,\mathbf{k}[2]} \otimes \tilde{\eta}_{j,\mathbf{k}[3]}, \quad (33)$$

where $\mathbf{k} = 2^j \alpha$. We also define

$$\varphi_{j,\mathbf{k}} := \varphi_{j,\mathbf{k}[1]} \otimes \varphi_{j,\mathbf{k}[2]} \otimes \varphi_{j,\mathbf{k}[3]}, \quad (34)$$

where $j \in \mathbb{Z}$ and $\mathbf{k} \in \mathbb{Z}^3$.

B. Backward and forward wavelet transforms

Let

$$f = \sum_{\alpha \in G} c_\alpha \zeta_\alpha, \quad (35)$$

where $c_\alpha \in \mathbb{R}$ for all $\alpha \in G$'s. Let $c = (c_\alpha)_{\alpha \in G}$. Define $v = (v_\alpha)_{\alpha \in G}$ by setting

$$v_\alpha = f(\alpha). \quad (36)$$

We define forward wavelet transform U and backward wavelet transform W by setting $U(v) = c$ and $W(c) = v$. Mappings U and W are linear. We compute the forward wavelet transform U using an algorithm somewhat similar to Ref. [41]. Define matrix $P^{(j)}$ by

$$P_{\alpha,\beta}^{(j)} = \delta_{\alpha,\beta}, \quad (37)$$

where $\alpha \in G_j$, $\beta \in G$, and matrix $E^{(j)}$ by

$$E_{\alpha,\beta}^{(j)} = \delta_{\alpha,\beta}, \quad (38)$$

where $\alpha \in G$ and $\beta \in G_j$. Define

$$W_{\alpha,\beta}^{(j,j')} = \zeta_\beta(\alpha), \quad (39)$$

where $\alpha \in G_j$ and $\beta \in G_{j'}$. See Eq. (27) for definition of G_j and Eq. (32) for the definition of ζ_β . We have

$$W = \sum_{j=j_{\min}}^{j_{\max}} \sum_{j'=j_{\min}}^j E^{(j)} W^{(j,j')} P^{(j')}. \quad (40)$$

For forward wavelet transform, we have

$$U = \sum_{j=j_{\min}}^{j_{\max}} E^{(j)} U^{(j)}, \quad (41)$$

$$U^{(j)} = J^{(j)} \left(P^{(j)} - \sum_{j'=j_{\min}}^{j-1} W^{(j,j')} U^{(j')} \right) \quad \text{for } j > j_{\min}, \quad (42)$$

$$U^{(j_{\min})} = P^{(j_{\min})}, \quad (43)$$

$$J^{(j)} = (W^{(j,j)})^{-1}. \quad (44)$$

When

$$f = \sum_{\beta \in G_j} c_\beta \zeta_\beta, \quad (45)$$

we have

$$c_\alpha = \langle \tilde{\zeta}_\alpha, f \rangle = \left\langle \tilde{\zeta}_\alpha, \sum_{\beta \in G_j} f(\beta) \varphi_{j,2^j \beta} \right\rangle = \sum_{\beta \in G_j} \langle \tilde{\zeta}_\alpha, \varphi_{j,2^j \beta} \rangle f(\beta). \quad (46)$$

Consequently,

$$J_{\alpha,\beta}^{(j)} = \langle \tilde{\zeta}_\alpha, \varphi_{j,2^j \beta} \rangle, \quad (47)$$

and we do not have to invert matrix $W^{(j,j)}$.

An operator representing pointwise multiplication of a function f by another in the given computation grid is

$$M = UDW, \quad (48)$$

where D is a diagonal matrix with values of the function f at the grid points in the diagonal. The local pseudopotentials are computed this way.

C. Matrix elements of the Laplacian operator

Laplacian operator,

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (49)$$

is approximated by linear operator $L = L^{(x)} + L^{(y)} + L^{(z)}$ where

$$L_{\alpha,\alpha'}^{(x)} = \int_{\mathbb{R}^3} \tilde{\zeta}_\alpha(\mathbf{x}) \frac{\partial^2}{\partial x^2} \zeta_{\alpha'}(\mathbf{x}) d\tau, \quad (50)$$

$$L_{\alpha,\alpha'}^{(y)} = \int_{\mathbb{R}^3} \tilde{\zeta}_\alpha(\mathbf{x}) \frac{\partial^2}{\partial y^2} \zeta_{\alpha'}(\mathbf{x}) d\tau, \quad (51)$$

$$L_{\alpha,\alpha'}^{(z)} = \int_{\mathbb{R}^3} \tilde{\zeta}_\alpha(\mathbf{x}) \frac{\partial^2}{\partial z^2} \zeta_{\alpha'}(\mathbf{x}) d\tau \quad (52)$$

for $\alpha, \alpha' \in G$. Let $\alpha = 2^{-j}(k_x, k_y, k_z) \in G \cap Q_j$ and $\alpha' = 2^{-j'}(k'_x, k'_y, k'_z) \in G \cap Q_{j'}$. We define

$$\iota = \begin{cases} j-1, & \text{if } j > j_{\min}, \\ j, & \text{if } j = j_{\min}, \end{cases} \quad (53)$$

$$l_x = \begin{cases} \frac{k_x}{2}, & \text{if } k_x \text{ even and } j > j_{\min}, \\ \frac{k_x-1}{2}, & \text{if } k_x \text{ odd and } j > j_{\min}, \\ k_x, & \text{if } j = j_{\min}, \end{cases} \quad (54)$$

$$t_x = \begin{cases} 0, & \text{if } j = j_{\min} \text{ or } j > j_{\min} \text{ and } k_x \text{ even}, \\ 1, & \text{if } j > j_{\min} \text{ and } k_x \text{ odd}, \end{cases} \quad (55)$$

$$l_y = \begin{cases} \frac{k_y}{2}, & \text{if } k_y \text{ even and } j > j_{\min}, \\ \frac{k_y-1}{2}, & \text{if } k_y \text{ odd and } j > j_{\min}, \\ k_y, & \text{if } j = j_{\min}, \end{cases} \quad (56)$$

$$t_y = \begin{cases} 0, & \text{if } j = j_{\min} \text{ or } j > j_{\min}, \text{ and } k_y \text{ even}, \\ 1, & \text{if } j > j_{\min}, \text{ and } k_y \text{ odd}, \end{cases} \quad (57)$$

$$l_z = \begin{cases} \frac{k_z}{2}, & \text{if } k_z \text{ even and } j > j_{\min}, \\ \frac{k_z-1}{2}, & \text{if } k_z \text{ odd and } j > j_{\min}, \\ k_z, & \text{if } j = j_{\min}, \end{cases} \quad (58)$$

$$t_z = \begin{cases} 0, & \text{if } j = j_{\min} \text{ or } j > j_{\min}, \text{ and } k_z \text{ even}, \\ 1, & \text{if } j > j_{\min} \text{ and } k_z \text{ odd}, \end{cases} \quad (59)$$

and similar definitions for $\iota', l'_x, t'_x, l'_y, t'_y, l'_z$, and t'_z . Elements of matrices are computed by

$$L_{\alpha, \alpha'}^{(x)} = \begin{cases} \begin{aligned} &2^{2\iota} a(t_x, t'_x, \iota' - \iota, l'_x - 2^{\iota'-\iota} l_x) \\ &\times s(t_y, t'_y, \iota' - \iota, l'_y - 2^{\iota'-\iota} l_y) \\ &\times s(t_z, t'_z, \iota' - \iota, l'_z - 2^{\iota'-\iota} l_z), \end{aligned} & \text{if } \iota \leq \iota', \\ \begin{aligned} &2^{2\iota'} a(t_x, t'_x, \iota' - \iota, l_x - 2^{\iota-\iota'} l'_x) \\ &\times s(t_y, t'_y, \iota' - \iota, l_y - 2^{\iota-\iota'} l'_y) \\ &\times s(t_z, t'_z, \iota' - \iota, l_z - 2^{\iota-\iota'} l'_z), \end{aligned} & \text{if } \iota > \iota', \end{cases} \quad (60)$$

$$L_{\alpha, \alpha'}^{(y)} = \begin{cases} \begin{aligned} &2^{2\iota} s(t_x, t'_x, \iota' - \iota, l'_x - 2^{\iota'-\iota} l_x) \\ &\times a(t_y, t'_y, \iota' - \iota, l'_y - 2^{\iota'-\iota} l_y) \\ &\times s(t_z, t'_z, \iota' - \iota, l'_z - 2^{\iota'-\iota} l_z), \end{aligned} & \text{if } \iota \leq \iota', \\ \begin{aligned} &2^{2\iota'} s(t_x, t'_x, \iota' - \iota, l_x - 2^{\iota-\iota'} l'_x) \\ &\times a(t_y, t'_y, \iota' - \iota, l_y - 2^{\iota-\iota'} l'_y) \\ &\times s(t_z, t'_z, \iota' - \iota, l_z - 2^{\iota-\iota'} l'_z), \end{aligned} & \text{if } \iota > \iota', \end{cases} \quad (61)$$

$$L_{\alpha, \alpha'}^{(z)} = \begin{cases} \begin{aligned} &2^{2\iota} s(t_x, t'_x, \iota' - \iota, l'_x - 2^{\iota'-\iota} l_x) \\ &\times s(t_y, t'_y, \iota' - \iota, l'_y - 2^{\iota'-\iota} l_y) \\ &\times a(t_z, t'_z, \iota' - \iota, l'_z - 2^{\iota'-\iota} l_z), \end{aligned} & \text{if } \iota \leq \iota', \\ \begin{aligned} &2^{2\iota'} s(t_x, t'_x, \iota' - \iota, l_x - 2^{\iota-\iota'} l'_x) \\ &\times s(t_y, t'_y, \iota' - \iota, l_y - 2^{\iota-\iota'} l'_y) \\ &\times a(t_z, t'_z, \iota' - \iota, l_z - 2^{\iota-\iota'} l'_z), \end{aligned} & \text{if } \iota > \iota'. \end{cases} \quad (62)$$

The filters a and s are defined by

$$a(t_1, t_2, j, k) = \int_{\mathbb{R}^3} \tilde{\psi}_{t_1, 0, 0}(x) \frac{\partial^2}{\partial x^2} \psi_{t_2, j, k}(x) d\tau, \quad \text{for } j \geq 0, \quad (63)$$

$$a(t_1, t_2, j, k) = \int_{\mathbb{R}^3} \tilde{\psi}_{t_1, -j, k}(x) \frac{\partial^2}{\partial x^2} \psi_{t_2, 0, 0}(x) d\tau, \quad \text{for } j < 0, \quad (64)$$

$$s(t_1, t_2, j, k) = \int_{\mathbb{R}^3} \tilde{\psi}_{t_1, 0, 0}(x) \psi_{t_2, j, k}(x) d\tau, \quad \text{for } j \geq 0, \quad (65)$$

$$s(t_1, t_2, j, k) = \int_{\mathbb{R}^3} \tilde{\psi}_{t_1, -j, k}(x) \psi_{t_2, 0, 0}(x) d\tau, \quad \text{for } j < 0. \quad (66)$$

