ADAPTIVE LOW-RANK WAVELET METHODS AND APPLICATIONS TO TWO-ELECTRON SCHRÖDINGER EQUATIONS

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Abstract

In this work, we develop methods for the numerical approximation of higher-dimensional functions, given as solutions of linear elliptic operator equations or as eigenfunctions of such operators. The approximations of these functions are generated by iterative schemes, where iterates are represented in a multiplicatively nonlinear tensor decomposition of their wavelet coefficients.

As a concrete application problem, we consider the stationary electronic Schrödinger equation, the fundamental equation of quantum chemistry, in model problems with one and two electrons, corresponding to three and six space dimensions, respectively. Besides the dimensionality of these problems, the characteristic singular behaviour of eigenfunctions at the singularities of the potential terms is of particular interest.

We first compare the convergence rates that can be achieved for two-electron model systems by different types of wavelet approximation: on the one hand, direct wavelet approximation with linearly parametrized wavelets, using uniform or adaptive refinement, and on the other hand, wavelet approximation with low-rank representation of coefficients, which yields the mentioned nonlinear parametrization of wavelets. In each case, the improvement of possible convergence rates by a combination with a problem-adapted, so-called explicitly correlated ansatz is studied as well.

The proposed adaptive methods for computing approximate solutions given by low-rank representations of wavelet coefficients have a structure analogous to known adaptive wavelet methods, based on a perturbed application of an iterative scheme to the wavelet representation of the underlying infinite-dimensional problem.

As common for wavelet methods, the transformation to a wavelet representation on ℓ_2 involves a diagonal rescaling of the corresponding representation matrices of operators. For finite-dimensional subproblems, this rescaling corresponds to a preconditioning. We consider, in particular, the difficulties that arise at this point in the context of low-rank representations, which leads us to a modification of the tensor representations of coefficients by an appropriate partitioning of wavelet index sets.

On this basis, algorithmic building blocks are developed that enable the realization of the basic operations required for adaptive wavelet methods also for suitable low-rank tensor representations. This concerns, in particular, the approximate evaluation of residuals, and the approximation of given iterates with lower representation complexity. We prove the convergence of the resulting methods for suitable step sizes and error tolerances. Here, all parameters controlling the iteration depend only on the infinite-dimensional problem and the wavelet basis, but not on a concrete discretization.

The adaptive eigenvalue solver is tested numerically for the electronic Schrödinger equation in the cases of hydrogen and helium, as well as for further model problems. In all those cases, a suitable low-rank format for the approximation of solution coefficients is the Tucker tensor format; however, attention is paid to the applicability of the methods in combination with recently discovered tensor formats that are suitable for very high dimensions.

In the realization of the method, the approximation of operators plays a central role. For the particular Coulomb potential terms arising in the Schrödinger equations, we construct approximations by a combination of separable expansions by exponential sums and wavelet matrix compression, and also study a specialized integration scheme for the required integrals.

Zusammenfassung

In dieser Arbeit werden Verfahren für die numerische Approximation höherdimensionaler Funktionen entwickelt, die als Lösungen linearer elliptischer Operatorgleichungen oder als Eigenfunktionen solcher Operatoren auftreten. Die Näherungen dieser Funktionen werden durch iterative Verfahren erzeugt, wobei die Iterierten in einer multiplikativ nichtlinearen Tensorzerlegung ihrer Waveletkoeffizienten dargestellt werden.

Als konkretes Anwendungsproblem betrachten wir dabei die stationäre elektronische Schrödingergleichung, die Grundgleichung der Quantenchemie, in Modellproblemen mit ein und zwei Elektronen in drei beziehungsweise sechs Raumdimensionen. Neben der Dimensionalität dieser Probleme ist dabei insbesondere das charakteristische singuläre Verhalten der Eigenfunktionen an den Singularitäten der Potentialterme von Interesse.

Wir vergleichen zunächst die durch verschiedene Arten der Waveletapproximation für Wellenfunktionen von Zweielektronen-Modellsystemen erreichbaren Konvergenzraten: einerseits direkte Waveletapproximationen mit linear parametrisierten Wavelets, bei uniformer und bei adaptiver Verfeinerung, sowie andererseits Waveletapproximation mit Niedrigrang-Tensordarstellung der Koeffizienten, was die erwähnte nichtlineare Parametrisierung der Wavelets ergibt. Dabei wird jeweils auch die Verbesserung der möglichen Konvergenzraten durch die Kombination mit einem dem Problem angepassten, sogenannten explizit korrelierten Ansatz untersucht.

Die vorgestellten adaptive Verfahren zur Berechnung von Niedrigrang-Tensordarstellungen der Waveletkoeffizienten von Näherungslösungen folgen in ihrer Grundstruktur bekannten adaptiven Waveletmethoden, basierend auf einer approximativen Anwendung eines iterativen Verfahrens auf die Waveletdarstellung der zugrundeliegenden unendlichdimensionalen Probleme.

Die Überführung in eine solche Waveletdarstellung auf ℓ_2, was für endlichdimensionale Teilprobleme einer Präkonditionierung entspricht, erfolgt wie bei Waveletmethoden üblich durch eine Diagonalskalierung der Darstellungsmatrizen der Operatoren. Wir betrachten insbesondere die Schwierigkeiten, die sich dabei im Kontext von Niedrigrang-Zerlegungen ergeben, was uns auf eine Modifikation der Tensordarstellung der Koeffizienten durch eine geeignete Unterteilung der Waveletindexmengen führt.

Darauf aufbauend werden algorithmische Grundbausteine entwickelt, mittels derer sich die in adaptiven Waveletverfahren erforderlichen Operationen auch für geeignete Niedrigrang-Darstellungen realisieren lassen. Dies betrifft insbesondere die näherungsweise Auswertung von Residuen sowie die Approximation gegebener Iterierter durch solche mit niedrigerer Darstellungskomplexität. Die Konvergenz des resultierenden Verfahren wird für geeignete Schrittweiten und Fehlertoleranzen nachgewiesen. Alle Parameter zur Steuerung der Iteration hängen dabei nur vom unendlichdimensionalen Problem und der verwendeten Waveletbasis, aber nicht von einer bestimmten Diskretisierung ab.

Der entsprechende adaptive Eigenwertlöser wird für die elektronische Schrödingergleichung für Wasserstoff und Helium sowie für weitere Modellprobleme umgesetzt. Für die betrachteten Fälle ist insbesondere die Approximation der Lösungskoeffizienten im Tucker-Tensorformat relevant, es wird aber auf die Anwendbarkeit der Methoden in Verbindung mit neueren, auch für sehr hohe Dimensionen geeigneten Tensorformaten geachtet.

Eine zentrale Rolle in der Realisierung des Verfahrens kommt der Approximation von Operatoren zu. Insbesondere betrachten wir für die in den Schrödingergleichungen auftretenden Coulomb-Potentialterme eine Kombination von separablen Entwicklungen mittels Exponentialsummen und Wavelet-Matrixkompression, sowie ein spezialisiertes Verfahren zur Auswertung der benötigten Integrale.

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Contents

1 Introduction

Numerical methods designed for problems in up to three spatial dimensions become infeasible with increasing dimensionality. This concerns, for instance, standard finite difference or finite element discretizations of partial differential equations. The typical observation is that the number of degrees of freedom and of operations required for achieving a certain accuracy increases exponentially with the dimension of the problem, which is usually referred to as the *curse of dimensionality.*

Classical adaptive schemes can exploit data sparsity of solutions that are, for instance, smooth up to localized singularities. However, adaptivity based on localization alone cannot prevent an exponential growth of the computational complexity with respect to the spatial dimension.

The convergence analysis of such discretization methods typically relies on standard Sobolev and Besov regularity of the solutions. The problem is therefore connected to the fact that these regularity notions, at a given order of smoothness, with increasing dimension impose increasingly weaker restrictions on the approximands. Functions of many variables are thus computationally tractable only if they exhibit some sort of structural sparsity beyond these types of regularity. A central task is therefore to identify relevant sparsity structures.

One possible approach centers on more appropriate regularity measures. It turns out that under certain conditions on the mixed derivatives of approximands, dimension-independent convergence rates can be achieved using tensor product multilevel bases. For instance, if $\{\psi_\nu\}_{\nu\in\nabla}$ is a wavelet basis on $\mathbb{R}$, then this type of regularity can be exploited for efficient approximation by the d-dimensional tensor product wavelets

$$\{\psi_{\nu_1} \otimes \cdots \otimes \psi_{\nu_d}\}_{(\nu_1,\ldots,\nu_d)\in\nabla^d} \,. \tag{1.1}$$

Note that such a tensor product basis contains functions with strongly anisotropic supports.

In the context of linear approximation, the resulting numerical schemes are known as sparse grid methods [133, 158, 21]. Such an approach can also be combined with adaptivity. In particular, adaptive wavelet schemes are applicable in the setting of anisotropic tensor product wavelet bases [129, 44]. Under certain conditions this leads to the expected dimension-independent convergence rates, that is, the increase in complexity for reducing the error by a certain factor becomes dimension-independent. However, as can be seen, in particular, from the numerical experiments in [44], the total complexity for achieving a *fixed* error still increases *exponentially* with space dimension. This observation is related to the general complexity results for approximation of high-dimensional functions in [118].

For the complexity to scale reasonably in d, one therefore needs to exploit further structural features of the problem at hand. For instance, in a wide range of problems one can exploit separability properties. As the simplest example of this type, let us consider the approximation of a function f on $\mathbb{R}^d$ of the form $f(x) = f_1(x_1)\, f_2(x_2) \cdots f_d(x_d)$. This may be done by an expansion in a tensor product multilevel basis (1.1), that is, by choosing $\Lambda \subset \nabla^d$ and $c_{(\nu_1,\ldots,\nu_d)} \in \mathbb{R}$ for $(\nu_1,\ldots,\nu_d) \in \Lambda$ with

$$f \approx \sum_{(\nu_1,\ldots,\nu_d)\in\Lambda} c_{(\nu_1,\ldots,\nu_d)} \, (\psi_{\nu_1} \otimes \cdots \otimes \psi_{\nu_d}) \,. \tag{1.2}$$

Although the choice of Λ depends on the given f in adaptive approximation schemes, for given Λ the mapping of coefficients $c_{(\nu_1,\ldots,\nu_d)}$ to the corresponding approximation is linear. We shall refer to this as a *linear parametrization* by the approximation parameters.

An expansion (1.2) will in general require a substantially higher number of nonzero coefficients for the same accuracy than approximating instead the factors f_i in a one-dimensional basis,

$$f \approx \bigotimes_{i=1}^{d} \Bigl(\sum_{\nu \in \Lambda^{(i)} \subset \nabla} c^{(i)}_\nu \, \psi_\nu \Bigr) = \sum_{(\nu_1,\ldots,\nu_d) \in \Lambda^{(1)} \times \cdots \times \Lambda^{(d)}} (c^{(1)}_{\nu_1} \cdots c^{(d)}_{\nu_d}) (\psi_{\nu_1} \otimes \cdots \otimes \psi_{\nu_d}) \,.$$

Note that in such an approximation, which exploits separability, the mapping from approximation parameters to basis coefficients is (multiplicatively) nonlinear. We shall refer to this as a *nonlinear parametrization* of wavelet coefficients with respect to the basis (1.1).

In problems of interest, the solution can typically not be represented or well approximated by a single separable function, but in many cases instead has good approximations by sums of several separable functions. In order to make effective use of this property in the solution of operator equations, the involved operators need to be approximable by sums of tensor product operators as well.

The main contribution of this work is an adaptive method that exploits both approximability by separable expansions, and near-sparsity of the arising lower-dimensional factors in a given reference basis. Essentially, we seek an approximation to the solution u in the form

$$u \approx \sum_{k=1}^{r} \bigotimes_{i=1}^{d} \Bigl(\sum_{\nu \in \Lambda^{(i)}_k} c^{(i)}_{k,\nu} \psi_\nu \Bigr) \,. \tag{1.3}$$

For our computational purposes, however, such a simple sum of separable terms turns out to be insufficient; one needs to introduce additional structure to obtain a representation with certain stability properties. Leaving these further issues aside in the present informal discussion, our aim is roughly speaking the construction of a scheme that simultaneously finds the required number of summands r, sets of nonzero wavelet coefficients $\Lambda^{(i)}_k \subset \nabla$, and the corresponding approximation coefficients $c^{(i)}_{k,\nu}$.

The adaptive refinement obtained in this manner is of particular interest if the functions under consideration have some localized lack of smoothness. A motivating example of a class of higher-dimensional problems with nonsmooth, but highly structured solutions is provided by the electronic Schrödinger equation, which in the stationary case is an eigenvalue problem for a second-order elliptic operator with singular potential terms. It is posed on $\mathbb{R}^{3n}$, where n is the number of electrons in the considered physical system. In this work we consider in detail one- and two-electron model problems in three and six spatial dimensions, respectively.

A particular challenge in the case of two or more electrons is the cusp in the eigenfunction caused by the singular Coulomb interaction between electrons. A natural approach for obtaining approximate solutions is to expand eigenfunctions in terms of tensor products of single-electron functions, and this is in fact the basis of most established standard methods. The interaction cusps, however, are diagonal with respect to this type of tensor product structure, which leads to a rather severe limitation of the convergence rates of such expansions.

This issue is a major limiting factor for the accuracy attained by standard approximation schemes for the electronic Schrödinger problem, which are almost exclusively based on antisymmetrized tensor products of Gaussian-type orbitals (GTOs). These GTOs can be written as sums of terms of the form $p(x)e^{-\gamma|x-a|^2}$ for $x \in \mathbb{R}^3$, where p is a multivariate polynomial, and $\gamma > 0$, $a \in \mathbb{R}^3$ are fixed parameters. A major practical advantage of GTOs is that all arising integrals required in a Galerkin discretization can then be computed analytically. The surprising approximation efficiency of such basis functions for electronic Schrödinger eigenfunctions depends to a great deal on the appropriate choice of the exponents $\gamma > 0$. In certain basic one-electron systems, it is known that almost exponential convergence of eigenvalues with respect to the number of such orbitals can be achieved [105]. In general, however, the convergence properties of such basis functions are still not well understood, and there is no systematic procedure for refining given approximations to higher accuracy.

In recent years, alternative methods based on more mathematically founded constructions have been developed. In [150], Yserentant showed that electronic Schrödinger eigenfunctions have square-integrable high-order mixed derivatives, which means that they are in principle amenable to approximation by anisotropic tensor product bases. A general construction of sparse grid-type wavelet approximations, based on this property and the exponential spatial decay of solutions, was given in [157].

Previous wavelet discretizations of the electronic Schrödinger equation using such concepts have been based, e.g., on orthonormal Meyer wavelets [65], and on semiorthogonal piecewise linear prewavelets [154]. However, in addition to the inherent difficulties for such generic basis functions in competing with highly optimized existing GTO-based quantum chemistry packages, it can be observed that such an approach requires a very large number of degrees of freedom even for two-electron systems. Combining such a sparse grid-type discretization with heuristic concepts, a scheme with better practical efficiency using approximately orthogonal Gaussian frames was obtained in [76, 66]. A different hybrid strategy combining GTOs and a refined approximation of interaction cusps by wavelets has also been studied in [49, 109].

The approximation of many-electron wavefunctions by sums of separable functions has been considered in [14, 112, 113]. These works focus on the algorithmic complexity of manipulating such expansions; however, the corresponding approximability of electronic Schrödinger eigenfunctions by separable expansions to the author's knowledge currently remains an open problem. With focus on the approximation of given model functions – as, e.g., in density fitting schemes in quantum chemistry – the combination of separable expansions with wavelet approximation of lower-dimensional factors has been considered in [25, 26, 24, 27].

A quantum-chemical method is called *explicitly correlated* if it takes special care of the electron interaction cusp in order to improve convergence. In this work we additionally consider an approach in this direction which amounts to multiplying the wavelet basis functions by an additional term that captures the behaviour of the interaction cusp to first order. In the model cases we shall consider, an improvement of the convergence rate with respect to the number of degrees of freedom compared to a direct approximation by tensor product wavelets can be quantified rigorously.

Furthermore, we investigate the convergence of nonlinearly parametrized wavelet approximations of the form (1.3) for model problems with explicit solutions. Here we find that, if the variables are separated in an appropriate way (in the two-electron case, by separating into bivariate factors), one can obtain improved convergence – as compared to a linearly parametrized wavelet expansion – with respect to the total number of nonzero coefficients.

The adaptive low-rank solvers for finding such nonlinearly parametrized representations proposed in this work follow in their basic structure the methodology of known adaptive wavelet methods [31]. They do not use a sequence of fixed discretizations, but are based on the approximate application of an iterative scheme for the underlying infinite-dimensional problem. Following this strategy, we obtain a rigorous convergence analysis for the resulting low-rank scheme. In contrast to known methods based on tensor representations for fixed discretizations, the analysis yields a choice of parameters for the iteration for which convergence is ensured up to any desired accuracy, where these parameters depend only on the given infinite-dimensional problem and the wavelet basis, but not on the particular discretization.

As in standard adaptive wavelet methods, the approximate application of operators is a central part of the algorithm, and can here also be done in a similar way based on wavelet compression techniques. The compression of the Laplacian term in the model problems is covered by existing results. For the Coulomb potential terms, we develop new approximations that are suitable for the adaptive low-rank algorithms. In our case, this involves two steps: approximation of the potential functions by sums of separable terms, and compression of the wavelet representations of the factors in the corresponding summands. The first step is based on the established technique of exponential sum approximations, where we give an error analysis in operator norm tailored to our setting. For the second step, we develop wavelet compression schemes for multiplication operators induced by certain Gaussian-type functions. In addition, we propose a specialized integration scheme for the evaluation of the corresponding matrix entries.

1.1 Outline

In Chapter 2, we give an overview of the *electronic Schrödinger equation* in the general many-particle case, and of the particular model problems that will be considered in more detail.

Chapter 3 provides a summary of general results concerning *approximation by tensor product wavelet bases*, and of a construction of adaptive wavelet schemes that we will build on later.

In Chapter 4, we consider several types of *wavelet approximation for the solutions of the electronic Schrödinger model problems* singled out in Chapter 2. In particular, we consider what can potentially be gained by explicitly correlated schemes and by nonlinear parameterization of wavelet coefficients in a low-rank tensor format.

In Chapter 5, we propose *adaptive wavelet schemes based on low-rank tensor representations* of wavelet coefficients for linear operator equations and for eigenvalue problems. Here we follow the general principles of the established adaptive wavelet methods reviewed in Chapter 3, but replace all building blocks by operations on low-rank representations.

A central role in this regard is played by the adaptive approximation of the action of operators on finite vectors of wavelet coefficients. After a discussion of suitable choices of wavelet bases, the *approximation of the particular operators arising in our electronic Schrödinger model problems* is studied in detail in Chapter 6.

In Chapter 7, we discuss the *numerical realization* of the methods considered in Chapter 5 and the numerical results obtained for the model problems.

1.2 Notation

In this section, we collect some basic notation that will be used throughout this work.

The standard sets of numbers are denoted by $\mathbb{N}$, $\mathbb{Z}$, $\mathbb{R}$ and $\mathbb{C}$; in addition, we shall use $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$, $\mathbb{R}^+ = (0,\infty)$ and $\mathbb{R}_0^+ = [0,\infty)$. We write $A \lesssim B$ to express $A \leq cB$ with some generic constant $c > 0$, analogously $A \gtrsim B$ for $A \geq cB$, and $A \sim B$ if and only if $A \lesssim B$ and $A \gtrsim B$. For $x \in \mathbb{R}$, we define $(\cdot)_+ := \max\{0, x\}$. For $x \in \mathbb{R}^d$, $|x|$ denotes the Euclidean norm. The open ball of radius R and center x is denoted by $B_R(x)$.

For $d \in \mathbb{N}$ and a domain $\Omega \subseteq \mathbb{R}^d$, we denote by $\mathrm{L}_p(\Omega)$ for $p \in (0,\infty]$ the standard Lebesgue spaces on Ω. The notation $\langle\cdot,\cdot\rangle$ by default denotes the duality pairing induced by the L_2–inner product. This duality pairing reduces to the L_2–inner product if both arguments are in L_2. The inner product of a Hilbert space $\mathcal{H}$ is denoted by $\langle\cdot,\cdot\rangle_{\mathcal{H}}$.

The gradient is denoted by D, and the partial derivative with respect to the variable x is denoted by D_x. Note that ∇ is used to denote the index sets of one-dimensional wavelet bases (cf. (3.6)). For further notational conventions related to wavelet bases, see Chapter 3.

The space of continuous functions on Ω is denoted by $\mathrm{C}(\Omega)$, the space of k times continuous functions by $\mathrm{C}^k(\Omega)$, and the Hölder spaces, for $\alpha \in [0,1]$, by $\mathrm{C}^{k,\alpha}(\Omega)$. Furthermore, $\mathrm{C}_0^\infty(\Omega)$ is the space of infinitely differentiable test functions of compact support in Ω, and $\mathcal{S}(\mathbb{R}^d)$ denotes the Schwartz space of rapidly decreasing functions; $\mathcal{S}'(\mathbb{R}^d)$ is the space of tempered distributions.

The Fourier transform of $u\colon \mathbb{R}^d \to \mathbb{C}$ is denoted by $\hat{u}$, defined with the scaling convention

$$\hat{u}(\xi) = (2\pi)^{-\frac{d}{2}} \int_{\mathbb{R}^d} u(x) e^{-ix\cdot\xi}\,\mathrm{d}x$$

for $u \in \mathrm{L}_1(\mathbb{R}^d)$ and extended to an isometric isomorphism on $\mathrm{L}_2(\mathbb{R}^d)$. For the product of functions u, v, we denote the Fourier transform by $(uv)^\wedge$.

The Sobolev spaces of order $k \in \mathbb{N}$ are denoted as $\mathrm{W}_p^k(\Omega)$ for $p \in [1, \infty]$; in the case $p = 2$, we denote these spaces as $\mathrm{H}^k(\Omega)$. Furthermore, we shall use the abbreviations $\|\cdot\|_k := \|\cdot\|_{\mathrm{H}^k(\Omega)}$ and $|\cdot|_k := |\cdot|_{\mathrm{H}^k(\Omega)}$ for norm and seminorm if the domain is clear from the context.

For $s \in \mathbb{R}$, the fractional order Sobolev space $\mathrm{H}^s(\mathbb{R}^d)$ comprises those $u \in \mathcal{S}'(\mathbb{R}^d)$ for which

$$\|u\|^2_{\mathrm{H}^s(\mathbb{R}^d)} := \int_{\mathbb{R}^d} \bigl(1 + |\xi|^2\bigr)^s |\hat{u}|^2 \,\mathrm{d}\xi < \infty\,.$$

Recall that for integer s, by Parseval's theorem this definition is equivalent to the standard Sobolev norm defined in terms of integrability of weak derivatives.

The standard Besov spaces on Ω are denoted by $\mathrm{B}^s_{p,q}(\Omega)$ [9, 143, 29]. Additional Sobolev and Besov spaces of dominating mixed regularity will be introduced in Section 3.4.

2 The Electronic Schrödinger Equation

The Schrödinger equation is the basic equation of non-relativistic quantum physics. In its time-dependent form, it describes the time evolution of quantum states; in the stationary case, with which we shall be dealing exclusively, it becomes an eigenvalue problem which has as its solutions the possible quantum states that the described physical system can attain. In this chapter, an overview is given of the electronic Schrödinger equation, which serves as the fundamental model of molecular systems in quantum chemistry, of some of its most important features, and of the model systems on which we will later focus.

The states of a single quantum-mechanical particle moving in an external potential $V\colon \mathbb{R}^3 \to \mathbb{R}$ are described by the solutions $u\colon \mathbb{R}^3 \to \mathbb{R}$ of the eigenvalue problem

$$-\tfrac{1}{2}\Delta u + Vu = \lambda u\,. \tag{2.1}$$

As the two terms on the left hand side correspond to kinetic and potential energy of the particle, the eigenvalue λ represents the total energy of the state u. The Coulomb potential

$$V(x) = -\frac{1}{|x|} \tag{2.2}$$

models the attractive force that a fixed charge located at the origin exerts on the particle. When using appropriately scaled units, equation (2.1) with the potential (2.2) provides a model for the hydrogen atom, i.e., a negatively charged electron moving in the electric field of an atomic nucleus consisting of a single positively charged proton. This model is based on the assumption that it suffices to consider only the electron as a quantum-mechanical particle, whereas the proton is modelled as a classical point charge. Since the proton is by orders of magnitude more massive than the electron, this so-called *Born-Oppenheimer approximation* [15] turns out to be sufficient in practice even for more complicated molecular systems.

2.1 The General Case

For a molecule composed of several nuclei and electrons, the same reasoning leads to the general electronic Schrödinger equation for n electrons. Assuming nuclei at given positions $a_\nu \in \mathbb{R}^3$ with charges Z_ν, it reads

$$Hu := \Biggl\{ -\frac{1}{2}\sum_{i=1}^{n} \Delta_{x_i} - \sum_{i=1}^{n}\sum_{\nu} \frac{Z_\nu}{|x_i - a_\nu|} + \sum_{\substack{i,j=1\\ i<j}}^{n} \frac{1}{|x_i - x_j|} \Biggr\} u = \lambda u\,. \tag{2.3}$$

In addition to the Coulomb attraction of the nuclei, the potential now contains terms depending on $|x_i - x_j|$ that model the repulsion between the equally charged electrons. In this context, the operator H is called *Hamiltonian.* The *wave function* u in (2.3) is a high-dimensional object: for n electrons,

$$u\colon (\mathbb{R}^3 \times \{-\tfrac{1}{2}, \tfrac{1}{2}\})^n \to \mathbb{C}\,,\ \bigl((x_1,\sigma_1),\dots,(x_n,\sigma_n)\bigr) \mapsto u\bigl((x_1,\sigma_1),\dots,(x_n,\sigma_n)\bigr)\,.$$

The $x_i \in \mathbb{R}^3$ correspond to spatial coordinates of each particle, and $\sigma_i \in \{-\tfrac{1}{2}, \tfrac{1}{2}\}$ represent electron spin. Since electrons are fermions, a physically meaningful solution u needs to be antisymmetric under permutation of electron coordinates (x_i, σ_i). Note that since H is real and self-adjoint, it suffices to consider real-valued u in this case.

A priori, such a wave function has 2^n components u_σ corresponding to all possible choices of spins $\sigma \in \{-\frac{1}{2}, \frac{1}{2}\}^n$. However, the Hamiltonian operator H in (2.3) is symmetric with respect to spatial electron coordinates and independent of the spins[1], and as a consequence the full wave function can immediately be recovered from only $\lfloor n/2 \rfloor$ spin components that are actually independent, see [152] for a detailed treatment.