Filter a is computed with formulas

$$a(0, 0, j, k) = 2^{2j} a_0(k) \quad \text{for } j \geq 0, \quad (67)$$

$$a(0, 0, -1, k) = 4 \sum_{\mu=-m}^m h_\mu a(0, 0, 0, \mu - k) \quad \text{for } j = -1, \quad (68)$$

$$a(0, 0, j, k) = 4 \sum_{\mu=-m}^m h_\mu a(0, 0, j+1, k - 2^{-j-1} \mu) \quad \text{for } j < -1, \quad (69)$$

$$a(0, 1, j, k) = a(0, 0, j+1, 2k+1) \quad \text{for } j \geq 0, \quad (70)$$

$$a(0, 1, -1, k) = 4a_0(1-k), \quad (71)$$

$$a(0, 1, j, k) = 4a(0, 0, j+1, k - 2^{-j-1}) \quad \text{for } j < -1, \quad (72)$$

$$a(1, 0, 0, k) = \sum_{v=-m}^m \tilde{g}_v a(0, 0, -1, v - 2k), \quad (73)$$

$$a(1, 0, j, k) = 4 \sum_{v=-m}^m \tilde{g}_v a(0, 0, j-1, k - 2^{j-1} v) \quad \text{for } j > 0, \quad (74)$$

$$a(1, 0, j, k) = \sum_{v=-m}^m \tilde{g}_v a(0, 0, j-1, 2k+v) \quad \text{for } j < 0, \quad (75)$$

$$a(1, 1, j, k) = a(1, 0, j+1, 2k+1) \quad \text{for } j \geq 0, \quad (76)$$

$$a(1, 1, -1, k) = 4a(1, 0, 0, 1-k), \quad (77)$$

$$a(1, 1, j, k) = 4a(1, 0, j+1, k - 2^{-j-1}) \quad \text{for } j < -1, \quad (78)$$

where

$$a_0(k) := \int_{\mathbb{R}} \tilde{\varphi}(x) \frac{\partial^2}{\partial x^2} \varphi(x-k) dx. \quad (79)$$

Filter s is computed with formulas,

$$s(0, 0, j, k) = \delta_{k,0} \quad \text{for } j \geq 0, \quad (80)$$

$$s(0, 0, -1, k) = h_k, \quad (81)$$

$$s(0, 0, j, k) = \sum_{\mu=-m}^m h_{\mu} s(0, 0, j+1, k-2^{-j-1}\mu) \quad \text{for } j < -1, \quad (82)$$

$$s(0, 1, j, k) = 0 \quad \text{for } j \geq 0, \quad (83)$$

$$s(0, 1, -1, k) = \delta_{k,1}, \quad (84)$$

$$s(0, 1, j, k) = s(0, 0, j+1, k-2^{-j-1}) \quad \text{for } j < -1, \quad (85)$$

$$s(1, 0, 0, k) = 0, \quad (86)$$

$$s(1, 0, j, k) = \sum_{v=-m}^m \tilde{g}_v \delta_{k, 2^{j-1}v} \quad \text{for } j > 0, \quad (87)$$

$$s(1, 0, j, k) = 0 \quad \text{for } j < 0, \quad (88)$$

$$s(1, 1, 0, k) = \delta_{k,0}, \quad (89)$$

$$s(1, 1, j, k) = 0 \quad \text{for } j \neq 0. \quad (90)$$

IV. CONSTANT AND INTERPOLATED PSEUDOPOTENTIALS

The Coulomb potential arising from a single nucleus is

$$V(r) = -\frac{Z}{r}, \quad (91)$$

where Z is the charge of the nucleus.

We avoid the singularity by using a pseudopotential. We define c to be the cutoff point of the pseudopotential, and D to be the degree of the interpolating polynomial used in the pseudopotential. Actually, we use $c = 2^{-j_{\max}}$ where $j_{\max}$ is the highest resolution level in the wavelet basis. Parameter D has to be an odd integer, and we define $n = (D+1)/2$. We define

$$V_1(r) := -\frac{1}{r}, \quad r \geq 0, \quad (92)$$

$$\mathbf{s} := [-nc, -(n-1)c, \dots, -2c, -c, c, 2c, \dots, (n-1)c, nc], \quad (93)$$

and

$$\mathbf{t}[i] := V_1(\mathbf{s}[i]), \quad (94)$$

where $i = 1, \dots, 2n$. Let P be the interpolating polynomial of degree at most D having value $\mathbf{t}[i]$ at point $\mathbf{s}[i]$ for $i = 1, \dots, 2n$. Now, we define the interpolated pseudopotential with

$$V_{\text{interp}}(r) := \begin{cases} V_1(r), & r \geq c, \\ P(r), & r < c. \end{cases} \quad (95)$$

The actual pseudopotential of a nucleus with charge Z and location $\mathbf{R}$ is then

$$V(\mathbf{r}) = ZV_{\text{interp}}(|\mathbf{r} - \mathbf{R}|). \quad (96)$$

Function V_{interp} with different values of c is plotted in Fig. 1. We may also use the cut pseudopotential defined by

$$V_{\text{cut}}(r) := \begin{cases} V_1(r), & r \geq c, \\ -\frac{1}{c}, & r < c, \end{cases} \quad (97)$$

where $c = 2^{-j_{\max}-1}$.

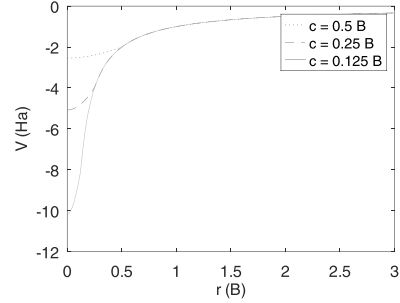


FIG. 1. Pseudopotentials V_{interp} with $D = 7$. Parameter c is the cutoff value, see Sec. IV.

V. HARTWIGSEN-GOEDECKER-HUTTER PSEUDOPOTENTIAL

By using pseudopotentials the number of computed orbitals can be reduced and since the pseudo wave functions are smoother than all-electron wave functions the basis function set can also be reduced. In a pseudopotential computation only, the valence electrons are actually computed, and the effect of the core electrons is handled by replacing the nuclear potential with a pseudopotential. We use the Hartwigsen-Goedecker-Hutter (HGH) pseudopotential [33,42] in these computations.

The HGH pseudopotential consists of a local and a non-local part. The local part is a function of the position as the nuclear potential. The nonlocal part is a linear operator, and it is not a function of position. The local pseudopotential is given by

$$V_{\text{loc}}(r) = \frac{-Z_{\text{ion}}}{r} \text{erf}\left(\frac{r}{\sqrt{2}r_{\text{loc}}}\right) + \exp\left[-\frac{1}{2}\left(\frac{r}{r_{\text{loc}}}\right)^2\right] \times \left[C_1 + C_2\left(\frac{r}{r_{\text{loc}}}\right)^2 + C_3\left(\frac{r}{r_{\text{loc}}}\right)^4 + C_4\left(\frac{r}{r_{\text{loc}}}\right)^6\right]$$

where r is the distance from the nucleus. Note that

$$\lim_{r \rightarrow 0} \frac{-Z_{\text{ion}}}{r} \text{erf}\left(\frac{r}{\sqrt{2}r_{\text{loc}}}\right) = \frac{-Z_{\text{ion}}}{r_{\text{loc}}} \sqrt{\frac{2}{\pi}}, \quad (98)$$

and the local pseudopotential is defined at the origin (nucleus), too.

The nonlocal pseudopotential is defined by

$$V_{\text{nonlocal}}[\phi] = \mathbf{r} \in \mathbb{R}^3 \mapsto \sum_l \int V_l(\mathbf{r}, \mathbf{r}') \phi(\mathbf{r}') d^3 \mathbf{r}', \quad (99)$$

where

$$V_l(\mathbf{r}, \mathbf{r}') = \sum_{i=1}^3 \sum_{j=1}^3 \sum_{m=-l}^l Y_{l,m}(\hat{\mathbf{r}}) p_i^l(r) h_{i,j}^l p_j^l(r') Y_{l,m}^*(\hat{\mathbf{r}}') \quad (100)$$

TABLE I. Computation grids. We define $Z(n) := \{k \in \mathbb{Z} : |k| \leq n\}$.

Number	Grid points
1	$\frac{1}{2}(Z(20))^3$
2	$\frac{1}{2}(Z(20))^3 \cup \frac{1}{4}(Z(10))^3$
3	$\frac{1}{2}(Z(20))^3 \cup \frac{1}{4}(Z(10))^3 \cup \frac{1}{8}(Z(4) \times Z(4) \times Z(10))$
4	$\frac{1}{4}(Z(60))^3$
5	$\frac{1}{2}(Z(30))^3 \cup \frac{1}{4}(Z(15))^3$
6	$(Z(38))^3 \cup \frac{1}{2}(Z(19))^3$
7	$\frac{1}{4}(Z(40))^3$
8	$(Z(10))^3 \cup \frac{1}{2}(Z(10))^3$
9	$\frac{1}{2}(Z(20))^3 \cup \frac{1}{4}(Z(20))^3$
10	$\frac{1}{4}(Z(40))^3 \cup \frac{1}{8}(Z(40))^3$
11	$(Z(10))^3 \cup \frac{1}{2}(Z(5))^3$
12	$\frac{1}{2}(Z(20))^3 \cup \frac{1}{4}(Z(10))^3 \cup \frac{1}{8}(Z(4) \times Z(4) \times Z(15))$
13	$\frac{1}{4}(Z(40))^3 \cup \frac{1}{8}(Z(20))^3$
14	$\frac{1}{4}(Z(60))^3 \cup \frac{1}{8}(Z(30))^3$

for each nucleus. The origin of the coordinate system in (100) is located at the nucleus. The functions p_l^j are defined by

$$p_l^j(r) = \frac{\sqrt{2}r^{l+2(i-1)} \exp\left(-\frac{r^2}{2r_l^2}\right)}{r_l^{l+(4i-1)/2} \sqrt{\Gamma\left(l + \frac{4i-1}{2}\right)}}, \quad (101)$$

where parameter r_l is given in Bohrs. The range of values l is determined by the actual pseudopotential. The spherical harmonics $Y_{l,m}$ in Eq. (100) can be replaced by orthonormal linear combinations of $Y_{l,m}$, $m = -l, \dots, l$. This allows us to avoid computation with complex valued functions.

VI. ATOMIC AND MOLECULAR ORBITALS

The hydrogen atom, hydrogen molecule ion, and lithium HGH computations presented here have been performed with the Arnoldi method. The helium, hydrogen molecule, and lithium hydride computations have been performed with self-consistent iteration and the Arnoldi method. When there is only one resolution level in the basis the Hamiltonian and Laplacian matrices are Hermitian and the Arnoldi method reduces to a variant of the Lanczos method. Furthermore, the ordinary conjugate gradient method could be used for the Poisson equation. Two methods have been used for solving the Poisson equation for the general case: CGNR and GMRES. We ran a benchmark for these methods and GMRES was eight times faster when the accuracies of the results were approximately the same. This is because the GMRES code is parallelized better than CGNR. All the computations use eighth order Deslauriers-Dubuc wavelets (polynomial span 7). We use interpolating polynomials of degree 7 for the pseudopotentials. In some computations, the Arnoldi method did not find the desired eigenvalues. This was solved by rising the number of computed eigenvalues and the number of basis vectors in the Arnoldi method. The basis function sets (computation point grids) are presented in Table I. The grid spacing for a wavelet basis is defined to be $g = 2^{-j_{\max}}a$ where $j_{\max}$ is the maximum resolution level in the basis and a is the size of

TABLE II. Total energy of the hydrogen atom. Quantity g is the distance between grid points in the highest resolution level. The numbers in column ‘Basis’ refer to Table I and ‘TH’ means this paper.

Source	Basis	g (B)	Pseudopot.	E (Ha)
TH	7	0.25	Const.	-0.487470
TH	8	0.5	Const.	-0.462247
TH	9	0.25	Const.	-0.487470
TH	10	0.125	Const.	-0.496380
TH	7	0.25	Interp.	-0.478328
TH	8	0.5	Interp.	-0.439146
TH	9	0.25	Interp.	-0.478328
TH	10	0.125	Interp.	-0.493471
TH	7	0.25	HGH	-0.499294
TH	8	0.5	HGH	-0.589957
TH	9	0.25	HGH	-0.499295
TH	10	0.125	HGH	-0.499899
CCCBDB [43]				-0.466582
BIGDFT [33,34]			HGH	-0.499969
Exact			None	-0.5

one unit in resolution level 0 in the wavelet basis in atomic units. See Sec. II A.

The data presented in the tables in this article were obtained from our own software (denoted by TH), our own computations with BIGDFT [33,34], and CCCBDB [43]. BIGDFT is a quantum-mechanical computation package using Daubechies wavelets. CCCBDB is large database containing atomic and molecular data. The CCCBDB energies and internuclear distances in this article use the (slater-type orbital) STO-3G basis set. Quantity g is the distance between grid points in the highest resolution level, and quantity d is the distance between the nuclei in the result tables. E_{system} is the total energy of the system, and E_{binding} is the binding energy. We used grid spacing 0.45 B (finer grid spacing 0.225 B) in all our BIGDFT computations. The BIGDFT parameters for determining the size of the basis set were $\text{crmult}=10.0$ and $\text{frmult}=16.0$. Parameter crmult is used to specify the size of the coarse region and parameter frmult the size of the fine region around atoms. The

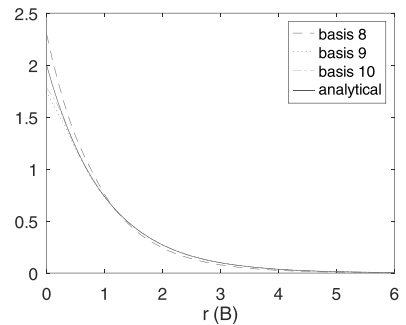


FIG. 2. Radially averaged wave functions of the hydrogen atom for several bases. The solid line is the analytical radial wave function. The basis numbers refer to Table I.

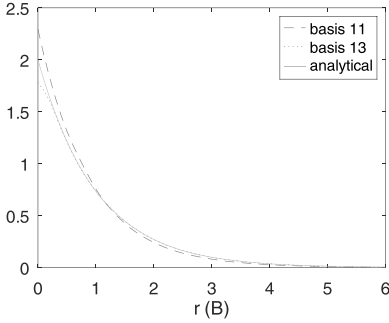


FIG. 3. Radially averaged wave functions of the hydrogen atom for some bases. The solid line is the analytical radial wave function. The basis numbers refer to Table I.

computations were also performed with values $\text{crm} = 5.0$ and $\text{frm} = 8.0$, but the results did not differ significantly. Note that the total energy does not include the energies of the core electrons in the lithium hydride HGH computations. Computations using our own software use interpolating wavelets and BIGDFT computations orthonormal Daubechies wavelets.

For the molecular computations, the energy of the system as a function of the distance between the nuclei is computed in three points near the energy minimum, and a second degree polynomial is fitted into these points. The distance between the nuclei is then the minimum point of the polynomial, and the energy of the system is computed at the minimum distance. We locate the nuclei at points $(0, 0, \pm \frac{d}{2})$ where d is the distance between the nuclei in Bohrs. When binding energies of molecules were computed the energies of atoms were usually computed with the basis set as the molecule. When the basis was unsymmetric, it was modified. For example, grid $Z(4) \times Z(4) \times Z(10)$ becomes $Z(4) \times Z(4) \times Z(4)$ for the atoms. See the caption of Table I for the definition of $Z(n)$.

The results for hydrogen atom ground state are presented in Table II. The radially averaged ground state wave functions

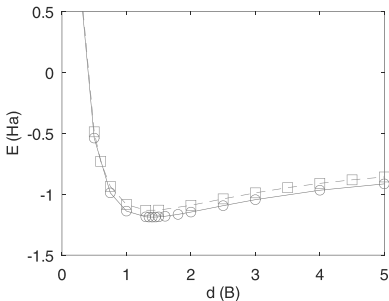


FIG. 4. Energy of H_2 as a function of internuclear distance calculated with the Hartree-Fock method and HGH pseudopotential. The solid line is our computation with interpolating wavelets and basis set 5, $g = 0.25$ B, and the dashed line is computed with BIGDFT and (fine) grid spacing $g = 0.225$ B.

TABLE III. Hydrogen atom orbital energies with the HGH pseudopotential. We labeled the resulting $2p$ orbitals with a , b , and c . All the orbitals presented are approximately orthogonal.

Orbital	Computed energy (Ha)	Exact energy (Ha)
$1s$	-0.499295	-0.5
$2s$	-0.120957	-0.125
$2p_a$	-0.123045	-0.125
$2p_b$	-0.123045	-0.125
$2p_c$	-0.123045	-0.125

of the hydrogen atom are plotted in Figs. 2 and 3. A radial average of a function $f: \mathbb{R}^3 \rightarrow \mathbb{R}$ is computed by

$$\bar{f}(r) := \frac{1}{4\pi} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} f(r, \theta, \phi) \sin \theta \, d\phi \, d\theta, \quad (102)$$

where $r \in [0, \infty[$. As the angular part of a s -type wave function is $\frac{1}{\sqrt{4\pi}}$, we estimate a radial wave function by

$$\bar{g}(r) := \frac{1}{2\sqrt{\pi}} \int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} f(r, \theta, \phi) \sin \theta \, d\phi \, d\theta. \quad (103)$$

The calculation of hydrogen excited states uses HGH pseudopotential and basis 9. Results are presented in Table III. The names of the excited states were obtained by computing inner products between the computed states and analytical states. The resulting orbitals are approximately orthonormal and the computed $2p$ states are approximately linear combinations of the analytical $2p$ states. The largest (in absolute value) inner product between different orbitals is $\langle 2p_a | 2p_c \rangle = 5.428 \times 10^{-4}$. The quality of the linear combinations can be measured by a quantity $\sqrt{1 - \|Pf\|_2^2}$ where P is the orthogonal projection from $L^2(\mathbb{R}^3)$ onto the space spanned by $2p_x$, $2p_y$, and $2p_z$. The value of this quantity is 0.1265 for all the computed orbitals $2p_a$, $2p_b$, and $2p_c$. Analytical expressions for hydrogenic orbitals can be found for example in Ref. [46].

Helium atom has been computed using the HGH pseudopotential. Results are presented in Table IV. Grid spacing $g = 0.5$ B does not give sensible results with the HGH pseudopotential. We suppose that Froese Fischer's results [44]

TABLE IV. Energetics of the helium atom. All our and BIGDFT computations use the HGH pseudopotential. The numbers in column Basis refer to Table I and TH means this paper.

Source	Basis	g (B)	Exchange potential	E (Ha)	E_{orb} (Ha)
TH	4	0.25	HF	-2.901959	-0.971927
TH	5	0.25	HF	-2.901180	-0.970247
TH	4	0.25	LDA	-2.821511	-0.629713
TH	5	0.25	LDA	-2.819951	-0.628152
TH	14	0.125	HF	-2.916129	-0.974768
CCCBDB [43]			HF	-2.807584	
CCCBDB [43]			LSDA	-2.809599	
BIGDFT [33,34]			HF	-2.862303	
BIGDFT [33,34]			LDA	-2.833895	
HF limit [44]			HF	-2.862	-0.918

TABLE V. Hydrogen molecule. The numbers in column Basis refer to Table I and TH means this paper.

Source	Basis	a (B)	g (B)	Pseudopot.	Exch.	E_{system} (Ha)	E_{binding} (Ha)	d (B)
TH	1	1.0	0.5	interp.	HF	-1.045883	0.167601	1.855140
TH	2	1.0	0.25	interp.	HF	-1.156554	0.199450	1.501870
TH	3	1.0	0.125	interp.	HF	-1.186176	0.210390	1.454593
TH	4	1.0	0.25	HGH	HF	-1.188779	0.190189	1.397995
TH	5	1.0	0.25	HGH	HF	-1.187995	0.189405	1.397991
TH	6	0.4	0.20	HGH	HF	-1.188547	0.189383	1.389890
TH	4	1.0	0.25	HGH	LDA	-1.157528	0.158938	1.485861
TH	5	1.0	0.25	HGH	LDA	-1.155960	0.157378	1.485851
CCCBDB ^a					HF	-1.117506	0.184342	1.345
CCCBDB ^a					LSDA	-1.157014	0.248654	1.391
BIGDFT ^b				HGH	HF	-1.133393	0.133455	1.386175
BIGDFT ^b				HGH	LDA	-1.136870	0.136932	1.445097
Experimental ^c							0.166	1.40

^aReference [43].^bReference [33,34].^cReference [45], Chap. 5.2.

can be regarded as the Hartree-Fock limit for helium. The computed total energies of the helium atom are quite good.

We calculated the hydrogen molecule with the interpolated and HGH pseudopotentials. The computation results for the hydrogen molecule are presented in Table V. The resulting dissociation curve with the HF method, HGH pseudopotential, and basis set 5 is plotted in Fig. 4. When the HGH pseudopotential was used the computation worked for grid spacing $g = 0.25$ B but did not work for spacing $g = 0.5$ B. The minimum energy of the curve is $E_0 = -1.188$ Ha, and it is located at internuclear distance $d_0 = 1.398$ B. The corresponding values for the BIGDFT reference curve are $E_0 = -1.132$ Ha and $d_0 = 1.385$ B. The results for the hydrogen molecule ion are presented in Table VI.

The calculations for lithium hydride molecule are presented in Table VII. Grid spacing $g = 0.5$ B did not yield a physical dissociation curve for the HGH pseudopotential. Neither $g = 0.5$ B nor $g = 0.25$ B yielded a physical dissociation curve for the interpolated pseudopotential. The dissociation curve of lithium hydride computed with the Hartree-Fock

method and basis set 5 is plotted in Fig. 5. The minimum energy of the curve is $E_0 = -0.817$ Ha, and it is located at internuclear distance $d_0 = 2.880$ B. The corresponding values for the BIGDFT reference curve are $E_0 = -0.760$ Ha and $d_0 = 2.921$ B.

The energies of the hydrogen atom converge to the exact value for the constant, interpolated, and HGH pseudopotentials with grid spacings $g = 0.5$, 0.25 , and 0.125 B (Table II). The Hartree-Fock helium computations yield approximately same results for $g = 0.25$ B and $g = 0.125$ B (Table IV). The Hartree-Fock computations of the hydrogen molecule using the HGH pseudopotential give approximately same energies for $g = 0.25$ B and $g = 0.2$ B (Table V). The calculations of the hydrogen molecule ion using the HGH pseudopotential yield approximately same energies and internuclear distances for $g = 0.25$ B and $g = 0.125$ B (Table VI). The Hartree-Fock computations of the lithium hydride molecule give approximately same results for $g = 0.25$ B and $g = 0.2$ B (Table VII).