For given σ, let $S^\pm_\sigma := \{i \colon \sigma_i = \pm\frac{1}{2}\}$. The antisymmetry requirement for the full wave function u, which is also known as Pauli's exclusion principle, translates to the partial antisymmetry requirement

$$u_\sigma(\ldots, x_i, \ldots, x_j, \ldots) = -u_\sigma(\ldots, x_j, \ldots, x_i, \ldots) \quad \text{if } i,j \in S^+_\sigma \text{ or } i,j \in S^-_\sigma, \tag{2.4}$$

in other words, the components u_σ need to be antisymmetric under exchange of electrons with equal spin. Note that this means in particular that u_σ vanishes on the set

$$\Big\{(x_1, \ldots, x_n) \in (\mathbb{R}^3)^n \colon \prod_{\substack{i,j \in S^+_\sigma \\ i<j}} (x_i - x_j) \prod_{\substack{i,j \in S^-_\sigma \\ i<j}} (x_i - x_j) = 0\Big\}.$$

In what follows, we shall therefore always assume some fixed choice of $\sigma = (\sigma_1, \ldots, \sigma_n)$ to be given, and only consider the single component $u_\sigma \colon \mathbb{R}^{3n} \to \mathbb{R}$; for simplicity, we again refer to such a spatial component as a wave function and write u in place of u_σ. In summary, we thus consider eigenfunctions $u \colon \mathbb{R}^{3n} \to \mathbb{R}$ of H as in (2.3) that additionally satisfy the partial antisymmetry requirement (2.4) for a certain fixed partition $\{S^+_\sigma, S^-_\sigma\}$ of $\{1, \ldots, n\}$.

In mathematical physics, the Hamiltonian H is usually considered as an unbounded, self-adjoint operator mapping $\mathrm{L}_2(\mathbb{R}^{3n})$ to itself, with domain $\mathrm{H}^2(\mathbb{R}^{3n})$. That H as in (2.3) can be treated in this framework is shown in [86, 87]; see also [123, 125].

For the weak formulation of the eigenvalue problem, we define the bilinear form a for $u, v \in \mathrm{H}^1(\mathbb{R}^{3n})$ as

$$a(u,v) := \frac{1}{2} \int \mathrm{D}u \cdot \mathrm{D}v \,\mathrm{d}x + \int (V_{\mathrm{ne}} + V_{\mathrm{ee}})\, u\, v \,\mathrm{d}x$$

with the potential terms

$$V_{\mathrm{ne}}(x) := -\sum_{i,\nu} \frac{Z_\nu}{|x_i - a_\nu|}, \quad V_{\mathrm{ee}}(x) := \sum_{i<j} \frac{1}{|x_i - x_j|}, \quad x = (x_1, \ldots, x_n) \in (\mathbb{R}^3)^n. \tag{2.5}$$

The following Hardy-type inequality plays a central role in the analysis of the bilinear form a.

Lemma 2.1. *For $v \in \mathrm{H}^1(\mathbb{R}^3)$,*

$$\int_{\mathbb{R}^3} \frac{1}{|x|^2} |v|^2 \,\mathrm{d}x \le 4 \int_{\mathbb{R}^3} |\mathrm{D}v|^2 \,\mathrm{d}x.$$

We refer to [125, p. 169] or [150, Lemma 1] for a proof, see also [152]. Note that in these references, Lemma 2.1 is formulated explicitly for infinitely differentiable functions with compact support. The extension to $\mathrm{H}^1(\mathbb{R}^3)$ follows by a density argument.

As a consequence of Lemma 2.1, the bilinear form a is bounded on $\mathrm{H}^1(\mathbb{R}^{3n})$, and there exists a $\mu > 0$ such that for some $c_{a,\mu} > 0$ we have

$$a(v,v) + \mu \langle v, v \rangle_{\mathrm{L}_2} \ge c_{a,\mu} \|v\|^2_{\mathrm{H}^1}, \quad v \in \mathrm{H}^1(\mathbb{R}^{3n}). \tag{2.6}$$

---

[1] In certain situations, explicit dependencies of H on the spin variables are possible, e.g., in the presence of external magnetic fields.

In other words, a can be made H^1–elliptic by an appropriate shift. For the details, including the dependence of the involved constants on n, see [89, 152].

We say that $u \in \mathrm{H}^1(\mathbb{R}^{3n})$, $u \neq 0$ is an eigenfunction of a with eigenvalue λ if

$$a(u,v) = \lambda \langle u, v\rangle_{\mathrm{L}_2} \quad \text{for all } v \in \mathrm{H}^1(\mathbb{R}^{3n}). \tag{2.7}$$

The weak formulation is equivalent to the classical eigenvalue problem for H as an unbounded operator on L_2, in the sense that the eigenfunctions in both formulations are the same, see [152, Section 2.5].

Concerning the structure of the spectrum of H, which since H is self-adjoint is a subset of $\mathbb{R}$, note that (2.6) implies that it is bounded from below. Furthermore, it can be shown that there exists a threshold $\Sigma \leq 0$ depending on the spin configuration such that any $\lambda < \Sigma$ in the spectrum is necessarily an eigenvalue, and Σ equals the infimum of the essential spectrum. In practice, the quantity of interest in the problem (2.7) is the lowest eigenvalue

$$\lambda_0 := \inf_{\substack{v\in\mathrm{H}^1\\ \|v\|_{\mathrm{L}_2}=1}} a(v,v)\,,$$

and quantities derived from the corresponding eigenspace, which is referred to as *ground state.*

2.1.1 Decay and Regularity Properties of Eigenfunctions

The threshold Σ is closely connected to the decay behavior of eigenfunctions of Schrödinger operators. We quote a result on exponential decay in the L_2–sense given in [152] that is most appropriate for our purposes.

Theorem 2.2. *If* $u \in \mathrm{H}^1(\mathbb{R}^{3n})$ *is an eigenfunction belonging to an eigenvalue* λ *in the discrete spectrum of* (2.3)*, then for any* $\delta > 0$ *with* $\delta < \sqrt{2d_\lambda}$*,*

$$\int e^{2\delta|x|}\bigl(|u|^2 + |\mathrm{D}u|^2\bigr)\,\mathrm{d}x \; < \infty\,, \tag{2.8}$$

where $d_\lambda = \Sigma - \lambda$*.*

For a detailed treatment of decay properties of eigenfunctions and of the above characterization of Σ, we refer to the monograph [2] and to [152]; concerning further qualitative results on the spectrum of electronic Schrödinger operators, see also [126].

Besides their exponential decay, a further feature of the eigenfunctions of interest that is of central importance in their numerical approximation are their specific regularity properties: essentially, the eigenfunctions are smooth except at locations of singularities of the potential terms, where they are not continuously differentiable.

More precisely, as a consequence of standard results [83, Section III.7.5], eigenfunctions of H are real analytic on the complement of the set

$$\Bigl\{x \in (\mathbb{R}^3)^n \colon \prod_{i,\nu}(x_i - a_\nu)\prod_{i<j}(x_i - x_j) = 0\Bigr\}$$

corresponding to the locations of singularities. Here points $x \in \mathbb{R}^{3n}$ for which $x_i = a_\nu$ for exactly one i and one ν are referred to as electron-nucleus coalescence points, and points for which $x_i = x_j$ for exactly one pair i, j are called two-electron coalescence points.

A first characterization of the smoothness properties at the singularities was obtained by Kato [88], who showed that wavefunctions are continuous on $\mathbb{R}^{3n}$ with first derivatives that are potentially discontinuous at the singularities of the potentials. The behaviour of these cusps at two-particle coalescence points is characterized by the celebrated Kato cusp condition in terms of spherical averages.

The latter result was sharpened in [53], where it was shown that one has a representation

$$u = \exp(F_2 + F_3)\, w$$

where

$$F_2(x) = -\sum_i \sum_\nu Z_\nu |x_i - a_\nu| + \frac{1}{2} \sum_{i<j} |x_i - x_j|\,,$$

$$F_3(x) = \frac{2-\pi}{3} \sum_{i<j} \sum_\nu Z_\nu\, (x_i - a_\nu) \cdot (x_j - a_\nu) \ln(|x_i - a_\nu|^2 + |x_j - a_\nu|^2)$$

and $w \in \mathrm{C}^{1,1}(\mathbb{R}^{3n})$. Intuitively this means that near electron-nucleus coalescence points with $x_i = a_\nu$, the wave function behaves essentially like $\exp(-Z_\nu |x_i - a_\nu|)$, whereas near electron-electron coalescence points with $x_i = x_j$, the cusps look to first order like $\exp(\frac{1}{2}|x_i - x_j|)$. At electron-electron-nucleus coalescence points, the additional correction factor F_3 comes into play.

In [54], it was shown that a sharper local result holds near two-particle coalescence points. For electron-nucleus coalescence points, there exists a neighborhood in which one has a representation of the form

$$u(x) = \phi_1(x) + |x_i - a_\nu| \phi_2(x)$$

with real analytic functions ϕ_1, ϕ_2; and for electron-electron coalescence points there exists a neighborhood in which

$$u(x) = \phi_3(x) + |x_i - x_j| \phi_4(x)$$

with real analytic ϕ_3, ϕ_4. Note, however, that this result breaks down at points where three or more particles meet.

Standard approximation schemes for wave functions are based on expansions into sums of antisymmetrized tensor products of basis functions depending on a single electron coordinate. For the moment, let us thus assume $\{\phi_i\}_{i\in\mathbb{N}}$ to be a suitable family of single-electron basis functions on $\mathbb{R}^3$. Then for a given spin configuration σ, a basis function satisfying the partial antisymmetry requirement (2.4) can be obtained by a so-called *Slater determinant*,

$$\Phi_{i_1,\ldots,i_n}(x) := (|S^+_\sigma||S^-_\sigma|)^{-\frac{1}{2}} \det\bigl(\phi_{i_k}(x_l)\bigr)_{k,l\in S^+_\sigma} \det\bigl(\phi_{i_k}(x_l)\bigr)_{k,l\in S^-_\sigma}\,, \tag{2.9}$$

where the indices $i_1, \ldots, i_n \in \mathbb{N}$ combined in each determinant need to be pairwise different.

With appropriately chosen ϕ_i, the electron-nuclear cusps, which are aligned to this type of tensor product structure, can be approximated very efficiently; this is true in particular when Gaussian-type basis functions as mentioned in Chapter 1 are used for the ϕ_i, see [105] for an analysis of certain basic special cases.

In the Hartree-Fock approximation, one makes an ansatz by a single Slater determinant with unknowns ϕ_i in the original Schrödinger equation to obtain a reduced nonlinear eigenvalue problem on $\mathbb{R}^3$ for the ϕ_i. In this mean-field approximation, the electron interaction enters only in an averaged manner. The eigenvalues obtained from this model are always strictly greater than the exact solution, where this difference is usually referred to as the *correlation energy*; correspondingly, electron interaction cusps are also called *correlation cusps.*

Unfortunately, for the approximation of these electron-electron cusps, which are diagonal with respect to the tensor product structure, by sums of functions of the form (2.9), one obtains only very slow convergence – with a strictly limited algebraic rate – regardless of the choice of ϕ_i. The results in [51] concerning this point will be considered in more detail in Section 4.2.

Methods that go beyond such expansions for obtaining more efficient approximations are called *explicitly correlated.* One possible remedy is to switch to different coordinates in which the inter-electronic distances become axes in the coordinate system, enabling efficient approximations of the transformed wave functions by basis functions that have a tensor product structure in the new coordinates. An early instance of such a scheme was given by Hylleraas [84], which we shall touch upon in Section 2.3; currently, such methods are applicable to small systems with simple geometries up to four-electron atoms.

A second possible way of approaching the problem is to work in the original spatial coordinates, but using basis functions that capture to some extent the known structure of the electron-electron cusps. In the well-known *R12 methods* [104, 99, 106], factors linear in $|x_i - x_j|$ are combined with standard basis functions of the form (2.9); in *F12 methods* [128], this is generalized to more general dependencies on the interelectronic distances. In *Gaussian geminal methods* [16, 132, 138, 122], products of Slater determinants with factors of the form $\exp(-\gamma|x_i - x_j|^2)$, with suitable exponents γ, are used as basis functions. A major difficulty in all of these methods is that the additional factors lead to integrals over up to four electron coordinates, that is, in up to twelve spatial dimensions.

In Section 4.3, we shall consider a type of approximation that is closely connected to Gaussian geminal expansions. In the next section, we consider in more detail a different explicitly correlated scheme based on ansatz functions including a factor of the form $\exp(\frac{1}{2}\sum_{i<j}|x_i - x_j|)$. It has the advantage of requiring only integrals over at most three electron coordinates, but leads to a nonsymmetric eigenvalue problem.

2.2 An Explicitly Correlated Formulation

In this section, we consider a specific way of incorporating information on the electron-electron cusp into approximations of wave functions. The electron-electron singularities are eliminated at the price of introducing additional nonsymmetric first-order two-electron terms and symmetric zero-order three-electron terms, whereas the single-electron parts of the Hamiltonian are unchanged.

In explicitly correlated methods, an ansatz for u is made that explicitly includes the correct first-order behavior of the electron-electron cusp, and v is chosen accordingly to obtain a favorable modified bilinear form. For the further discussion, let

$$F(x) := \frac{1}{2}\sum_{i<j} |x_i - x_j|\,. \tag{2.10}$$

A first option, related to R12 methods in quantum chemistry, would be a substitution $u = (1 + F)\varphi$, $v = (1 + F)\tau$ with modified solution φ and test function τ in (2.7). This preserves symmetry of the Hamiltonian, but leads to rather complicated four-electron integrals.

The approach we will follow here corresponds to taking $u = \exp(F)\varphi$, $v = \exp(-F)\tau$ instead, which can be interpreted as a similarity transformation and in the computational chemistry literature is referred to as a *transcorrelated method*. Although it entails loss of symmetry of the bilinear form, it completely eliminates the two-electron singularities and avoids four-electron integrals.

It is also possible to modify the correlation factor $\exp(F)$ to a uniformly bounded function and still achieve the same effect. This is particularly important for modelling the correct decay behaviour when using Gaussian basis sets, but, as we will see in more detail below, is not required in the two-electron case. Therefore, and to avoid more complicated expressions, we use the unbounded correlation factor $\exp(F)$ in what follows.