TABLE VI. Hydrogen molecule ion H_2^+ . The analytical results are equal to the experimental results. The numbers in column Basis refer to Table I and TH means this paper.

Source	Basis	g (B)	Pseudopot.	E_{system} (Ha)	E_{binding} (Ha)	d (B)
TH	1	0.5	interp.	-0.520169	0.082028	2.371005
TH	2	0.25	interp.	-0.573665	0.095310	2.021654
TH	12	0.125	interp.	-0.589135	0.101242	2.015143
TH	11	0.5	HGH	-0.712279	0.121898	2.007951
TH	2	0.25	HGH	-0.601783	0.102460	2.006845
TH	7	0.25	HGH	-0.601636	0.102342	2.005329
TH	13	0.125	HGH	-0.602448	0.102549	1.999338
CCCBDB ^a				-0.582697	0.116115	2.005
BigDFT ^b			HGH	-0.602489	0.102520	1.995677
Experimental ^c					0.103	2.00

^aReference [43].^bReference [33,34].^cReference [45], Chap. 4.6.

TABLE VII. Lithium hydride molecule. All our and BIGDFT computations were performed with the HGH pseudopotential. The CCCBDB all-electron total energies are not presented in the table because the energies calculated by us do not include the energies of the core electrons. The numbers in column Basis refer to Table I and TH means this paper.

Source	Basis	a (B)	g (B)	Exch.	E_{system} (Ha)	E_{binding} (Ha)	d (B)
TH	4	1.0	0.25	HF	-0.817817	0.117472	2.879961
TH	5	1.0	0.25	HF	-0.817030	0.116686	2.880018
TH	4	1.0	0.25	LDA	-0.811482	0.111137	3.013411
TH	5	1.0	0.25	LDA	-0.809904	0.109560	3.013474
TH	6	0.4	0.2	HF	-0.817007	0.116370	2.863496
CCCBDB ^a				HF		0.081274	2.855
CCCBDB ^b				LSDA		0.135698	2.899
BIGDFT ^b				HF	-0.760938	0.059911	2.866004
BIGDFT ^b				LDA	-0.776416	0.075389	2.930745

^aReference [43].^bReferences [33,34].

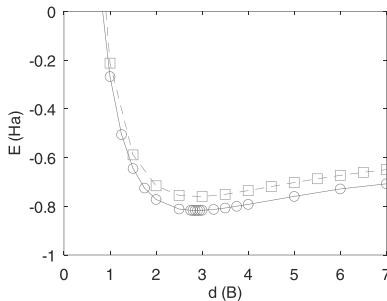


FIG. 5. Total energy of the lithium hydride molecule as a function of the internuclear distance calculated with the Hartree-Fock method and HGH pseudopotential. The solid line has been computed with interpolating wavelets and basis set 5, $g = 0.25$ B, and the dashed line with BIGDFT and (fine) grid spacing $g = 0.225$ B.

VII. CONCLUSIONS

We have shown how to solve the wave equations of hydrogen and helium atoms, hydrogen molecule ion, and hydrogen and lithium hydride molecules in a three-dimensional interpolating tensor product wavelet basis. As far the authors know,

only Arias [10] and Engeness and Arias [11] have performed this before. However, they do not use the dual interpolating MRA to evaluate matrix elements. We do that, and it allows us to neglect the overlap integrals of the basis functions.

It seems to require large basis sets to obtain numerically good orbitals for quantum physical systems. Roughly, the description requires, at least, 10 000 basis functions. The most accurate computed bond length of the hydrogen molecule is good and the energy satisfactory. The most accurate binding energies and internuclear distances for the hydrogen molecule ion in Table VI are very accurate. The calculations with the HGH pseudopotential performed very well with grid spacing $g = 0.25$ B but not with $g = 0.5$ B. The same phenomenon was observed with BIGDFT, too.

We tested the H and He atom computations with BIGDFT so that the coarse grid spacing was changed from 0.45 to 0.225 B. For some reason, we got slightly worse energies. We also found that one level basis set can be replaced with considerably smaller two-level basis set without a significant effect on the results.

Note that having no more than two resolution levels in the basis makes the computation of the Laplacian operator simpler and faster because in that case the $s(\cdots)$ terms in the Laplacian operator, equations (60)–(62), are either Kronecker δ s or zero.

- [1] I. Daubechies, *Ten Lectures on Wavelets*, CBMS-NSF Regional Conference Series in Applied Mathematics 61 (SIAM, Philadelphia, 1992).
- [2] C. K. Chui and C. Li, *SIAM J. Math. Anal.* **27**, 865 (1996).
- [3] D. L. Donoho, *Interpolating Wavelet Transforms*, Technical Report No. 408 (Department of Statistics, Stanford University, Stanford, 1992).
- [4] G. Deslauriers and S. Dubuc, *Constr. Approx.* **5**, 49 (1989).
- [5] S. Dubuc, *J. Math. Anal. Appl.* **114**, 185 (1986).
- [6] T. Höynälänmaa, *Int. J. Wavelets Multiresolut Inf. Process.* **13**, 1550010 (2015).
- [7] S. Goedecker, *Wavelets and Their Application for the Solution of Partial Differential Equations in Physics* (EPFL Press, Lausanne, 1998).
- [8] N. Fukuda, T. Kinoshita, and T. Suzuki, *Int. J. Wavelets Multiresolut Inf. Process.* **14**, 1650007 (2016).
- [9] R. S. Pathak, *Int. J. Wavelets Multiresolut Inf. Process.* **9**, 905 (2011).
- [10] T. A. Arias, *Rev. Mod. Phys.* **71**, 267 (1999).
- [11] T. D. Engeness and T. A. Arias, *Phys. Rev. B* **65**, 165106 (2002).
- [12] R. A. Lippert, T. A. Arias, and A. Edelman, *J. Comput. Phys.* **140**, 278 (1998).
- [13] P. Fischer and M. Defranceschi, *SIAM J. Numer. Anal.* **35**, 1 (1998).
- [14] P. Fischer and M. Defranceschi, *Wavelet Analysis and Its Applications*, Vol. 5 (Academic Press, 1994), pp. 495–506.
- [15] P. Fischer and M. Defranceschi, *Appl. Comput. Harmon. Anal.* **1**, 232 (1994).
- [16] S. Wei and M. Y. Chou, *Phys. Rev. Lett.* **76**, 2650 (1996).
- [17] C. J. Tymczak and X.-Q. Wang, *Phys. Rev. Lett.* **78**, 3654 (1997).
- [18] K. Yamaguchi and T. Mukoyama, *Nucl. Instrum. Methods Phys. Res. Sect. B* **124**, 361 (1997).
- [19] T. Höynälänmaa, T. T. Rantala, and K. Ruotsalainen, *Phys. Rev. E* **70**, 066701 (2004).
- [20] T. Höynälänmaa and T. T. Rantala, *Atoms* **11**, 9 (2023).
- [21] S. S. Iyengar and M. J. Frisch, *J. Chem. Phys.* **121**, 5061 (2004).
- [22] C. J. Tymczak, A. M. N. Niklasson, and H. Röder, *J. Comput. Phys.* **175**, 363 (2002).
- [23] G. Strang and V. Strela, *Opt. Eng.* **33**, 2104 (1994).
- [24] F. Gossler, B. Oliveira, M. Duarte, J. Vieira Filho, F. Villarreal, and R. Lamblém, *Trends Comput. Appl. Math.* **22**, 139 (2021).
- [25] A. Singh and J. Singh, *Indian J. Sci. Technol.* **9**, 1 (2016).
- [26] R. J. Harrison, G. I. Fann, T. Yanai, and G. Beylkin, in *Computational Science—ICCS 2003: International Conference, Melbourne, Australia and St. Petersburg, Russia, June 2–4, 2003 Proceedings, Part IV 3* (Springer, Berlin, Heidelberg, 2003), pp. 103–110.
- [27] T. Yanai, G. I. Fann, Z. Gan, R. J. Harrison, and G. Beylkin, *J. Chem. Phys.* **121**, 6680 (2004).
- [28] T. Yanai, R. J. Harrison, and N. C. Handy, *Mol. Phys.* **103**, 413 (2005).
- [29] T. Yanai, G. I. Fann, G. Beylkin, and R. J. Harrison, *Phys. Chem. Chem. Phys.* **17**, 31405 (2015).
- [30] S. R. Jensen, S. Saha, J. A. Flores-Livas, W. Huhn, V. Blum, S. Goedecker, and L. Frediani, *J. Phys. Chem. Lett.* **8**, 1449 (2017).
- [31] S. R. Jensen, T. Flå, D. Jonsson, R. S. Monstad, K. Ruud, and L. Frediani, *Phys. Chem. Chem. Phys.* **18**, 21145 (2016).
- [32] S. Han, K. Cho, and J. Ihm, *Phys. Rev. B* **60**, 1437 (1999).
- [33] L. Genovese *et al.*, *J. Chem. Phys.* **129**, 014109 (2008).
- [34] S. Mohr *et al.*, *J. Chem. Phys.* **140**, 204110 (2014).

- [35] W. E. Arnoldi, Q. Appl. Math. **9**, 17 (1951).
- [36] R. B. Lehoucq and D. C. Sorensen, SIAM J. Matrix Anal. Appl. **17**, 789 (1996).
- [37] Y. Saad, J. R. Chelikowsky, and S. M. Shontz, SIAM Rev. **52**, 3 (2010).
- [38] Y. Saad and M. H. Schultz, SIAM J. Sci. Statist. Comput. **7**, 856 (1986).
- [39] W. Kohn, Rev. Mod. Phys. **71**, 1253 (1999).
- [40] J. M. Soler, E. Artacho, J. D. Gale, A. García, J. Junquera, P. Ordejón, and D. Sánchez-Portal, J. Phys.: Condens. Matter **14**, 2745 (2002).
- [41] O. V. Vasilyev and P. Paolucci, J. Comput. Phys. **125**, 498 (1996).
- [42] C. Hartwigsen, S. Goedecker, and J. Hutter, Phys. Rev. B **58**, 3641 (1998).
- [43] <http://cccbdb.nist.gov>
- [44] C. Froese Fischer, *The Hartree-Fock Method for Atoms—A Numerical Approach* (Wiley, New York, 1977).
- [45] L. van Dommelen, Quantum Mechanics for Engineers, <http://www.umich.edu/~ners312/CourseLibrary/Dommelen.pdf>
- [46] P. Atkins and R. Friedman, *Molecular Quantum Mechanics* (Oxford University Press, New York, 2005).

PUBLICATION

V

Fourier transform and wavelet approaches to the path integral formulation

Tommi Höynälänmaa

Communications in Computational Physics (2024), submitted

Publication reprinted with the permission of the copyright holders.

Fourier transform and wavelet approaches to the path integral formulation

Tommi Höynälänmaa
Computational Physics,
P. O. Box 692, FI-33014 Tampere University, Finland

October 1, 2023

Abstract

We calculate energies and wavefunctions of several systems using the path integral formulation of quantum physics. The systems considered are one-dimensional and three-dimensional harmonic oscillators and hydrogen atom in one and three dimensions. We represent the time-evolution operator as matrix in a basis consisting of Deslauriers–Dubuc or Daubechies wavelets. We use Trotter kernels and we also develop an own approximation for the path integral kernel. For the one-dimensional harmonic oscillator we use the exact kernel, too. We also develop a method to calculate wavefunctions with the path integral formulation.