For $\varphi, \tau \in \mathrm{H}^1(\mathbb{R}^{3n})$, the modified bilinear form is given by

$$\tilde{a}(\varphi,\tau) := \frac{1}{2}\int \mathrm{D}\varphi \cdot \mathrm{D}\tau \,\mathrm{d}x + \int (V_{\mathrm{ne}} + V_{\mathrm{ee}} - \frac{1}{2}\Delta F)\,\varphi\,\tau\,\mathrm{d}x - \int (\mathrm{D}F \cdot \mathrm{D}\varphi)\tau\,\mathrm{d}x - \frac{1}{2}\int |\mathrm{D}F|^2 \varphi\tau\,\mathrm{d}x\,,$$

with F as in (2.10), and consequently $V_{\mathrm{ee}} = \frac{1}{2}\Delta F$. Written out in full, in this case we have

$$\begin{aligned} \tilde{a}(\varphi,\tau) = {} & \frac{1}{2}\int \mathrm{D}\varphi \cdot \mathrm{D}\tau \,\mathrm{d}x - \sum_{i,\nu}\int \frac{Z_\nu}{|x_i - a_\nu|}\varphi\,\tau\,\mathrm{d}x \\ & - \frac{1}{2}\sum_i \int \sum_{k\neq i} \frac{x_i - x_k}{|x_i - x_k|}\cdot \mathrm{D}_{x_i}\varphi\,\tau\,\mathrm{d}x - \frac{1}{8}\sum_i\int\sum_{k,l\neq i}\frac{x_i - x_k}{|x_i - x_k|}\cdot\frac{x_i - x_l}{|x_i - x_l|}\varphi\,\tau\,\mathrm{d}x\,. \end{aligned} \tag{2.11}$$

The strong form of the modified problem (2.11) was also used to obtain the regularity results in [53] already mentioned above. In the quantum chemistry literature, the formulation seems to appear first in [81]. It was used in a similar form in computational schemes for Gaussian-type orbitals for instance in [17, 117, 139, 159]. Quite promising numerical results using Gaussian basis sets for the helium model system for the particular Hamiltonian corresponding to (2.11) are given in [98].

We next establish the connection between a and $\tilde{a}$, see also [153].

Proposition 2.3. *Let $u \in \mathrm{H}^1(\mathbb{R}^{3n})$ be an eigenfunction of the bilinear form a with eigenvalue λ, then $w = e^{-F}u \in \mathrm{H}^1(\mathbb{R}^{3n})$ is an eigenfunction of $\tilde{a}$ with the same eigenvalue,*

$$\tilde{a}(w,\tau) = \lambda\langle w,\tau\rangle \quad \textit{for all } \tau \in \mathrm{H}^1(\mathbb{R}^{3n}). \tag{2.12}$$

Proof. From Lipschitz continuity of $e^{-|\cdot|}$ and the chain and product rules for weak differentiation (cf. [61]) it follows that $e^{-F}u \in \mathrm{H}^1(\mathbb{R}^{3n})$. For any $\tau \in \mathrm{C}_0^\infty(\mathbb{R}^{3n})$,

$$\begin{aligned} \tilde{a}(e^{-F}u,\tau) &= \frac{1}{2}\int e^{-F}(\mathrm{D}u - u\,\mathrm{D}F)\cdot\mathrm{D}\tau\,\mathrm{d}x - \int e^{-F}\mathrm{D}F\cdot(\mathrm{D}u - u\,\mathrm{D}F)\tau\,\mathrm{d}x \\ &\quad + \frac{1}{2}\int e^{-F}(2V_{\mathrm{ne}} - |\mathrm{D}F|^2)u\,\tau\,\mathrm{d}x \\ &= \frac{1}{2}\int e^{-F}\mathrm{D}u\cdot\mathrm{D}\tau\,\mathrm{d}x - \frac{1}{2}\int e^{-F}u\,\mathrm{D}F\cdot\mathrm{D}\tau\,\mathrm{d}x - \int e^{-F}\mathrm{D}F\cdot\mathrm{D}u\,\tau\,\mathrm{d}x \\ &\quad + \frac{1}{2}\int e^{-F}|\mathrm{D}F|^2 u\,\tau\,\mathrm{d}x + \int e^{-F}V_{\mathrm{ne}}\,u\,\tau\,\mathrm{d}x\,. \end{aligned}$$

Now on the one hand,

$$\frac{1}{2}\int e^{-F}\mathrm{D}u\cdot\mathrm{D}\tau\,\mathrm{d}x - \frac{1}{2}\int e^{-F}\mathrm{D}F\cdot\mathrm{D}u\,\tau\,\mathrm{d}x = \frac{1}{2}\int \mathrm{D}u\cdot\mathrm{D}(e^{-F}\tau)\,\mathrm{d}x\,,$$

on the other hand, by integration by parts and noting that $\Delta F = 2V_{\mathrm{ee}}$,

$$\begin{aligned} -\frac{1}{2}\int e^{-F}u\mathrm{D}F\cdot\mathrm{D}\tau\,\mathrm{d}x &= \frac{1}{2}\int \mathrm{D}(e^{-F}u)\cdot\mathrm{D}F\,\tau\,\mathrm{d}x + \frac{1}{2}\int e^{-F}\Delta F\,u\,\tau\,\mathrm{d}x \\ &= \frac{1}{2}\int e^{-F}(\mathrm{D}u\cdot\mathrm{D}F)\tau\,\mathrm{d}x - \frac{1}{2}\int e^{-F}|\mathrm{D}F|^2u\,\tau\,\mathrm{d}x + \int e^{-F}V_{\mathrm{ee}}u\,\tau\,\mathrm{d}x\,. \end{aligned}$$

Putting this together, using that $e^{-F}\tau \in \mathrm{H}^1(\mathbb{R}^{3n})$ and that u solves (2.7), we obtain

$$\begin{aligned} \tilde{a}(e^{-F}u,\tau) &= \frac{1}{2}\int \mathrm{D}u\cdot\mathrm{D}(e^{-F}\tau)\,\mathrm{d}x + \int e^{-F}(V_{\mathrm{ne}} + V_{\mathrm{ee}})u\,\tau\,\mathrm{d}x \\ &= a(u, e^{-F}\tau) = \lambda\langle u, e^{-F}\tau\rangle = \lambda\langle e^{-F}u,\tau\rangle\,. \end{aligned}$$

By a density argument we obtain the assertion. □

As mentioned before, the disadvantage of the modified problem for $\tilde{a}$ is that the symmetry of the bilinear form a is lost. This has the further consequence that for an eigenfunction u with eigenvalue

λ of a, the solutions of the adjoint problem

$$\tilde{a}(\tau, w^*) = \lambda\langle w^*, \tau\rangle \quad \text{for all } \tau \in \mathrm{H}^1(\mathbb{R}^{3n}) \tag{2.13}$$

are different from those of (2.12). It will be shown below that (2.13) is solved by $w^* = e^F u$, given that this product is contained in $\mathrm{H}^1(\mathbb{R}^{3n})$. Whereas $e^F u \in \mathrm{H}^1_{\mathrm{loc}}(\mathbb{R}^{3n})$ follows as in the proof of Proposition 2.3 from $u \in \mathrm{H}^1(\mathbb{R}^{3n})$, for unbounded functions F as in (2.10), global integrability of $|w^*|^2$ and $|\mathrm{D}w^*|^2$ now depends on the decay properties of u.

Theorem 2.2 can be used to verify the assumptions of the following Proposition, see also Remark 2.5.

Proposition 2.4. *If* $w^* = e^F u \in \mathrm{H}^1(\mathbb{R}^{3n})$, *where* u *is an eigenfunction of* a *with eigenvalue* λ, *then* w^* *solves the adjoint modified problem* (2.13).

Proof. We proceed as above to rewrite $\tilde{a}(\tau, e^F u)$ for $\tau \in \mathrm{C}^\infty_0(\mathbb{R}^{3n})$, using integration by parts,

$$-\frac{1}{2}\int e^F(\mathrm{D}F\cdot \mathrm{D}\tau)u\,\mathrm{d}x = \frac{1}{2}\int e^F(\mathrm{D}F\cdot\mathrm{D}u)\tau\,\mathrm{d}x + \frac{1}{2}\int e^F|\mathrm{D}F|^2 u\,\tau\,\mathrm{d}x + \int e^F V_{\mathrm{ee}}\,u\,\tau\,\mathrm{d}x\,,$$

and that for the compactly supported functions τ, we have $e^F\tau \in \mathrm{H}^1(\mathbb{R}^{3n})$. □

We shall see in Remark 2.5 below that for the ground state of the two-electron model system of helium, the assumption $w^* \in \mathrm{H}^1(\mathbb{R}^{3n})$ in Proposition 2.4 is satisfied with F defined as in (2.10). It should be noted, however, that this integrability condition on w^* need no longer hold for higher eigenvalues and systems with more electrons. In general, it will therefore be preferable to replace F by a suitable bounded functions, see also Remark 6.14 concerning computational implications of different correlation factors.

2.3 One- and Two-Electron Model Cases

Our main interest concerning the approximation of electronic wave functions in this work lies in the approximation of electron interaction cusps, and in methods for achieving higher convergence rates than achievable by a direct discretization by tensor product basis functions. We shall study this problem in the simplest case where it arises, namely that of two-electron atomic systems in six spatial dimensions.

In this section, we give an overview of the one- and two-electron model problems that we shall consider in detail in this work. As a general comprehensive reference on the quantum mechanical background of one- and two-electron systems, see [10].

A basic example of a one-electron system is provided by the hydrogen atom with Hamiltonian given by (2.1) and (2.2), that is,

$$-\frac{1}{2}\Delta u - \frac{1}{|x|}u = \lambda u\,.$$

In this case, the eigenvalue problem can be completely solved analytically. We shall only consider the ground state eigenfunction

$$u_0 \sim e^{-|x|}$$

with ground state eigenvalue $\lambda_0 = -\frac{1}{2}$; the higher eigenvalues are given by $\lambda_n := -\frac{1}{2n^2}$.

The two-electron model problem of main interest to us is the helium atom with one nucleus of charge 2 at the coordinate origin. The eigenvalue problem reads

$$-\frac{1}{2}\Delta u - 2\left(\frac{1}{|x_1|} + \frac{1}{|x_2|}\right)u + \frac{1}{|x_1 - x_2|}u = \lambda u\,, \tag{2.14}$$

where here and in the remainder of this section, $x = (x_1, x_2) \in (\mathbb{R}^3)^2$. For this system, no analytical solutions are known. However, there exist highly accurate approximations to the lowest eigenvalue:

in [100], the approximation

$$\lambda_0 \approx -2.903724377034119598311159 \tag{2.15}$$

for the ground state eigenvalue is given, which on the basis of comparisons to other calculations is expected to be exact to 24 significant digits.

Note that for the ground state of a two-electron system, antisymmetry does not play a role: as demonstrated in detail in [10], the ground state needs to be symmetric with respect to exchange of spatial electron coordinates, which corresponds to the two electrons having opposite spins.

In the case of helium, the explicitly correlated formulation (2.12), with unbounded correlation factor as in (2.10), reads

$$-\frac{1}{2}\Delta w - 2\biggl(\frac{1}{|x_1|} + \frac{1}{|x_2|}\biggr) w - \frac{1}{2}\frac{x_1 - x_2}{|x_1 - x_2|} \cdot (\mathrm{D}_{x_1} - \mathrm{D}_{x_2}) w = \biggl(\lambda + \frac{1}{4}\biggr) w\,. \tag{2.16}$$

The relevant difference in regularity between u and $w = \exp(-\frac{1}{2}|x_1 - x_2|)u$ will be considered in more detail in Chapter 4. Concerning the decay of the corresponding adjoint eigenfunction w^* as required in Proposition 2.4, in this particular example we obtain the following result.

Remark 2.5. *To give a specific example of what the exponential decay property* (2.8) *means for the adjoint eigenfunction in the explicitly correlated formulation, i.e., for* w^* *from Proposition 2.4 with* F *as in* (2.10)*, we consider the corresponding formulation for helium as in* (2.16)*. Here we have*[2] $\Sigma = -2$*, and* λ_0 *as in* (2.15)*. Since* $\sqrt{2d_{\lambda_0}}|x| - \frac{1}{2}|x_1 - x_2| \geq \Bigl(\sqrt{2d_{\lambda_0}} - \frac{1}{\sqrt{2}}\Bigr)|x|$*, an estimate of the form* (2.8) *is satisfied also for* w^* *with* $\delta < \sqrt{2d_{\lambda_0}} - \frac{1}{\sqrt{2}} \approx 0.637$*.*

For helium, the Hylleraas method [84] provides a specialized discretization scheme that yields highly efficient approximate wave functions. By a coordinate change, and exploiting symmetries of the helium eigenproblem, the six-dimensional problem (2.14) can be rewritten in terms of the three variables $s = |x_1| + |x_2|$, $t = |x_1| - |x_2|$, and $u = |x_1 - x_2|$. The solution is approximated by sums of functions of the form $e^{-\zeta s} s^n t^{2l} u^m$, with some fixed $\zeta > 0$, that are parameterized by $n, l, m \in \mathbb{N}_0$. Details of this scheme can also be found in [10]. A method based on such a coordinate transformation was also used for the high-precision result (2.15). This approach thus turns out to be extremely efficient for two-electron atomic systems, but, as mentioned before, it is very difficult to extend to more than four electrons or to arbitrary molecular systems. See for instance [97] for recent results of such calculations for four-electron atomic systems, and for a discussion of the restrictions in applicability of such an approach.