Keywords: path integral, wavelet, harmonic oscillator, hydrogen atom, quantum physics, Fourier transform

1 Introduction

The path integral formulation was developed by Richard Feynman in 1948. It generalizes the action principle of classical mechanics. In path integral formulation the transient state at time t of a quantum mechanical system is obtained from the initial state by formula

$$\Psi(\mathbf{y}, t) = \int e^{iS[\mathbf{x}, \dot{\mathbf{x}}]} \psi_0(\mathbf{x}(t)) \mathcal{D}\mathbf{x}. \quad (1)$$

Here the integration is done over all paths beginning with $\mathbf{x}(0) = \mathbf{y}$, the action is given by

$$S[\mathbf{x}, \dot{\mathbf{x}}] = \int L(\mathbf{x}(t), \dot{\mathbf{x}}(t)) dt, \quad (2)$$

$L(\mathbf{x}(t), \dot{\mathbf{x}}(t))$ is the Lagrangian of the system, and ψ_0 is the initial state. See [1] for an introduction to the path integral formulation.

The method is often applied by using an imaginary time variable [2]. Ruokosenmäki and Rantala [3, 2] have developed a real-time diffusion method for the path integral formulation. Ruokosenmäki et al. [4] and Gholizadehkalkhoran et al. [5] have also used the path integral method for the calculation of the Hooke's atom. Svensson [6] discusses the computation of the hydrogen atom with the

path integral method. Ho and Inomata [7] and Steiner [8] present an exact treatment of the hydrogen atom with path integral formulation. Path integral treatment of the quantum mechanical harmonic oscillator has been given for example by Ruokosenmäki and Rantala [3].

Wavelets are a basis function set constructed by dilatations and translations of so called mother scaling function and mother wavelet. Mathematical theory of interpolating wavelets has been developed by Chui and Li [9] and Donoho [10]. Höynälänmaa [11] has generalized these results for the multivariate case. Goedecker [12] gives an application-oriented introduction to interpolating wavelets. Höynälänmaa et al. [13] have made Hartree–Fock calculations of atoms using an interpolating wavelet basis. Höynälänmaa and Rantala [14] have also made three-dimensional Hartree-Fock and Density Functional Theory calculations for some atoms and two-atom molecules.

We use the Deslauriers-Dubuc interpolating wavelets [15, 16] in this article. We use atomic units ($e = m_e = \hbar = 4\pi\epsilon_0 = 1$) and the unitary angular frequency definition of the Fourier transform throughout this article. We abbreviate “atomic units” by a.u and units “Hartree” and “Bohr” by Ha and B. This research did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

2 Path Integral Formulation

The time-evolution operator defines the evolution of quantum mechanical system [1]:

$$\Psi(\mathbf{x}, t_b) = \hat{U}(t_b, t_a)\Psi(\mathbf{x}, t_a). \quad (3)$$

For a stationary system it is given by

$$\hat{U}(t_b, t_a) = \exp(-i(t_b - t_a)\hat{H}) \quad (4)$$

where $\hat{H}$ is the Hamiltonian operator of the system. The time evolution of an eigenstate of a stationary system is given by

$$\Psi_a(\mathbf{x}, t) = \exp(-iE_a t)\psi_a(\mathbf{x}) \quad (5)$$

where ψ_a is an eigenstate of the time-independent Hamiltonian and E_a is its energy.

The time-evolution operator can be represented as [1]

$$\hat{U}(t_b, t_a)\Psi_a = \int_{\mathbb{R}^d} K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a)\Psi_a(\mathbf{x}_a, t_a)d\mathbf{x}_a \quad (6)$$

where d is the dimensionality of the system (1, 2, or 3) and function K is called the kernel. In path integral formulation the kernel is given by

$$K(\mathbf{x}_b, t_b; \mathbf{x}_a, t_a) = \lim_{N \rightarrow \infty} \sqrt{\frac{m}{2\pi i \epsilon}}^{Nd} \int_{\mathbb{R}^d} \cdots \int_{\mathbb{R}^d} \exp(iS_N) d\mathbf{x}_1 \cdots d\mathbf{x}_{N-1}. \quad (7)$$

For a one-particle system the quantity S_N is given by [17]

$$S_N = \epsilon \sum_{n=1}^N \left(\frac{m}{2} \left(\frac{\mathbf{x}_n - \mathbf{x}_{n-1}}{\epsilon} \right)^2 - V(\mathbf{x}_n, t_n) \right) \quad (8)$$

and

$$\epsilon = \frac{t_b - t_a}{N}. \quad (9)$$

We also define $\Delta t = t_b - t_a$. The Trotter kernel is an approximation of the path-integral kernel given by [3]

$$K(\mathbf{x}_b, \mathbf{x}_a; \Delta t) = \left(\frac{m}{2\pi i \Delta t} \right)^{d/2} \exp \left(i \left(\frac{m}{2\Delta t} |\mathbf{x}_b - \mathbf{x}_a|^2 - \frac{\Delta t}{2} (V(\mathbf{x}_b) + V(\mathbf{x}_a)) \right) \right). \quad (10)$$

3 Stationary State Energies and Wavefunctions

Fourier transform has been used to determine the energy spectrum of a quantum mechanical system with path integral formulation e.g. by Gholizadehkalkhoran et al. [5].

A stationary state ψ of a quantum mechanical system can be represented by

$$\psi(\mathbf{x}) = \sum_{k=0}^{\infty} c_k f_k(\mathbf{x}) \quad (11)$$

where functions f_k are the eigenstates of the Hamiltonian operator of the system and c_k are complex numbers. The time evolution of the stationary states is given by

$$\Psi(\mathbf{x}, t) = \sum_{k=0}^{\infty} c_k \exp(-iE_k t) f_k(\mathbf{x}) \quad (12)$$

where E_k are the energies of the eigenstates. Suppose that we have a fixed point $\mathbf{x}_0 \in \mathbb{R}^d$ and define $g(t) := \Psi(\mathbf{x}_0, t)$. By making a Fourier transform we obtain

$$\hat{g}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{t=-\infty}^{\infty} g(t) \exp(-i\omega t) dt \quad (13)$$

$$= \frac{1}{\sqrt{2\pi}} \sum_{k=0}^{\infty} c_k f_k(\mathbf{x}_0) \int_{t=-\infty}^{\infty} \exp(-iE_k t) \exp(-i\omega t) dt \quad (14)$$

$$= \sqrt{2\pi} \sum_{k=0}^{\infty} c_k f_k(\mathbf{x}_0) \delta(\omega + E_k). \quad (15)$$

Thus we may compute the eigenenergies of the system from the Fourier spectrum of function g .

Suppose that we have a stationary system with initial state $\psi_i(\mathbf{x}) = \Psi(\mathbf{x}, t_i)$ and final state $\psi_f(\mathbf{x}) = \Psi(\mathbf{x}, t_f)$ and assume that the time interval $\Delta t := t_b - t_a$ is small. We have

$$\psi_f(\mathbf{x}) - \psi_i(\mathbf{x}) = (\exp(-iEt) - 1) \psi_i(\mathbf{x}) \approx -iEt \psi_i(\mathbf{x}) \quad (16)$$

from which we obtain

$$E \approx -\frac{1}{\Delta t} \text{Im} \frac{\psi_f(\mathbf{x}) - \psi_i(\mathbf{x})}{\psi_i(\mathbf{x})} \quad (17)$$

and

$$\langle E \rangle \approx -\frac{1}{\Delta t} \text{Im} \int_{\mathbb{R}^d} (\psi_f(\mathbf{x}) - \psi_i(\mathbf{x})) (\psi_i(\mathbf{x}))^* d\mathbf{x}. \quad (18)$$

The initial function of the time evolution should be chosen so that it has a broad Fourier spectrum and it should also contain both even and odd terms. So we chose to approximate the sum of delta function and its derivative at the origin with a scaling function centred at the origin and its derivative in the one-dimensional case. In some calculations we use function $-\varphi_{j_{\min},-1} + \varphi_{j_{\min},1}$ instead of the derivative. In three dimensions we use the tensor products of functions $(-1-i)\varphi_{j_{\min},-1} + (1+i)\varphi_{j_{\min},0} + (1+i)\varphi_{j_{\min},1}$.

We use the method described in [18, section 2] to compute the continuous Fourier transform. We have also generalized it into three dimensions.

Let $\mathbf{x}_j$, $j = 1, \dots, N$ be the points where we calculate the wavefunction of state k . Let $g_j(t) := \Psi(\mathbf{x}_j, t)$ and ΔE be the spacing between points in the Fourier spectrum $\hat{g}_j(E)$. We fit the peak k to the Lorentzian distribution

$$L(E) = \frac{1}{\pi} \frac{\gamma}{(E + E_k)^2 + \gamma^2}. \quad (19)$$

Define

$$p_{k,j} = |\hat{g}_j(-E_k)|^2, \quad (20)$$

$$p'_{k,j} = \frac{1}{2} \left(|\hat{g}_j(-E_k + \Delta E)|^2 + |\hat{g}_j(-E_k - \Delta E)|^2 \right), \quad (21)$$

and

$$L_{k,j}(E) = \frac{1}{\pi} \frac{\gamma_{k,j}}{(E + E_k)^2 + \gamma_{k,j}^2}. \quad (22)$$

Note that $|\hat{g}_j(E)|^2$ is the Fourier transform of the autocorrelation function of $g_j(t)$ multiplied by a constant. Let $d_{k,j} = |c_k f_k(\mathbf{x}_j)|^2$ be the undefined variables. We now set

$$p_{k,j} = d_{k,j} L_{k,j}(-E_k) = d_{k,j} \frac{1}{\pi} \frac{1}{\gamma_{k,j}} \quad (23)$$

and

$$p'_{k,j} = d_{k,j} L_{k,j}(-E_k + \Delta E) = d_{k,j} \frac{1}{\pi} \frac{\gamma_{k,j}}{\Delta E^2 + \gamma_{k,j}^2}. \quad (24)$$

It follows that

$$d_{k,j} = \pi \gamma_{k,j} p_{k,j} \quad (25)$$

where

$$\gamma_{k,j} = \sqrt{\frac{q_{k,j}}{1 - q_{k,j}}} |\Delta E| \quad (26)$$

and

$$q_{k,j} = \frac{p'_{k,j}}{p_{k,j}}. \quad (27)$$

4 Approximation of the Path Integral Kernel

We assume that the potential V does not depend on time. We approximate the kernel by setting $N = 2$ and we get

$$K_2(\mathbf{x}_b, \mathbf{x}_a; \epsilon) := \left(\frac{m}{2\pi i \epsilon} \right)^d \int_{\mathbb{R}^d} \exp(iS_2) d\mathbf{x}_1. \quad (28)$$