The so-called *Hooke's law atom*, also referred to as *hookium* or *harmonium*, is a commonly used simplified model problem for helium. It has a similar electron interaction cusp, but can be solved analytically. The corresponding eigenvalue problem has the same basic form as that for helium, but the nuclear Coulomb potentials are replaced by appropriately scaled quadratic (harmonic oscillator) potentials [91, 28, 120], which leads to

$$-\frac{1}{2}\Delta u + \frac{1}{8}|x|^2 u + \frac{1}{|x_1 - x_2|} u = \lambda u\,. \tag{2.17}$$

The eigenpair for the lowest eigenvalue is given by

$$\lambda_0 = 2\,, \quad u_0 \sim \bigl(1 + \tfrac{1}{2}|x_1 - x_2|\bigr) \exp\bigl(-\tfrac{1}{4}|x|^2\bigr)\,. \tag{2.18}$$

It can thus be seen that the ground state has an electron-electron cusp satisfying the same first-order Kato cusp condition as the ground state of helium. The eigenvalue problem (2.17) has been been used as a test problem for the approximation of electron-electron cusps, e.g., in [51] and [103]. Of

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[2] See [126, XIII.3.A]; note the different scaling convention for the Laplacian term in the Hamiltonian.

course, in this particular example the electron-electron cusp problem could easily be circumvented by a coordinate rotation. However, note that this is not possible in the case of helium, where such a rotation would lead to the same difficulties in the approximation of electron-nuclear cusps instead.

In the case of (2.17), we can obtain an explicitly correlated formulation analogous to (2.16),

$$-\frac{1}{2}\Delta w + \frac{1}{8}|x|^2 w - \frac{1}{2}\frac{x_1 - x_2}{|x_1 - x_2|} \cdot (\mathrm{D}_{x_1} - \mathrm{D}_{x_2}) w = \Bigl(\lambda + \frac{1}{4}\Bigr) w \,. \tag{2.19}$$

The corresponding modified ground state reads

$$w_0 \sim \exp\bigl(-\tfrac{1}{2}|x_1 - x_2|\bigr)\bigl(1 + \tfrac{1}{2}|x_1 - x_2|\bigr) \exp\bigl(-\tfrac{1}{4}|x|^2\bigr) \,. \tag{2.20}$$

In Chapter 4, the availability of explicit solutions will allow a more detailed investigation of the approximability of the ground states u_0 in (2.18) and w_0 in (2.20).

3 Higher-Dimensional Approximation and Adaptive Wavelet Methods

In this chapter, we first introduce basic concepts and collect relevant facts concerning the approximation of higher-dimensional functions by wavelet-type tensor product multilevel bases. We review the construction of wavelet bases on the real line in Section 3.1, consider general properties of tensor products of Hilbert spaces in Section 3.2, and finally turn to the construction and approximation properties of tensor product wavelets in Sections 3.3 and 3.4. In Sections 3.5 and 3.6, we summarize a construction of adaptive wavelet schemes that serves as a basis for our further developments in Chapter 5.

3.1 Wavelets on $\mathbb{R}$

The characterization of function spaces in terms of the coefficients in basis expansions plays an important role in this work. For Hilbert spaces, a central concept in this regard are Riesz bases.

Definition 3.1. Let $\mathcal{H}$ be a Hilbert space. A family $\{f_i\}_{i\in\mathcal{I}}$ with countable $\mathcal{I}$ is a *Riesz basis* of $\mathcal{H}$ if and only if $\overline{\operatorname{span}\{f_i\}_{i\in\mathcal{I}}} = \mathcal{H}$ and there exist $0 < c \leq C$ such that for any finitely supported sequence $(a_i)_{i\in\mathcal{I}}$, we have

$$c\|(a_i)\|_{\ell_2(\mathcal{I})} \leq \Big\|\sum_{i\in\mathcal{I}} a_i f_i\Big\|_{\mathcal{H}} \leq C\|(a_i)\|_{\ell_2(\mathcal{I})}\,. \tag{3.1}$$

The quantity $c^{-1}C$ is called the *condition number* of the Riesz basis. Note that $\{f_i\}_{i\in\mathcal{I}}$ is an orthonormal basis if and only if $c = C = 1$. The wavelet bases on $\mathbb{R}$ considered in this work are Riesz bases of $\mathrm{L}_2(\mathbb{R})$ and, when rescaled appropriately, of a certain range of Sobolev spaces. They are all derived from the basic framework of a *multiresolution analysis*; in the following definition, we follow [29].

Definition 3.2. A sequence $(V_j)_{j\in\mathbb{Z}}$ of closed subspaces of $\mathrm{L}_2(\mathbb{R})$ is a *multiresolution analysis* if the following properties are satisfied:

(i) The subspaces are nested, that is, $V_j \subset V_{j+1}$ for all $j \in \mathbb{Z}$.

(ii) For all $j \in \mathbb{Z}$, $f \in V_j$ if and only if $f(2\,\cdot) \in V_{j+1}$.

(iii) Denoting by P_j the L_2–orthogonal projection onto V_j, for all $f \in \mathrm{L}_2$ we have

$$\lim_{j\to\infty} \|f - P_j f\|_{\mathrm{L}_2(\mathbb{R})} \to 0\,, \qquad \lim_{j\to-\infty} \|P_j f\|_{\mathrm{L}_2(\mathbb{R})} \to 0\,.$$

(iv) There exists a function $\varphi \in V_0$ such that $\big\{\varphi(\cdot - k)\big\}_{k\in\mathbb{Z}}$ is a Riesz basis of V_0.

Remark 3.3. *Property (ii) can be rephrased as the requirement that $f(2^j\cdot) \in V_j$ if and only if $f \in V_0$. Property (iii) can also be formulated as*

$$\overline{\bigcup_{j\in\mathbb{Z}} V_j} = \mathrm{L}_2(\mathbb{R})\,, \qquad \bigcap_{j\in\mathbb{Z}} V_j = \{0\}\,,$$

that is, the union of the V_j is dense in $\mathrm{L}_2(\mathbb{R})$, *whereas their intersection contains only the zero function.*

Combining properties (ii) and (iv) in Definition 3.2, setting $\varphi_{j,k} := 2^{j/2}\varphi(2^j \cdot -k)$ one finds that $\{\varphi_{j,k}\}_{k\in\mathbb{Z}}$ are a Riesz basis of V_j. A multiresolution analysis is therefore completely determined by the choice of the so-called *scaling function* φ. By property (i), there exists a sequence $(h_k)_{k\in\mathbb{Z}} \in \ell_2(\mathbb{Z})$ such that one has the *refinement equation*

$$\varphi = \sum_k h_k\, \varphi_{1,k} = \sqrt{2}\sum_k h_k\, \varphi(2\cdot -k)\,. \tag{3.2}$$

A standard approach to the construction of wavelet bases that affords some flexibility for numerical purposes are biorthogonal wavelets, where one considers pairs of scaling functions φ, $\tilde\varphi$, each satisfying the properties in Definition 3.2, such that

$$\langle \varphi, \tilde\varphi(\cdot - k)\rangle_{\mathrm{L}_2} = \delta_{0,k}\,, \quad k \in \mathbb{Z}\,.$$

Such pairs of wavelet bases will appear later in the computation of certain integrals, see Section 6.6.

However, for a number of reasons that will be discussed in more detail later, in particular in Section 6.1, as basis functions for numerical schemes we shall be exclusively interested in wavelet bases that satisfy a stronger requirement than property (iv), namely orthonormality: if φ satisfies properties (i)–(iii) and in addition its translates are L_2–orthonormal, that is,

$$\text{(iv')} \qquad \langle \varphi(\cdot - k), \varphi(\cdot - l)\rangle = \delta_{kl}\,,$$

then φ immediately yields a construction of orthonormal bases for $\mathrm{L}_2(\mathbb{R})$. To this end, let $g_k := (-1)^k h_{-k+1}$ for $k \in \mathbb{Z}$ and let the so-called *mother wavelet* be defined by

$$\psi := \sum_k g_k\, \varphi_{1,k}\,. \tag{3.3}$$

For $j \in \mathbb{Z}$, let W_j be the orthogonal complement of V_j in V_{j+1}, i.e., $V_{j+1} = V_j \oplus W_j$. Then $\{\psi(\cdot - k)\}_{k\in\mathbb{Z}}$ with ψ as in (3.3) is an orthonormal basis of W_0, and for each $j \in \mathbb{Z}$, $\{\psi_{j,k}\}_{k\in\mathbb{Z}}$ with $\psi_{j,k} := 2^{j/2}\psi(2^j\cdot -k)$ is an orthonormal basis for W_j. We thus obtain that $\{\psi_{j,k}\}_{j,k\in\mathbb{Z}}$ and, for any $j_0 \in \mathbb{Z}$,

$$\{\varphi_{j_0,k}\}_{k\in\mathbb{Z}} \cup \{\psi_{j,k}\}_{j\geq j_0, k\in\mathbb{Z}} \tag{3.4}$$

are both orthonormal bases of $\mathrm{L}_2(\mathbb{R})$, corresponding to the decompositions

$$\mathrm{L}_2(\mathbb{R}) = \bigoplus_{j\in\mathbb{Z}} W_j = V_{j_0} \oplus \bigoplus_{j\geq j_0} W_j$$

of $\mathrm{L}_2(\mathbb{R})$ into pairwise orthogonal subspaces.

Given a scaling function φ and a wavelet ψ, we set

$$\psi_{j,k,0} := 2^{j/2}\varphi(2^j\cdot -k)\,, \quad \psi_{j,k,1} := 2^{j/2}\psi(2^j\cdot -k)\,,$$

and with the notation

$$\mathbb{Z}_{j_0} = \{j \in \mathbb{Z}\colon\ j \geq j_0\}\,, \quad j_0 \in \mathbb{Z}\,, \tag{3.5}$$

we define the index set

$$\nabla = \nabla(j_0) := \{(j_0, k, 0)\colon k \in \mathbb{Z}\} \cup \{(j,k,1)\colon j \geq j_0, k \in \mathbb{Z}\}\,. \tag{3.6}$$

In this work we exclusively use wavelet bases with scaling functions at a suitable level $j_0 \in \mathbb{Z}$ as in (3.4) which, using the above definitions, can be denoted more concisely by $\{\psi_\lambda\}_{\lambda\in\nabla}$. Note that for simplicity, we do not indicate the dependence of the wavelet basis on the choice of j_0 in this notation.

We furthermore introduce the abbreviations $|\lambda| := j$, $\mathrm{k}(\lambda) := k$, $\mathrm{s}(\lambda) := s$ for $\lambda = (j,k,s) \in \nabla$, and set

$$\nabla_j := \{\nu \in \nabla \colon |\nu| = j\} \tag{3.7}$$

for $j \in \mathbb{Z}_{j_0}$. A wavelet ψ is said to have m *vanishing moments* if

$$\int_{\mathbb{R}} x^k \psi \, dx = 0\,, \quad k = 0,\dots,m-1\,. \tag{3.8}$$

A scaling function φ is said to have *order of polynomial reproduction* $m-1$ if for $k = 0,\dots,m-1$ there exist monic polynomials p_k such that

$$x^k = \sum_{n\in\mathbb{Z}} p_k(n)\, \varphi(x-n)\,.$$

In the case of orthonormal wavelets, the number of vanishing moments determines the order of polynomial reproduction: (3.8) holds for the wavelet if and only if the corresponding scaling function has order of polynomial reproduction $m-1$.

The property (3.8) can be used in the following form: For $v \in \mathrm{L}_2(\mathbb{R})$ and $p,q \in [1,\infty]$ such that $p^{-1} + q^{-1} = 1$, with (3.8) and Hölder's inequality one obtains

$$\left|\int_{\mathbb{R}} v\, \psi_{j,k}\, \mathrm{d}x\right| \leq \|\psi_{j,k}\|_{\mathrm{L}_p(\mathbb{R})} \inf\bigl\{ \|v-g\|_{\mathrm{L}_q(\operatorname{supp}\psi_{j,k})} \colon g \text{ polynomial of degree} < m \bigr\}\,.$$

The infimum on the right hand side can now be estimated by standard results on local polynomial approximation, making use of the smoothness properties of v – in particular, by the Deny-Lions theorem and the more general theorem of Whitney, see [29, Section 3.2]. This basic technique plays a central role in Chapters 4 and 6.

Remark 3.4. *For compactly supported wavelets obtained from a multiresolution analysis,* $\varphi \in \mathrm{H}^k(\mathbb{R})$ *for* $k \in \mathbb{N}$ *implies that* φ *has order of polynomial reproduction at least* k*, cf. [29, Theorem 2.8.2]. For orthonormal wavelets, the corresponding* ψ *then has* $k+1$ *vanishing moments.*

In the remainder of this work we shall, unless stated otherwise, assume the wavelet basis functions under consideration to be compactly supported and L_2–orthonormal. The motivation for these restrictions will be discussed in detail in Section 6.1.

3.1.1 Linear and Nonlinear Approximation by Wavelets

Let $\varphi \in \mathrm{H}^t(\mathbb{R})$ satisfy the polynomial reproduction property of order $m-1$, then there exists $C > 0$ such that for $0 < t < s \leq m$ and any $u \in \mathrm{H}^s(\mathbb{R})$, we have the *direct estimate*

$$\inf_{u_j \in V_j} \|u - u_j\|_{\mathrm{H}^t(\mathbb{R})} \leq C 2^{-(s-t)j} |u|_{\mathrm{H}^s(\mathbb{R})}\,, \tag{3.9}$$

see [29, Section 3.3]. Sobolev regularity thus yields a certain rate of *linear* approximation by wavelets, where the set of basis functions is chosen solely based on the known regularity, but independently of the concrete function under consideration.

If in addition to the direct estimate (3.9), the wavelet basis has sufficient regularity, one obtains norm equivalences of a range of Sobolev norms to the ℓ_2-norms of appropriately rescaled wavelet coefficients. The following result follows as a special case of [29, Theorems 3.7.7 and 3.8.1]; we shall use it in particular in the case $s = 1$.