We have

$$K_2(\mathbf{x}_b, \mathbf{x}_a; \epsilon) = \left(\frac{m}{2\pi i \epsilon} \right)^d I \quad (29)$$

where

$$I := \int_{\mathbf{x}_1 \in \mathbb{R}^d} \exp(iS_2) d\mathbf{x}_1 \quad (30)$$

$$= \int_{\mathbf{x}_1 \in \mathbb{R}^d} \exp \left(i\epsilon \left(\frac{m}{2} \left(\frac{\mathbf{x}_1 - \mathbf{x}_a}{\epsilon} \right)^2 - V(\mathbf{x}_1) + \frac{m}{2} \left(\frac{\mathbf{x}_b - \mathbf{x}_1}{\epsilon} \right)^2 - V(\mathbf{x}_b) \right) \right) d\mathbf{x}_1 \quad (31)$$

$$= \exp \left(i \left(\frac{m}{2\epsilon} (\mathbf{x}_b^2 + \mathbf{x}_a^2) - \epsilon V(\mathbf{x}_b) \right) \right) \int_{\mathbf{x}_1 \in \mathbb{R}^d} \exp \left(i \left(\frac{m}{\epsilon} \mathbf{x}_1^2 - \epsilon V(\mathbf{x}_1) \right) \right) \exp \left(-i \frac{m}{\epsilon} (\mathbf{x}_b + \mathbf{x}_a) \cdot \mathbf{x}_1 \right) d\mathbf{x}_1 \quad (32)$$

$$= \sqrt{2\pi}^d \exp \left(i \left(\frac{m}{2\epsilon} (\mathbf{x}_b^2 + \mathbf{x}_a^2) - \epsilon V(\mathbf{x}_b) \right) \right) \hat{h} \left(\frac{m}{\epsilon} (\mathbf{x}_b + \mathbf{x}_a) \right) \quad (33)$$

and

$$h(\mathbf{x}_1) := \exp \left(i \left(\frac{m}{\epsilon} \mathbf{x}_1^2 - \epsilon V(\mathbf{x}_1) \right) \right). \quad (34)$$

Now

$$K_2(\mathbf{x}_b, \mathbf{x}_a; \epsilon) = \left(\frac{m}{2\pi i \epsilon} \sqrt{2\pi} \right)^d \exp \left(i \left(\frac{m}{2\epsilon} (\mathbf{x}_b^2 + \mathbf{x}_a^2) - \epsilon V(\mathbf{x}_b) \right) \right) \hat{h} \left(\frac{m}{\epsilon} (\mathbf{x}_b + \mathbf{x}_a) \right). \quad (35)$$

We call this kernel the *midpoint kernel*.

If function h is radially symmetric (i.e. the potential is radially symmetric) we have

$$\hat{h}(\mathbf{k}) = \frac{i}{2k} \left(\hat{f}(k) - \hat{f}(-k) \right), \quad (36)$$

where $f(r) = r h_{\text{rad}}(|r|)$ and $h(\mathbf{r}) = h_{\text{rad}}(|\mathbf{r}|)$. Note that the Fourier transform of f in equation (36) is one-dimensional.

5 Quantum Harmonic Oscillator and Hydrogen-like Atom

The potential of the one-dimensional harmonic oscillator is

$$V(x) = \frac{m\omega_0^2}{2} x^2 \quad (37)$$

where m is the mass of the particle and ω_0 is the angular frequency. The potential of the isotropic three-dimensional harmonic oscillator is

$$V(\mathbf{x}) = \frac{m\omega_0^2}{2}|\mathbf{x}|^2. \quad (38)$$

The kernel for the one-dimensional harmonic oscillator can be computed exactly [1]. We have

$$K(x_b, x_a; t) = \left(\frac{m\omega_0}{2\pi i \sin(\omega_0 t)} \right)^{1/2} \exp(iS_{\text{cl}}), \quad (39)$$

where S_{cl} is the classical action given by

$$S_{\text{cl}} = \frac{m\omega_0}{2\sin(\omega_0 t)} ((x_b^2 + x_a^2) \cos(\omega_0 t) - 2x_b x_a). \quad (40)$$

By substituting the potential of the one-dimensional harmonic oscillator to equation (34) we obtain

$$h(x_1) = \exp \left(i \frac{m}{\epsilon} \left(1 - \frac{\epsilon^2 \omega_0^2}{2} \right) x_1^2 \right). \quad (41)$$

Define

$$a := \frac{m}{\epsilon} \left(1 - \frac{\epsilon^2 \omega_0^2}{2} \right) \quad (42)$$

and assume that $a > 0$. Now

$$\hat{h}(k) = \frac{1}{2}(1 + i) \frac{1}{\sqrt{a}} \exp \left(-i \frac{k^2}{4a} \right). \quad (43)$$

Similarly, in the three-dimensional case we have

$$\hat{h}(\mathbf{k}) = \frac{1}{4}(-1 + i)a^{-3/2} \exp \left(-i \frac{k^2}{4a} \right) \quad (44)$$

using equation (36).

The potential of a hydrogen-like atom is

$$V(x) = -\frac{Z}{|x|} \quad (45)$$

in one dimension and

$$V(\mathbf{x}) = -\frac{Z}{|\mathbf{x}|} \quad (46)$$

in three dimensions. Here Z is the atomic number.

6 Wavelet Bases

6.1 Interpolating Wavelets

We construct the basis function set in the same way as in [14, section 3]. We assume that φ is some Deslauriers–Dubuc mother scaling function [9, 10, 11, 15,

16] and d is the dimensionality of the domain $\mathbb{R}^d$. We use only bases with one or two resolution levels in this article. Constant $j_{\min}$ is the minimum resolution level in the basis, see [14]. We define G to be the whole basis, $G = G_{j_{\min}}$ or $G = G_{j_{\min}} \cup G_{j_{\min}+1}$.

The interpolating mother scaling function can be represented as [9, 11]

$$\varphi(x) = \sum_{\alpha \in \mathbb{Z}} s[\alpha] \varphi(2^J x - \alpha) \quad (47)$$

where J is some nonnegative integer and $s[\alpha]$, $\alpha \in \mathbb{Z}$, are constants that depend on the mother scaling function and J . We define $s_0[\alpha]$ to be the coefficients for J and $s_1[\alpha]$ for $J-1$. We now have

$$\eta_{j_{\min},k}(2^{-J-j_{\min}}p) = s_0[p - 2^J k] \quad (48)$$

for all $p \in \mathbb{Z}$,

$$\eta_{j_{\min}+1,k}(2^{-J-j_{\min}}p) = s_0[p - 2^{J-1}k] \quad (49)$$

for all $p \in \mathbb{Z}$ and k even integer, and

$$\eta_{j_{\min}+1,k}(2^{-J-j_{\min}}p) = s_1[p - 2^{J-1}k] \quad (50)$$

for all $p \in \mathbb{Z}$ and k odd integer. We also have

$$\tilde{\eta}_{j_{\min},\ell} = \tilde{\varphi}_{j_{\min},\ell} = \delta(\cdot - 2^{-j_{\min}}\ell) \quad (51)$$

for all $\ell \in \mathbb{Z}$,

$$\tilde{\eta}_{j_{\min}+1,\ell} = \delta(\cdot - 2^{-j_{\min}-1}\ell) = \sum_{\beta \in \mathbb{Z}} \tilde{h}_{\beta} \delta(\cdot - 2^{-j_{\min}-1}(\beta + \ell)) \quad (52)$$

for all $\ell \in 2\mathbb{Z}$, and

$$\tilde{\eta}_{j_{\min}+1,\ell} = \sum_{\beta \in \mathbb{Z}} \tilde{g}_{\beta} \delta(\cdot - 2^{-j_{\min}-1}(\beta + \ell - 1)) \quad (53)$$

for all $\ell \in 2\mathbb{Z} + 1$.

The matrix of the time evolution operator in the interpolating wavelet basis is

$$K_{\mathbf{r},\mathbf{q}} = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \tilde{\zeta}_{\mathbf{r}}(\mathbf{y}) K(\mathbf{y}, \mathbf{x}) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x} d\mathbf{y}. \quad (54)$$

Note that the dual wavelets $\tilde{\zeta}_{\mathbf{r}}$ are finite sums of delta distributions and consequently the integration over $\mathbf{y}$ is actually a weighted sum of values of the function

$$\int_{\mathbb{R}^d} K(\mathbf{y}, \mathbf{x}) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x}$$

in finite number of points $\mathbf{y}$. When $\mathbf{r} = 2^{-j_{\min}}\ell \in G_{j_{\min}}$ we have

$$K_{\mathbf{r},\mathbf{q}} = \int_{\mathbb{R}^d} K(2^{-j_{\min}}\ell, \mathbf{x}) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x}. \quad (55)$$

In one-dimensional case the integral over x is approximated by

$$\int_{\mathbb{R}} K(y, x) \zeta_q(x) dx \approx 2^{-j_{\min}-J} \sum_{p \in \mathbb{Z}} K(y, 2^{-j_{\min}-J}p) s_{t(q)}(p - 2^{J-t(q)}k) \quad (56)$$

where $k \in \mathbb{Z}$, $q = 2^{-j_{\min}}k \in G_{j_{\min}}$ or $q = 2^{-j_{\min}-1}k \in G_{j_{\min}+1}$, and

$$t(q) := \begin{cases} 1 & \text{if } q \in G_{j_{\min}+1} \\ 0 & \text{if } q \in G_{j_{\min}}. \end{cases} \quad (57)$$

For the three-dimensional case define

$$t_i(\mathbf{q}) := \begin{cases} 1 & \text{if } \mathbf{q} \in G_{j_{\min}+1} \text{ and } 2^{j_{\min}+1}\mathbf{q}[i] \text{ odd} \\ 0 & \text{otherwise} \end{cases} \quad (58)$$

for $i = 1, 2, 3$ and $\mathbf{t}(\mathbf{q}) := (t_1(\mathbf{q}), t_2(\mathbf{q}), t_3(\mathbf{q}))$. Define also

$$s_{\mathbf{t}}(\mathbf{z}) := s_{t[1]}(\mathbf{z}[1])s_{t[2]}(\mathbf{z}[2])s_{t[3]}(\mathbf{z}[3]). \quad (59)$$

Now we can approximate

$$\int_{\mathbb{R}^3} K(\mathbf{y}, \mathbf{x}) \zeta_{\mathbf{q}}(\mathbf{x}) d\mathbf{x} \approx 2^{-3(j_{\min}+J)} \sum_{\mathbf{p} \in \mathbb{Z}^3} K(\mathbf{y}, 2^{-j_{\min}-J}\mathbf{p}) s_{\mathbf{t}(\mathbf{q})}(\mathbf{p} - \mathbf{w} \cdot \mathbf{k}) \quad (60)$$

where $\mathbf{k} \in \mathbb{Z}^3$ and $\mathbf{q} = 2^{-j_{\min}}\mathbf{k} \in G_{j_{\min}}$ or $\mathbf{q} = 2^{-j_{\min}-1}\mathbf{k} \in G_{j_{\min}+1}$, and $\mathbf{w} := (2^{J-t_1(\mathbf{q})}, 2^{J-t_2(\mathbf{q})}, 2^{J-t_3(\mathbf{q})})^T$. We pick some value $J_0 \geq 2$ and for $\mathbf{r} \in G_{j_{\min}+1}$ we use value $J = J_0 - 1$ in equation (47) and $J = J_0$ otherwise. The lower accuracy is used because the matrix elements where $\mathbf{q}$ belongs to the finer grid are significantly more complex to compute as the ones in the coarser grid.

We use 8th order Deslauriers–Dubuc wavelets for one-dimensional calculations and 4th order Deslauriers–Dubuc wavelets for three-dimensional calculations.