Theorem 3.5. *If φ is the compactly supported, L_2–orthonormal scaling function of a multiresolution analysis and $\varphi \in \mathrm{H}^\tau(\mathbb{R})$ for some $\tau > 0$, then $\{2^{-s|\lambda|}\psi_\lambda\}_{\lambda\in\nabla}$ is a Riesz basis of $\mathrm{H}^s(\mathbb{R})$ for $-\tau < s < \tau$.*

A similar statement holds for biorthogonal wavelets, where the lower bound on s depends on the corresponding dual scaling function $\tilde\varphi$. Note that we shall make explicit use of Theorem 3.5 only for $s > 0$.

We next turn to best N-term approximation by wavelets, which is an instance of *nonlinear* approximation, since in this case the choice of basis functions depends on the given approximand. In this section, we consider the univariate setting. The main concepts, however, are essentially the same in the case of tensor product wavelet bases in higher dimensions, which will be treated in Section 3.4.

In this work, we shall mostly be concerned with approximation in the H^1–norm. That is, in the one-dimensional case presently under consideration, for $u \in \mathrm{H}^1(\mathbb{R})$ and each given $N \in \mathbb{N}$, we aim to find a sequence $(c_\lambda)_{\lambda\in\nabla}$ with $\#\operatorname{supp}(c_\lambda) \leq N$ such that

$$\Bigl\| u - \sum_{\lambda\in\nabla} c_\lambda \psi_\lambda \Bigr\|_{\mathrm{H}^1(\mathbb{R})}$$

is minimized. In view of Theorem 3.5, this problem can be reduced to the simpler problem of best N-term approximation in the sequence space $\ell_2(\nabla)$: Let $\tilde u_\lambda := 2^{|\lambda|}\langle u, \psi_\lambda\rangle$, and let $\Lambda_N \subset \nabla$ be the set of indices corresponding to the N largest absolute values[1] $|\tilde u_\lambda|$. Choose the approximation by $c_\lambda = \tilde u_\lambda$ for $\lambda \in \Lambda_N$, and $c_\lambda = 0$ otherwise. Then by the Riesz basis property,

$$\Bigl\| u - \sum_{\lambda\in\Lambda_N} \tilde u_\lambda (2^{-|\lambda|}\psi_\lambda) \Bigr\|_{\mathrm{H}^1(\mathbb{R})} \sim \|(\tilde u_\lambda) - (c_\lambda)\|_{\ell_2(\nabla)} = \Bigl(\sum_{\lambda\in\nabla\setminus\Lambda_N} |\tilde u_\lambda|^2 \Bigr)^{\frac12} .$$

As a consequence, the convergence with respect to N of best N-term approximation by wavelets can be characterized precisely by the decay of the (rescaled) wavelet coefficients, reordered by nonincreasing absolute value.

To make this more precise, we next introduce a standard definition of spaces of functions for which a certain convergence rate of best N-term approximation by a given basis is attained.

Definition 3.6 (see e.g. [41, 29])**.** Let $\mathcal{H}$ be a separable Hilbert space, and let $\Gamma := \{\gamma_\lambda\}_{\lambda\in\mathcal{I}}$ be a Riesz basis of $\mathcal{H}$. For $N \in \mathbb{N}$, let

$$\Sigma_N := \Bigl\{ \sum_{\lambda\in\mathcal{I}} c_\lambda\gamma_\lambda\colon\ \#\operatorname{supp}(c_\lambda) \leq N \Bigr\}, \quad \sigma_N(f)_{\mathcal{H}} := \inf_{g\in\Sigma_N} \|f-g\|_{\mathcal{H}} .$$

For $s > 0$ and $q \in (0,\infty]$, we define

$$\mathcal{A}^s_q(\mathcal{H}) := \bigl\{ f \in \mathcal{H}\colon\ \bigl(2^{sj}\sigma_{2^j}(f)_{\mathcal{H}}\bigr)_{j\geq 0} \in \ell_q(\mathbb{N}_0) \bigr\} .$$

Note that $\mathcal{A}^s_q(\mathcal{H}) \subset \mathcal{A}^s_\infty(\mathcal{H})$ for $q \in (0,\infty)$. As a consequence of the monotonicity of $\sigma_n(u)_{\mathcal{H}}$, we obtain furthermore that $u \in \mathcal{A}^s_\infty(\mathcal{H})$ if and only if $\sigma_n(u)_{\mathcal{H}} \lesssim n^{-s}$.

The sets $\mathcal{A}^s_q(\mathcal{H})$ become quasi-Banach spaces when endowed with an appropriate quasinorm. We shall use this explicitly only in the case $q = \infty$, where a quasinorm for $\mathcal{A}^s_\infty(\mathcal{H})$ is given by

$$\|\mathbf{v}\|_{\mathcal{A}^s_\infty(\mathcal{H})} := \|\mathbf{v}\|_{\mathcal{H}} + |\mathbf{v}|_{\mathcal{A}^s_\infty(\mathcal{H})} , \quad |\mathbf{v}|_{\mathcal{A}^s_\infty(\mathcal{H})} := \sup_{N\in\mathbb{N}} N^s \sigma_N(\mathbf{v})_{\mathcal{H}} .$$

For the special case of nonlinear approximation in ℓ_2–spaces, we additionally introduce an abbreviated notation for the corresponding approximation spaces.

---

[1] Note that these need not be uniquely determined, but in the case of coefficients with equal absolute values it suffices to pick one of the possible choices.

Definition 3.7. For a given index set $\mathcal{I}$, with s, q as in Definition 3.6 and with the underlying basis Γ chosen as the coordinate basis of $\ell_2(\mathcal{I})$, that is, $\Gamma = \{(\delta_{\nu,\lambda})_{\nu\in\mathcal{I}}\}_{\lambda\in\mathcal{I}}$, we set

$$\mathcal{A}^s_q := \mathcal{A}^s_q(\ell_2(\mathcal{I}))\,. \tag{3.10}$$

The sequence space $\mathcal{A}^s_\infty$ can be identified with a standard weak-ℓ_τ space for a certain relation between s and τ, where the latter spaces are defined as follows.

Definition 3.8. Let $\mathbf{v} = (v_\lambda)_{\lambda\in\mathcal{I}}$ be a sequence on $\mathcal{I}$, and let $(\lambda_n)_{n\in\mathbb{N}}$ be an enumeration of $\mathcal{I}$ such that

$$|v_{\lambda_1}| \geq |v_{\lambda_2}| \geq \dots\,,$$

then $\mathbf{v}^* := (|v_{\lambda_n}|)_{n\in\mathbb{N}}$ is called the *nonincreasing rearrangement* of $\mathbf{v}$. For $\tau \in (0,2)$, we define the sequence space $\mathrm{w}\ell_\tau$ by

$$\mathrm{w}\ell_\tau := \bigl\{\mathbf{v} = (v_\lambda)_\lambda \in \ell_2(\mathcal{I})\colon |\mathbf{v}|_{\mathrm{w}\ell_\tau(\mathcal{I})} < \infty\bigr\}\,,$$

where $|\mathbf{v}|_{\mathrm{w}\ell_\tau(\mathcal{I})} := \sup_{n\in\mathbb{N}} n^{\frac{1}{\tau}} v^*_n$.

We have

$$\mathcal{A}^s_\infty = \mathrm{w}\ell_\tau\,, \quad \text{if } \tau = (s+\tfrac{1}{2})^{-1}\,,$$

with equivalent quasinorms

$$\|\mathbf{v}\|_{\mathcal{A}^s_\infty} \sim \|\mathbf{v}\|_{\ell_2} + |\mathbf{v}|_{\mathrm{w}\ell_\tau}\,.$$

In other words, the elements of $\mathcal{A}^s_\infty$ are precisely those sequences $\mathbf{v} \in \ell_2$ whose decreasing rearrangements $\mathbf{v}^* = (v^*_n)_{n\in\mathbb{N}}$ decay at least proportionally to $n^{-(s+\frac{1}{2})}$.

As exemplified by (3.9), Sobolev spaces are related to the convergence rates of linear approximation by the family of uniformly refined subspaces V_j. In the context of best N-term approximation, a comparable role is played by the Besov spaces $\mathrm{B}^s_{p,q}(\mathbb{R})$. These spaces can be defined for any $s, p, q > 0$, but we shall use them only for $0 < p < \infty$, $p \leq q \leq \infty$, and $s \geq \frac{1}{p} - \frac{1}{2}$. They can be defined in a number of equivalent ways, see for instance [143, 29]. We shall only need the characterization of these spaces in terms of wavelet coefficients, as given in the following theorem, which follows as a special case of [29, Theorem 3.7.7].

Theorem 3.9. *Let φ be a compactly supported, continuous, and L_2–orthonormal scaling function of a multiresolution analysis, let $\{\psi_\nu\}_{\nu\in\nabla}$ be a corresponding wavelet basis, and let $p > 0$. If $\varphi \in \mathrm{B}^t_{p,p}$ for a $t > 0$ and ψ has at least $\lceil t\rceil$ vanishing moments, then for any $s > 0$ with $\frac{1}{p} - 1 < s < t$, we have the norm equivalence*

$$\|f\|_{\mathrm{B}^s_{p,p}(\mathbb{R})} \sim \bigl\|(2^{(s+\frac{1}{2}-\frac{1}{p})|\nu|}\langle f,\psi_\nu\rangle)_{\nu\in\nabla}\bigr\|_{\ell_p(\nabla)} = \Bigl(\sum_{\nu\in\nabla} 2^{(s+\frac{1}{2}-\frac{1}{p})p|\nu|}|\langle f,\psi_\nu\rangle|^p\Bigr)^{\frac{1}{p}} \tag{3.11}$$

for any $f \in \mathrm{L}_1(\mathbb{R})$.

Remark 3.10. *Note that combining Theorem 3.9 with Theorem 3.5 for sufficiently smooth wavelet bases, one obtains that $\mathrm{H}^s(\mathbb{R}) = \mathrm{B}^s_{2,2}(\mathbb{R})$ for any $s > 0$.*

Remark 3.11. *The Besov regularity requirements on φ in Theorem 3.9 are satisfied in particular if $\varphi \in \mathrm{H}^\tau(\mathbb{R})$ for a $\tau \geq t + \frac{1}{2} - \frac{1}{p}$, since then one has the imbedding $\mathrm{H}^\tau(\mathbb{R}) = \mathrm{B}^\tau_{2,2} \hookrightarrow \mathrm{B}^t_{p,p}$, cf. [29, Corollary 3.7.1].*

For a wavelet basis $\Gamma = \{\psi_\nu\}_{\nu\in\nabla}$ as in Theorem 3.9, using (3.11) it can be shown (cf. [42] and [29, Theorem 4.3.3]) that for each $s > 0$ we have

$$\mathrm{B}^s_{p,p}(\mathbb{R}) = \mathcal{A}^s_p(\mathrm{L}_2(\mathbb{R}))\,, \quad p^{-1} = s + \frac{1}{2}\,, \tag{3.12}$$

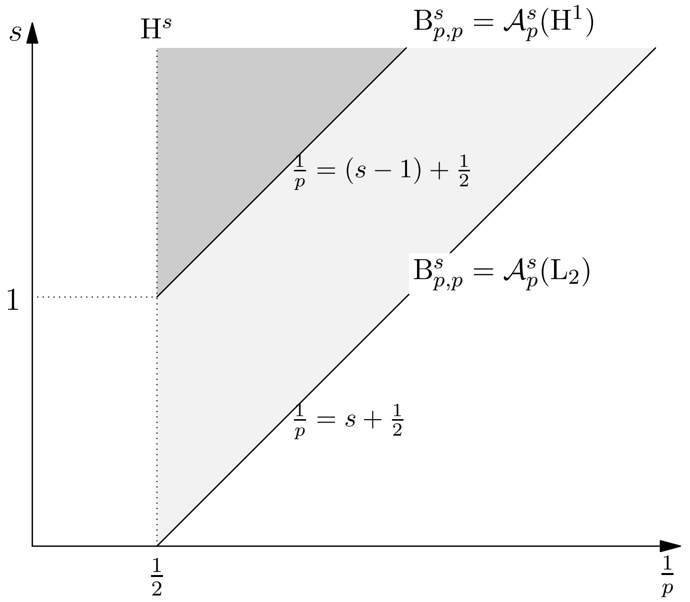

Figure 3.1. Relation of Besov spaces to approximation spaces corresponding to nonlinear approximation in L_2 and H^1 in the one-dimensional case.

and if $s > 1$ then

$$\mathrm{B}^s_{p,p}(\mathbb{R}) = \mathcal{A}^s_p(\mathrm{H}^1(\mathbb{R}))\,, \quad p^{-1} = (s-1) + \frac{1}{2}\,. \tag{3.13}$$

For the particular relations between s and p in (3.12) and (3.13), which imply $p \in (0,\infty)$, the spaces of nonlinear approximation from Definition 3.6 that are relevant in our setting can therefore be identified with Besov spaces. In both cases, for the corresponding spaces of coefficient sequences we have $\mathcal{A}^s_p = \ell_p$ for the respective values of p.

Under the hypotheses of Theorem 3.9 on $\{\psi_\lambda\}$, for $s > 0$ and $p = (s + \frac{1}{2})^{-1}$, as a consequence of (3.11) we obtain that if $u \in \mathrm{B}^s_{p,p}(\mathbb{R})$, then for the wavelet coefficients $u_\lambda := \langle u, \psi_\lambda \rangle$ we have

$$(u_\lambda)_{\lambda\in\nabla} \in \ell_p(\nabla) \subset \mathrm{w}\ell_p(\nabla)\,,$$

and thus $(u_\lambda) \in \mathcal{A}^s_\infty$, or equivalently, $u \in \mathcal{A}^s_\infty(\mathrm{L}_2(\mathbb{R}))$ with respect to the basis $\{\psi_\nu\}_{\nu\in\nabla}$.

Furthermore, if the wavelets are sufficiently regular to ensure that $\{2^{-|\lambda|}\psi_\lambda\}$ is a Riesz basis of $\mathrm{H}^1(\mathbb{R})$, we have that if $u \in \mathrm{B}^s_{p,p}(\mathbb{R})$ with $s > 1$ and $p = ((s-1) + \frac{1}{2})^{-1}$, then (3.11) yields

$$\bigl(2^{|\lambda|} u_\lambda\bigr)_{\lambda\in\nabla} \in \ell_p(\nabla) \subset \mathrm{w}\ell_p(\nabla)$$

and consequently $(2^{|\lambda|}u_\lambda) \in \mathcal{A}^s_\infty$ and $u \in \mathcal{A}^s_\infty(\mathrm{H}^1(\mathbb{R}))$.

The relation between the parameters s and p, juxtaposing the case of linear approximation to nonlinear approximation, is shown in Figure 3.1. The spaces in the shaded region – including the boundaries – are embedded in $\mathrm{L}_2(\mathbb{R})$, those in the darkly shaded region are also embedded in $\mathrm{H}^1(\mathbb{R})$. Whereas the Sobolev spaces $\mathrm{H}^s(\mathbb{R})$ related to linear approximation lie on the left boundaries of these regions, the Besov spaces related to the spaces of nonlinear approximation as discussed above lie on the right boundaries of the respective regions.

3.1.2 Compactly Supported and Orthonormal Wavelet Bases

We now come to a brief overview of concrete wavelets that are relevant for our purposes. The wavelets constructed by Daubechies [37] are L_2–orthonormal, the scaling functions φ are compactly supported, and a φ of this type can be constructed to have any prescribed orders of differentiability and polynomial reproduction, and thus for any prescribed number of vanishing moments of the corresponding wavelet ψ. However, these requirements entail some fairly strong restrictions on such φ. In particular, there exist no closed-form representations for these functions, but they are instead only given as fractals defined by a refinement equation (3.2).

Since the smoothness of the wavelets is a limiting factor in the compression of certain relevant operators, in our setting a variant of Daubechies wavelets constructed by Ojanen [119] is of interest. These wavelets are orthonormal as well, but trade some fixed number of vanishing moments for higher Sobolev regularity.

For numerical purposes, spline wavelets are in general preferable to such fractal functions. This concerns especially the computation of integrals and the compression of matrices based on vanishing moment properties, which will both be discussed in more detail in Chapter 6.

Although there exist no orthonormal wavelets that are piecewise polynomial, compactly supported, and sufficiently regular, basis functions that have these properties simultaneously have been constructed Donovan, Geronimo and Hardin in the framework of *multiwavelets* [45, 46].

In the case of multiwavelets, a multiresolution analysis is generated by a family of several different scaling functions and wavelets. An orthonormal basis for a corresponding space V_0 is given by the integer translates of a family of scaling functions

$$\varphi_{[\ell]}\,, \quad \ell = 1, \ldots, L\,,$$

for some $L > 1$, and the complements W_0 are spanned by the integer translates of L different wavelet functions $\psi_{[\ell]}$. Defining as before

$$\psi_{[\ell],\nu} := 2^{|\nu|/2} \begin{cases} \varphi_{[\ell]}(2^{|\nu|}\cdot - \mathrm{k}(\nu))\,, & \mathrm{s}(\nu) = 0\,, \\ \psi_{[\ell]}(2^{|\nu|}\cdot - \mathrm{k}(\nu))\,, & \mathrm{s}(\nu) = 1\,, \end{cases}$$

with the index set ∇ defined as above, the set of functions

$$\left\{\psi_{[\ell],\nu} \colon \nu \in \nabla\,,\ \ell = 1, \ldots, L\right\}$$

then yields an orthonormal basis of $\mathrm{L}_2(\mathbb{R})$. Although we restrict our considerations in this work to wavelet bases to simplify notation, all results equally apply to multiwavelets as well.

Implications of the choice of wavelet bases in our context, and in particular the advantages and disadvantages of Daubechies wavelets and Donovan-Geronimo-Hardin multiwavelets, are discussed in more detail in Section 6.1.

3.2 Tensor Product Hilbert Spaces

In this section, we collect some standard properties of tensor products of Hilbert spaces for later reference. For a detailed treatment of the formal definition of such tensor products and of tensor product operators, we refer to [108, 149, 124], and restrict ourselves here to a recapitulation of the most important properties.

One of several possible equivalent ways of defining the tensor product of two Hilbert spaces proceeds as follows. For given Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2$, one first defines an algebraic tensor product as the set of expressions

$$\sum_{i=1}^{n} v_i \otimes w_i\,, \quad n \in \mathbb{N},\ v_i \in \mathcal{H}_1,\ w_i \in \mathcal{H}_2\,, \tag{3.14}$$

that is, of sums of elementary tensor products, endowed with the following equivalence relation: $\sum_{i=1}^{n} v_i \otimes w_i$ is equivalent to $\sum_{i=1}^{n} \tilde{v}_i \otimes \tilde{w}_i$, with $v_i, \tilde{v}_i \in \mathcal{H}_1$ and $w_i, \tilde{w}_i \in \mathcal{H}_2$, if and only if the bilinear form

$$\sum_{i=1}^{n}\big(\langle v_i,\cdot\rangle_{\mathcal{H}_1}\langle w_i,\cdot\rangle_{\mathcal{H}_2} - \langle \tilde v_i,\cdot\rangle_{\mathcal{H}_1}\langle \tilde w_i,\cdot\rangle_{\mathcal{H}_2}\big)$$

vanishes identically. The tensor product Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ is subsequently defined as the closure of these equivalence classes of expressions (3.14) in the norm induced by the inner product

$$\langle v_1 \otimes v_2, w_1 \otimes w_2\rangle_{\mathcal{H}_1\otimes\mathcal{H}_2} := \langle v_1, w_1\rangle_{\mathcal{H}_1}\langle v_2, w_2\rangle_{\mathcal{H}_2}\,.$$

If $\mathcal{G}_1, \mathcal{G}_2$ are Hilbert spaces and $A\colon \mathcal{H}_1 \to \mathcal{G}_1$ and $B\colon \mathcal{H}_2 \to \mathcal{G}_2$ are bounded operators, then $A\otimes B$ is defined for sums of elementary tensor products (3.14) by

$$(A \otimes B)\sum_{i=1}^{n} v_i \otimes w_i = \sum_{i=1}^{n}(Av_i) \otimes (Bw_i)\,,$$

and uniquely extended to a bounded operator on $\mathcal{H}_1 \otimes \mathcal{H}_2$ by linearity and continuity.

Theorem 3.12. *Let $\mathcal{H}_1, \mathcal{H}_2$ and $\mathcal{G}_1, \mathcal{G}_2$ be separable Hilbert spaces and let $A_1\colon \mathcal{H}_1 \to \mathcal{G}_1$, $A_2\colon \mathcal{H}_2 \to \mathcal{G}_2$ be bounded linear operators. Then $A_1 \otimes A_2\colon \mathcal{H}_1 \otimes \mathcal{H}_2 \to \mathcal{G}_1 \otimes \mathcal{G}_2$ is a bounded linear operator with*

$$\|A_1 \otimes A_2\|_{\mathcal{H}_1\otimes\mathcal{H}_2\to\mathcal{G}_1\otimes\mathcal{G}_2} = \|A_1\|_{\mathcal{H}_1\to\mathcal{G}_1}\|A_2\|_{\mathcal{H}_2\to\mathcal{G}_2}\,. \tag{3.15}$$

If in addition A_1 and A_2 are isomorphisms, then $A_1\otimes A_2$ is an isomorphism with inverse $A_1^{-1}\otimes A_2^{-1}$.

Proof. See [108, Lemma 1.30] and [131, Lemma B.1]. □

Theorem 3.13. *For $n_1, n_2 \in \mathbb{N}$, we have $\ell_2(\mathbb{N}^{n_1+n_2}) = \ell_2(\mathbb{N}^{n_1})\otimes\ell_2(\mathbb{N}^{n_2})$, as well as $\mathrm{L}_2(\mathbb{R}^{n_1+n_2}) = \mathrm{L}_2(\mathbb{R}^{n_1}) \otimes \mathrm{L}_2(\mathbb{R}^{n_2})$.*

Proof. See [108, Theorem 1.39]. □

Theorem 3.14. *Let $\mathcal{H}_1, \mathcal{H}_2$ be separable Hilbert spaces, let $\{e^{(1)}_i\}_{i\in\mathbb{N}}$ be a Riesz basis for $\mathcal{H}_1$ with constants $C_1 \geq c_1 > 0$, and let $\{e^{(2)}_i\}_{i\in\mathbb{N}}$ be a Riesz basis for $\mathcal{H}_2$ with constants $C_2 \geq c_2 > 0$. Then $\{e^{(1)}_i \otimes e^{(2)}_j\}_{(i,j)\in\mathbb{N}^2}$ is a Riesz basis of $\mathcal{H}_1 \otimes \mathcal{H}_2$ with constants $C_1C_2 \geq c_1c_2 > 0$.*

Note that in particular, if $\{e^{(1)}_i\}_{i\in\mathbb{N}}$, $\{e^{(2)}_i\}_{i\in\mathbb{N}}$ are orthonormal bases of $\mathcal{H}_1$ and $\mathcal{H}_2$, then $\{e^{(1)}_i \otimes e^{(2)}_j\}_{(i,j)\in\mathbb{N}^2}$ is an orthonormal basis as well.

Proof. This can be obtained, for instance, by applying Theorem 3.12 to the corresponding Riesz isomorphisms. For a direct argument in the orthonormal case, see also [149, Theorem 3.12]. □

Unlike ℓ_2– and L_2–spaces, the Sobolev spaces H^s cannot be characterized as tensor products. From the definition of Sobolev norms in terms of the Fourier transform as in (3.24), however, one immediately obtains the following characterization of higher-dimensional Sobolev spaces as intersections of tensor product spaces. The result, which will be used in several places later, is shown in a similar form in [154], see also [69, 68] for the case of bounded domains.

Lemma 3.15. *Let $s > 0$, $n_i \in \mathbb{N}$ for $i = 1, \ldots, k$. Then*

$$\begin{aligned}\mathrm{H}^s(\mathbb{R}^{\sum_i n_i}) = \mathrm{H}^s(\mathbb{R}^{n_1}) \otimes \mathrm{L}_2(\mathbb{R}^{\sum_{i>1} n_i}) \;\cap\; \ldots\\ \cap\; \mathrm{L}_2(\mathbb{R}^{\sum_{i<j} n_i}) \otimes \mathrm{H}^s(\mathbb{R}^{n_j}) \otimes \mathrm{L}_2(\mathbb{R}^{\sum_{i>j} n_i}) \;\cap\; \ldots \;\cap\; \mathrm{L}_2(\mathbb{R}^{\sum_{i<k} n_i}) \otimes \mathrm{H}^s(\mathbb{R}^{n_k})\,.\end{aligned} \tag{3.16}$$

Proof. Let $N := \sum_i n_i$. Denoting the space on the right hand side of (3.16) by X, the canonical choice of norm for the intersection is given by

$$\|u\|_X^2 = \max_i \int_{\mathbb{R}^{n_1}\times\cdots\times\mathbb{R}^{n_k}} (1 + |\xi_i|^2)^s|\hat u|^2\,\mathrm{d}\xi\,, \quad \xi = (\xi_1, \ldots, \xi_k)\,.$$

On the one hand,

$$\|u\|_X^2 \geq k^{-1} \int_{\mathbb{R}^N} \sum_i \bigl(1+|\xi_i|^2\bigr)^s |\hat{u}|^2 \,\mathrm{d}\xi \geq k^{-1} k^{-(s-1)_+} \int_{\mathbb{R}^N} \Bigl(k + \sum_i |\xi_i|^2\Bigr)^s |\hat{u}|^2 \,\mathrm{d}\xi$$
$$\geq k^{-1-(s-1)_+} \|u\|^2_{\mathrm{H}^s(\mathbb{R}^N)}\,,$$

and on the other hand

$$\|u\|_X^2 \leq \int_{\mathbb{R}^N} \bigl(1+\max_i |\xi_i|^2\bigr)^s |\hat{u}|^2 \,\mathrm{d}\xi \leq \|u\|^2_{\mathrm{H}^s(\mathbb{R}^N)}\,. \qquad \square$$

We will also implicitly use tensor products of Banach and quasi-Banach spaces that arise in the characterization of approximation spaces corresponding to nonlinear approximation by tensor product bases, see Section 3.4. We refer to [116, 131] for further details on the construction of such tensor product spaces.

3.3 Tensor Product Wavelet Bases

The higher-dimensional wavelets we shall consider here are tensor products of lower-dimensional basis functions. This separable structure plays an important role in the following chapters.

A first approach to the construction of wavelets in higher dimensions yields bases that again fit into the multiresolution analysis framework of Definition 3.2. For dimensions $d \geq 1$, we define the index sets

$$\nabla^{(d)} := \bigl\{(j_0, k, 0)\bigr\} \cup \bigl\{(j,k,s)\colon j \geq j_0, s \in \{0,1\}^d \setminus \{0\}\bigr\} \subset \mathbb{Z} \times \mathbb{Z}^d \times \{0,1\}^d \tag{3.17}$$

and assign, analogously to the one-dimensional case, to each $\lambda \in \nabla^{(d)}$ a level $|\lambda| \in \mathbb{Z}$, a vector of translation indices $\mathrm{k}(\lambda) \in \mathbb{Z}^d$, and a binary vector $\mathrm{s}(\lambda) \in \{0,1\}^d$ encoding a choice of scaling function or wavelet for each coordinate direction. We define corresponding tensor product basis functions by

$$\Psi_\lambda := \bigotimes_{i=1}^d \psi_{|\lambda|, \mathrm{k}_i(\lambda), \mathrm{s}_i(\lambda)}\,, \quad \lambda \in \nabla^{(d)}\,. \tag{3.18}$$

Note that $\nabla^{(1)} = \nabla$ and $\Psi_\lambda = \psi_\lambda$ for $\lambda \in \nabla^{(1)}$. The basis functions have isotropic supports, that is, $\operatorname{diam}(\operatorname{supp}\Psi_\lambda) \sim 2^{-|\lambda|}$ and $|\operatorname{supp}\Psi_\lambda| \sim 2^{-d|\lambda|}$.