6.2 Orthonormal Wavelets

See [19] for more information on orthonormal wavelets. We define the basis indices by $I = I_{j_{\min}} \cup I_{j_{\min}+1}$ where $I_j = \{(j, k) : k \in K_j\}$ and K_j is a finite set of integer numbers (usually a range of integers). Now the basis functions are defined by

$$\zeta_{j,k} = \begin{cases} \varphi_{j_{\min},k} = 2^{j/2}\varphi(2^j \cdot -k) & j = j_{\min} \\ \psi_{j-1,k} = 2^{(j-1)/2}\psi(2^{j-1} \cdot -k) & j > j_{\min} \end{cases} \quad (61)$$

where $(j, k) \in I$, φ is the mother scaling function of the wavelet family, and ψ is the mother wavelet of the wavelet family. In order to compute the values of the orthonormal wavelets we use the representation

$$\varphi(x) = 2^{J/2} \sum_{\alpha \in \mathbb{Z}} w[\alpha] \varphi(2^J x - \alpha) \quad (62)$$

where J is some nonnegative integer and $w[\alpha]$, $\alpha \in \mathbb{Z}$, are constants that depend on the mother scaling function and J . The matrix elements of the time-evolution operator are given by

$$K_{j,k,j',k'} = \int_{\mathbb{R}} \int_{\mathbb{R}} \zeta_{j,k}(y) K(y, x) \zeta_{j',k'}(x) dx dy \quad (63)$$

with orthonormal wavelets. We use the 20th order Daubechies wavelets in this study. We use only one-dimensional orthonormal wavelets.

7 Application to the Harmonic Oscillator and Hydrogen Atom

Unless otherwise stated the calculations use Deslauriers–Dubuc wavelets.

We make calculations for the one-dimensional harmonic oscillator with the exact kernel, Trotter kernel, and midpoint kernel. We compute all these system with both one and two resolution levels of the basis functions for $\Delta t = 1.0$ a.u. and one resolution level for $\Delta t = 0.5$ a.u. and $\Delta t = 0.25$ a.u. The mass of the particle is 1 a.u. and the angular frequency 0.1 radians. All these calculations yield the ground state energy 0.050265 Ha and first excited state 0.150796 Ha or 0.149226 Ha. We use the basis $(1/4)\{-48, \dots, 48\}$ for one-level calculations and $(1/4)\{-48, \dots, 48\} \cup (1/8)\{-5, \dots, 5\}$ for two-level calculations. We use scaling function resolution $J = 3$. The energy spectrum for the exact kernel is plotted in Fig. 1 and for the midpoint kernel in Fig. 2. Both of these calculations use two resolution levels. The wavefunction of the one-dimensional harmonic oscillator calculated with the method described in section 3 is plotted in Fig. 3.

When the Deslauriers–Dubuc (interpolating) wavelets are used for the hydrogen atom the calculations work for parameter $\Delta t = 1$ a.u. but not for $\Delta t = 0.5$ a.u. So we calculated this system with Daubechies (orthonormal) wavelets using both Trotter and midpoint kernels. For one resolution level calculations we use the basis $\{(2, -48), \dots, (2, 48)\}$ and for the two-level calculations $\{(1, -24), \dots, (1, 24)\} \cup \{(2, -6), \dots, (2, 6)\}$. We set the mother scaling function resolution to $J = 5$. The resulting ground state energies are presented in Table 1. It can be seen that for the same time parameter the midpoint kernel yields usually better energy compared to the Trotter kernel but the Trotter kernel accepts smaller time parameters. The best energy for the Trotter kernel is $E_0 = -0.502655$ Ha and if the energies smaller than the exact energy are neglected we get $E_0 = -0.494801$ Ha. The best energy for the midpoint kernel is $E_0 = -0.496372$ Ha. The best energy spectrum for the Trotter kernel is plotted in Fig. 4 and for the midpoint kernel in Fig. 5. The radial probability density function of the hydrogen atom calculated in one dimension with the method described in section 3 is plotted in Fig. 6.

We make calculations for the three-dimensional harmonic oscillator using the midpoint kernel and the Trotter kernel. The mass of the particle is 1 a.u. and the angular frequency 0.1 radians. We use basis $\{-10, \dots, 10\}^3$ and mother scaling function resolution $J = 2$. The resulting ground state energy for the midpoint kernel is $E_0 = 0.150796$ Ha and the first excited state $E_1 = 0.249757$ Ha for $\Delta t = 4.0$ a.u.. For $\Delta t = 2.0$ a.u. the energies are $E_0 = 0.150796$ Ha and $E_1 = 0.251327$ Ha. The energy spectrum for $\Delta t = 2.0$ a.u. is plotted in Fig. 7. For the Trotter kernel the energies are $E_0 = 0.150796$ Ha and $E_1 = 0.251327$ Ha for both $\Delta t = 4.0$ a.u. and $\Delta t = 2.0$ a.u..

We make three-dimensional calculations of the hydrogen atom using the midpoint kernel and the Trotter kernel. The basis function set is $(1/2)\{-9, \dots, 9\} \cup (1/4)\{-4, \dots, 4\}$. The function $\hat{h}(\mathbf{k})$ for the midpoint kernel is calculated with formula (36). We have to invert the sign of the midpoint kernel (35) in order to get the energy computation to work. We get energy $E = -0.474380$ Ha for the midpoint kernel with parameter $\Delta t = 2.0$ a.u. and value $\Delta t = 1.5$ a.u. does not yield reasonable results. For the Trotter kernel we get $E = -0.477522$ Ha with parameter $\Delta t = 0.2$ a.u. and value $\Delta t = 0.125$ a.u. does not give reasonable

Table 1: Energies from the one-dimensional calculations of the hydrogen atom.

kernel	res. levels	Δt	E_0 (Ha)	E_1 (Ha)
midpoint	1	1	-0.446106	-0.131947
midpoint	2	1	-0.446106	-0.113097
Trotter	1	1	-0.402124	-0.106814
Trotter	2	1	-0.402124	-0.106814
midpoint	1	0.5	-0.471239	-0.119381
midpoint	2	0.5	-0.471239	-0.119310
Trotter	1	0.5	-0.446106	-0.113097
Trotter	2	0.5	-0.452389	-0.113097
midpoint	1	0.25	-0.490088	-0.119381
midpoint	2	0.25	-0.490088	-0.119381
Trotter	1	0.25	-0.471239	-0.119381
Trotter	2	0.25	-0.477522	-0.119381
midpoint	1	0.20	-0.490088	-0.131947
midpoint	2	0.20	-0.483805	-0.144513
Trotter	1	0.20	-0.477522	-0.119381
Trotter	2	0.20	-0.483805	-0.119381
midpoint	1	0.125	-0.496372	-0.113097
midpoint	2	0.125	-	-
Trotter	1	0.125	-0.490088	-0.119381
Trotter	2	0.125	-0.490088	-0.119381
midpoint	1	0.1	-0.510509	-
Trotter	1	0.1	-0.494801	-0.117810
Trotter	2	0.1	-0.494801	-0.117810
Trotter	1	0.0625	-0.490088	-0.125664
Trotter	2	0.0625	-	-
midpoint	1	0.05	-	-
Trotter	1	0.03125	-0.502655	-0.125664
Trotter	1	0.03	-	-

results.

Note that we get exactly same energy values for many different calculations because the energy spectrum $\hat{g}(-E)$ is approximated by the Discrete Fourier Transform, for which the energy values are discrete. Ruokosenmäki [17] has discussed the behavior of the path integral kernel with small values of Δt , too. It turned out that when the time step parameter Δt is the same the midpoint kernel gives usually better energy than the Trotter kernel for the hydrogen atom (one and three dimensions) but the Trotter kernel accepts smaller values for Δt . The two kernels yield approximately the same energy for the harmonic oscillator.

8 Acknowledgments

The author thanks professor Tapio T. Rantala for proofreading the article.

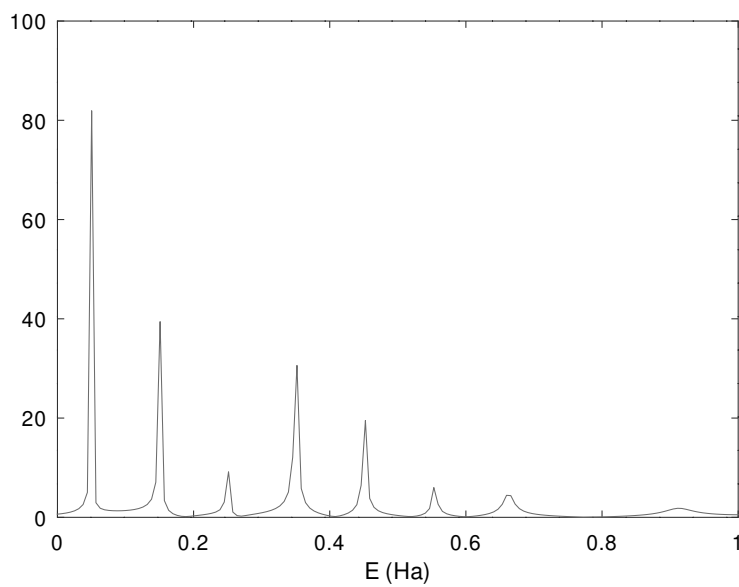


Figure 1: Energy spectrum of the one-dimensional harmonic oscillator computed with the exact kernel.

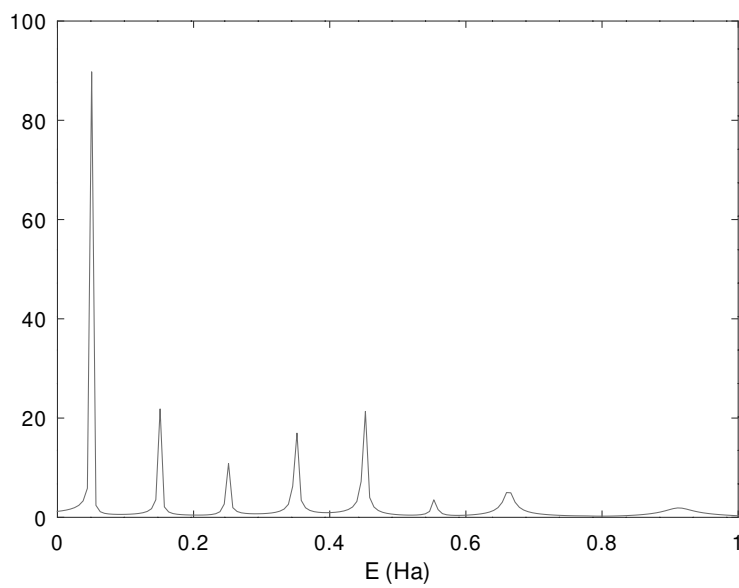


Figure 2: Energy spectrum of the one-dimensional harmonic oscillator computed with the midpoint kernel.

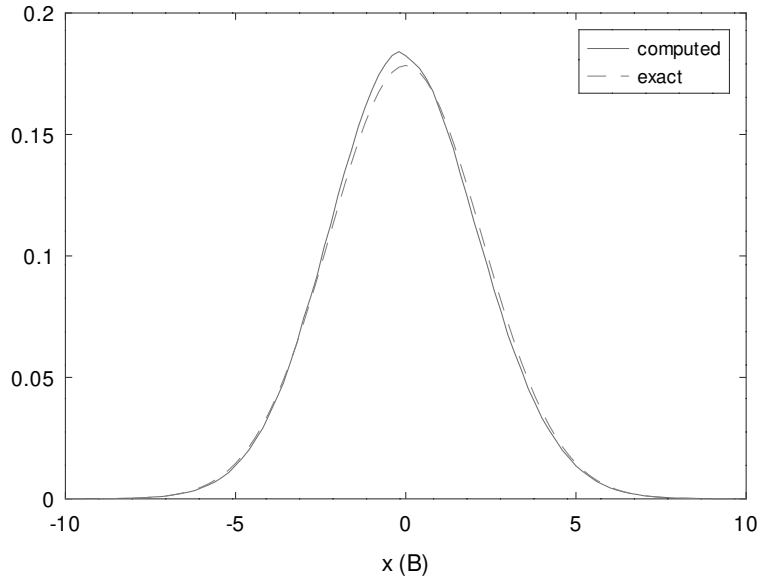


Figure 3: Probability density function $|\psi(x)|^2$ of the one-dimensional harmonic oscillator computed with the exact kernel.

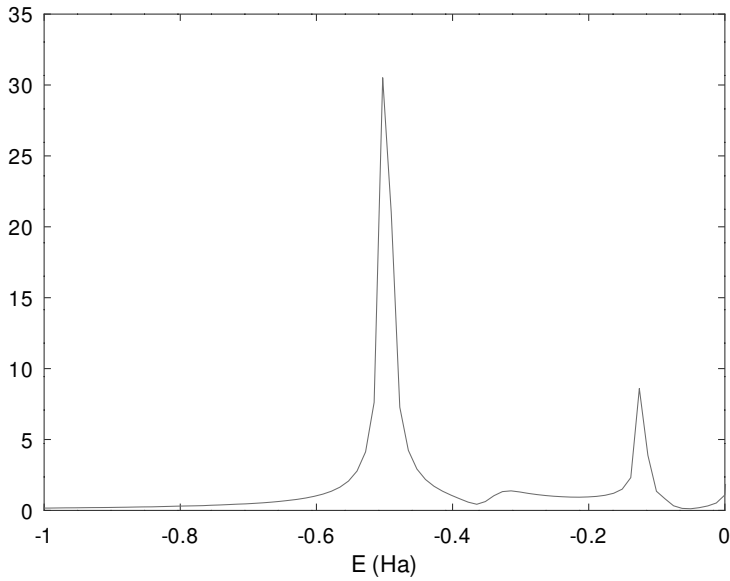


Figure 4: Energy spectrum of the hydrogen atom computed with the Trotter kernel in one dimension.

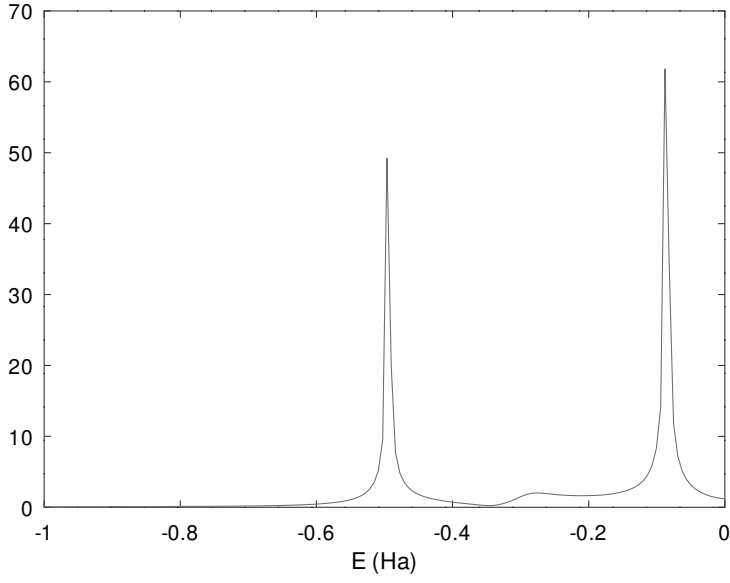


Figure 5: Energy spectrum of the hydrogen atom computed with the midpoint kernel in one dimension.

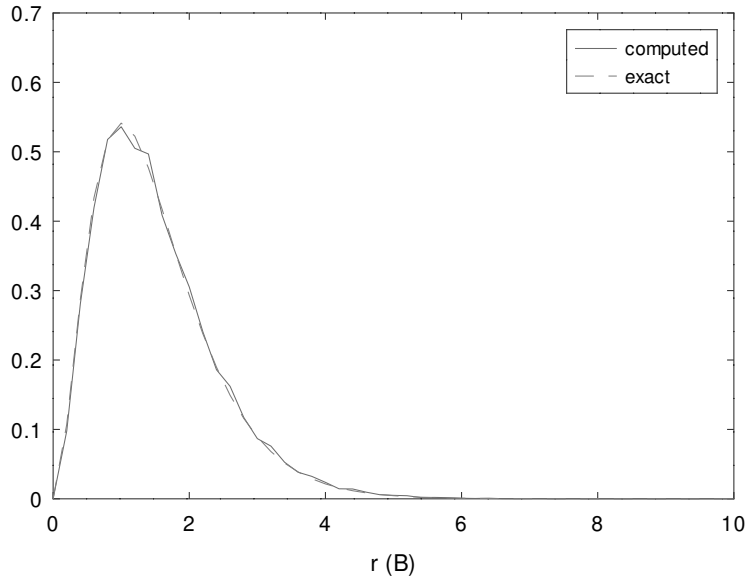


Figure 6: Radial probability density function $|P_{1s}(r)|^2$ of the hydrogen atom computed with the midpoint kernel in one dimension.

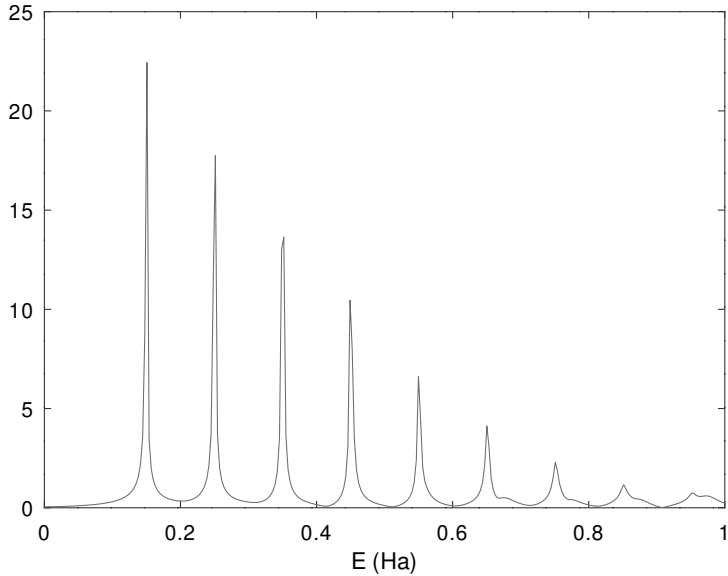


Figure 7: Energy spectrum of the three-dimensional harmonic oscillator calculated with the midpoint kernel.

References

- [1] Richard P. Feynman and Albert R. Hibbs and Daniel F. Styer. *Quantum Mechanics and Path Integrals*. Courier Corporation, 2010.
- [2] Ilkka Ruokosenmäki and Tapio T. Rantala. “Real-Time Diffusion Monte Carlo Method”. In: *Commun. Comput. Phys.* 25.2 (2019), pp. 347–360. DOI: 10.4208/cicp.0A-2018-0048.
- [3] Ilkka Ruokosenmäki and Tapio T. Rantala. “Numerical Path Integral Approach to Quantum Dynamics and Stationary Quantum States”. In: *Commun. Comput. Phys.* 18.1 (2015), pp. 91–103. DOI: 10.4208/cicp.180914.161214a.
- [4] Ilkka Ruokosenmäki et al. “Numerical path integral solution to strong Coulomb correlation in one dimensional Hooke’s atom”. In: *Computer Physics Communications* 210 (2017), pp. 45–53. DOI: 10.1016/j.cpc.2016.09.012.
- [5] Hossein Gholizadehkalkhoran, Ilkka Ruokosenmäki, and Tapio T. Rantala. “Eigenstates and dynamics of Hooke’s atom: Exact results and path integral simulations”. In: *J. Math. Phys.* 59 (2018), p. 052104. DOI: 10.1063/1.5028503.
- [6] Anders Svensson. “Path Integral for the Hydrogen Atom: Solutions in two and three dimensions”. B. S. Thesis. 2016. URL: <http://www.diva-portal.se/smash/get/diva2:947133/FULLTEXT01.pdf>.
- [7] Roger Ho and Akira Inomata. “Exact-Path-Integral Treatment of the Hydrogen Atom”. In: *Phys. Rev. Lett.* 48 (4 Jan. 1982), pp. 231–234. DOI:

- 10.1103/PhysRevLett.48.231. URL: <https://link.aps.org/doi/10.1103/PhysRevLett.48.231>.
- [8] F. Steiner. “Exact path integral treatment of the hydrogen atom”. In: *Physics Letters A* 106.8 (1984), pp. 363–367. ISSN: 0375-9601. DOI: [https://doi.org/10.1016/0375-9601\(84\)90917-4](https://doi.org/10.1016/0375-9601(84)90917-4). URL: <https://www.sciencedirect.com/science/article/pii/0375960184909174>.
 - [9] Charles K. Chui and Chun Li. “Dyadic Affine Decompositions and Functional Wavelet Transforms”. In: *SIAM J. Math. Anal.* 27.3 (1996), pp. 865–890. DOI: 10.1137/0527046.
 - [10] David L. Donoho. *Interpolating Wavelet Transforms*. Tech. rep. 408. Department of Statistics, Stanford University, 1992.
 - [11] Tommi Höynälänmaa. “Multiresolution Analysis for Compactly Supported Interpolating Tensor Product Wavelets”. In: *Int. J. Wavelets Multiresolut Inf. Process.* 13.2 (2015), p. 1550010. DOI: 10.1142/S0219691315500101.
 - [12] S. Goedecker. *Wavelets and their application for the solution of partial differential equations in physics*. Presses Polytechniques et Universitaires Romandes, 1998.
 - [13] Tommi Höynälänmaa, Tapio T. Rantala, and Keijo Ruotsalainen. “Solution of atomic orbitals in an interpolating wavelet basis”. In: *Phys. Rev. E* 70 (2004), p. 066701. DOI: 10.1103/PhysRevE.70.066701.
 - [14] Tommi Höynälänmaa and Tapio T. Rantala. “Electronic structure calculations with interpolating tensor product wavelet basis”. In: *Phys. Rev. E* 108 (2023), p. 025307. DOI: 10.1103/PhysRevE.108.025307.
 - [15] Serge Dubuc. “Interpolation through an Iterative Scheme”. In: *J. Math. Anal. Appl.* 114 (1986), pp. 185–204. DOI: 10.1016/0022-247X(86)90077-6.
 - [16] Gilles Deslauriers and Serge Dubuc. “Symmetric Iterative Interpolation Processes”. In: *Constr. Approx.* 5.1 (1989), pp. 49–68. DOI: 10.1007/BF01889598.
 - [17] Ilkka Ruokosenmäki. “Real Time Path Integral Simulation Methods for Quantum Particles”. PhD thesis. Tampere University, 2019.
 - [18] David H. Bailey and Paul N. Swarztrauber. “A Fast Method for the Numerical Evaluation of Continuous Fourier and Laplace Transforms”. In: *SIAM J. on Scientific Computing* 15.5 (1994), pp. 1105–1110.
 - [19] I. Daubechies. *Ten Lectures on Wavelets*. CBMS-NSF regional conference series in applied mathematics ; 61. SIAM, 1992. DOI: 10.1137/1.9781611970104.