The resulting higher-dimensional wavelet bases $\{\Psi_\lambda\}_{\lambda\in\nabla^{(d)}}$ again yield characterizations of relevant function spaces in terms of wavelet coefficients. In particular, if $\{\psi_\lambda\}_{\lambda\in\nabla}$ is an orthonormal basis of $\mathrm{L}_2(\mathbb{R})$, then $\{\Psi_\lambda\}_{\lambda\in\nabla^{(d)}}$ is an orthonormal basis of $\mathrm{L}_2(\mathbb{R}^d)$. Furthermore, if $\{2^{-s|\lambda|}\psi_\lambda\}_{\lambda\in\nabla}$ is a Riesz basis of $\mathrm{H}^s(\mathbb{R})$ for $-\tau < s < \tau$ for some $\tau > 0$, then for any $d \in \mathbb{N}$, we also have that $\{2^{-s|\lambda|}\Psi_\lambda\}_{\lambda\in\nabla^{(d)}}$ is a Riesz basis of $\mathrm{H}^s(\mathbb{R}^d)$ for these values of s.

For later reference, we define the auxiliary notation

$$\chi_d(\mu,\nu) := \begin{cases} 1\,, & \operatorname{supp}\Psi_\mu \cap \operatorname{supp}\Psi_\nu \neq \emptyset\,,\\ 0\,, & \text{otherwise.}\end{cases} \tag{3.19}$$

Furthermore, for $j \in \mathbb{Z}_{j_0}$, we denote the set of basis indices of level j by

$$\nabla^{(d)}_j := \{\lambda \in \nabla^{(d)}\colon\ |\lambda| = j\}\,. \tag{3.20}$$

In the construction of tensor product wavelets based on (3.17), each basis function is a tensor product of one-dimensional functions. A second approach to constructing wavelets in higher dimensions consists in forming tensor products of entire lower-dimensional wavelet bases.

To give a specific example, for a wavelet basis $\{\psi_\nu\}_{\nu\in\nabla}$ of $\mathrm{L}_2(\mathbb{R})$, it is essentially a consequence of Theorem 3.14 that the tensor product basis $\{\psi_{\nu_1}\otimes\psi_{\nu_2}\}_{(\nu_1,\nu_2)\in\nabla\times\nabla}$ is a wavelet basis for $\mathrm{L}_2(\mathbb{R}^2)$. Here, the basis functions are not assigned a unique level as in the construction of (3.17), (3.18), but may belong to different levels in each coordinate direction, which also means that these basis functions in general have anisotropic supports. As we shall see, they differ in their approximation properties quite substantially from the two-dimensional wavelets with isotropic support Ψ_ν, $\nu\in\nabla^{(2)}$, defined above.

Keeping in mind the aim of constructing basis functions for the approximation of n-electron wave functions, which are functions on $\mathbb{R}^{3n}$, there are two options that are of interest in our context: from the physical point of view, a natural approach are n-fold tensor products of single-electron basis functions from $\nabla^{(3)}$, indexed by $(\nabla^{(3)})^n$; for our purposes, however, the second option of $3n$-fold tensor products of univariate wavelet bases, indexed by ∇^{3n}, will turn out to be more appropriate. The first choice will also be referred to as a partially anisotropic, the second choice as a fully anisotropic tensor product basis. We shall consider both as special cases of index sets $(\nabla^{(d)})^D$ with $d,D\in\mathbb{N}$, where the above two cases correspond to $d=3$, $D=n$ and $d=1$, $D=3n$, respectively.

We define a class of tensor product wavelets on $\mathbb{R}^{dD}$ with anisotropic support comprising both cases by

$$\Psi_\lambda := \bigotimes_{i=1}^{D} \Psi_{\lambda_i}\,,\qquad \lambda=(\lambda_1,\dots,\lambda_D)\in(\nabla^{(d)})^D\,.$$

For $\lambda\in(\nabla^{(d)})^D$, we define $|\lambda|:=(|\lambda_1|,\dots,|\lambda_D|)$, and similarly $\mathrm{k}(\lambda)=(\mathrm{k}(\lambda_1),\dots,\mathrm{k}(\lambda_D))\in(\mathbb{Z}^d)^D$ and $\mathrm{s}(\lambda)=(\mathrm{s}(\lambda_1),\dots,\mathrm{s}(\lambda_D))$. For $j\in\mathbb{Z}^D_{j_0}$, analogously to (3.20) we introduce the notation

$$(\nabla^{(d)})^D_j := \bigl\{\nu\in(\nabla^{(d)})^D\colon |\nu|=(|\nu_1|,\dots,|\nu_D|)=(j_1,\dots,j_D)\bigr\}\,.$$

In addition, for $\nu\in(\nabla^{(d)})^D$ we shall use the abbreviations

$$\max|\nu| := \max_{i=1,\dots,D}|\nu_i|\,,\quad \min|\nu| := \min_{i=1,\dots,D}|\nu_i|\,. \tag{3.21}$$

Remark 3.16. *If the compactly supported,* L_2*–orthonormal scaling function* φ *satisfies* $\varphi\in\mathrm{H}^\tau(\mathbb{R})$ *for some* $\tau>0$*, with [29, Theorem 3.7.7] and Lemma 3.15 (see also [69, 68]) it follows similarly to Theorem 3.5 that*

$$\Bigl\{\Bigl(\sum_{i=1}^{D}2^{2s|\lambda_i|}\Bigr)^{-\frac12}\Psi_\lambda\Bigr\}_{\lambda\in(\nabla^{(d)})^D}\qquad \textit{and}\qquad \bigl\{2^{-s\max|\lambda|}\Psi_\lambda\bigr\}_{\lambda\in(\nabla^{(d)})^D}$$

are both Riesz bases of $\mathrm{H}^s(\mathbb{R}^{dD})$ *for* $-\tau<s<\tau$*. Note that the constants in the corresponding norm equivalences depend on the choice of scaling function level* j_0 *of the wavelet basis.*

Remark 3.17. *The case* $s=1$ *in Remark 3.16 is of central importance for our purposes. The Riesz basis property can be obtained for general biorthogonal wavelets. However, as shown in [44], the corresponding condition number is independent of* D *if and only if the underlying univariate wavelet basis* $\{\psi_\nu\}_{\nu\in\nabla}$ *is* L_2*–orthonormal, and grows exponentially in* D *otherwise. This is the main motivation for our restriction to orthonormal wavelets.*

For sufficiently regular L_2*–orthonormal wavelets, we thus have the norm equivalences*

$$c\sum_{\lambda\in(\nabla^{(d)})^D}\Bigl(\sum_{i=1}^{D}2^{2|\lambda_i|}\Bigr)|\langle u,\Psi_\lambda\rangle|^2 \le \|u\|_1^2 \le C\sum_{\lambda\in(\nabla^{(d)})^D}\Bigl(\sum_{i=1}^{D}2^{2|\lambda_i|}\Bigr)|\langle u,\Psi_\lambda\rangle|^2 \tag{3.22}$$

as well as

$$\hat{c} \sum_{\lambda\in(\nabla^{(d)})^D} 2^{2\max|\lambda|} |\langle u, \Psi_\lambda\rangle|^2 \leq \|u\|_1^2 \leq \hat{C} D \sum_{\lambda\in(\nabla^{(d)})^D} 2^{2\max|\lambda|} |\langle u, \Psi_\lambda\rangle|^2 \,, \tag{3.23}$$

where $c, C > 0$ *and* $\hat{c}, \hat{C} > 0$ *are* independent of D.

3.4 Approximation by Tensor Product Wavelets

For the isotropically supported higher-dimensional wavelets $\{\Psi_\lambda \colon \lambda \in \nabla^{(d)}\}$, one obtains estimates for linear approximation that are completely analogous to (3.9). Let $u \in \mathrm{H}^s(\mathbb{R}^d)$ for $s > 0$, and let the underlying scaling function $\varphi \in \mathrm{H}^t(\mathbb{R})$ satisfy the polynomial reproduction property of order $m-1$. Then for $0 < t < s \leq m$, we have the direct estimate

$$\inf_{u_j \in \operatorname{span}\{\Psi_\lambda \colon \lambda\in\nabla^{(d)}\,,\ |\lambda|\leq j\}} \|u_j - u\|_{\mathrm{H}^t(\mathbb{R}^d)} \lesssim 2^{-(s-t)j} |u|_{\mathrm{H}^s(\mathbb{R}^d)} \,.$$

To obtain an approximation to u, we additionally need to take spatial decay properties of u into account. For this discussion, let us assume for the sake of simplicity that u is compactly supported, then with the notation $\Lambda_u := \{\nu \in \nabla^{(d)} \colon \langle u, \Psi_\nu\rangle \neq 0\}$ we obtain

$$\#\bigl(\{\lambda \in \nabla^{(d)} \colon |\lambda| \leq j\} \cap \Lambda_u\bigr) \;\sim\; \#\bigl(\{\lambda \in \nabla^{(d)} \colon |\lambda| \leq j\} \cap \Lambda_u\bigr) \;\sim\; 2^{dj} \,,$$

where the constants depend on the wavelet bases and on $|\operatorname{supp} u|$. In terms of the number N of nonzero coefficients of u_j, we thus obtain the estimate

$$\|u_j - u\|_{\mathrm{H}^t(\mathbb{R}^d)} \lesssim N^{-\frac{s-t}{d}} \,,$$

or conversely, the number of coefficients required for an approximation error ε is proportional to $\varepsilon^{-\frac{d}{s-t}}$.

In this setting, a reduction of the approximation error by a prescribed factor requires a growth of the number of coefficients by a factor increasing exponentially with d. We shall briefly review a construction that addresses this problem based on dimension-dependent regularity information, or more specificially, on integrability of high-order mixed derivatives.

To this end, we introduce certain standard Sobolev spaces of dominating mixed derivatives. For $s, k > 0$ and $d, D \in \mathbb{N}$, we define the Sobolev space $\mathrm{H}^{s,k}_{\mathrm{mix}}(\mathbb{R}^d; D)$ to comprise those $f \in \mathrm{L}_2(\mathbb{R}^{dD})$ for which

$$\bigl\| f \,|\, \mathrm{H}^{s,k}_{\mathrm{mix}}(\mathbb{R}^d; D)\bigr\|^2 := \int_{\mathbb{R}^{dD}} \Bigl(1 + \prod_i |\xi_i|^{2s}\Bigr)\Bigl(1 + \sum_i |\xi_i|^2\Bigr)^k |\hat{f}|^2 \,\mathrm{d}(\xi_1, \dots, \xi_n) < \infty \,, \tag{3.24}$$

where $\xi_i \in \mathbb{R}^d$, $i = 1, \dots, D$. In other words, these are the functions for which the mixed derivative of order s, in the meaning of taking s derivatives for each x_i, is in $\mathrm{H}^k(\mathbb{R}^{dD})$. In what follows, we shall use the abbreviation $\|\cdot\|_{s,k}$ for the norm on $\mathrm{H}^{s,k}_{\mathrm{mix}}(\mathbb{R}^d; D)$.

For the spaces $\mathrm{H}^{s,k}_{\mathrm{mix}}(\mathbb{R}^d; D)$, provided that $\varphi \in \mathrm{H}^\tau(\mathbb{R})$, similarly to Remark 3.16, for $0 < s < \tau - k$ we have norm equivalences for fully and partially anisotropic tensor product wavelet bases,

$$\begin{aligned} \|u\|_{s,k}^2 &\sim \sum_{\lambda\in(\nabla^{(d)})^D} \Bigl(2^{2s\sum_{i=1}^D |\lambda_i|} \sum_{i=1}^D 2^{2k|\lambda_i|}\Bigr) |\langle u, \Psi_\lambda\rangle|^2 \\ &\sim \sum_{\lambda\in\nabla^{dD}} \Bigl(\prod_{i=0}^{D-1} \sum_{j=1}^d 2^{2s|\lambda_{di+j}|}\Bigr)\Bigl(\sum_{i=1}^{dD} 2^{2k|\lambda_i|}\Bigr) |\langle u, \Psi_\lambda\rangle|^2 \,. \end{aligned} \tag{3.25}$$

Proofs are given in [154], see also [68, 44] for the case of bounded domains.

The norm equivalences (3.25) give an indication of the relevance of such Sobolev spaces of mixed smoothness for higher-dimensional approximation. The coefficients with respect to anisotropic tensor product bases of functions with this type of regularity have a certain decay that can be exploited for the construction of so-called *sparse grid* approximations. This approach has its origins in higher-dimensional quadrature [133] and was later applied in the discretization of partial differential equations [158]; see also [21] for a review. In the context of wavelet approximation, one also finds the term *hyperbolic wavelets* [43].

In order to illustrate the idea by a simple example, we consider approximation by tensor product wavelets in $\mathrm{H}^1(\mathbb{R}^D)$. Defining for $j \in \mathbb{Z}$ the sparse grid or hyperbolic wavelet subspace

$$\hat{\Lambda}_j := \Bigl\{ \nu \in \nabla^D \colon \sum_{i=1}^{D} |\nu_i| \leq j \Bigr\}, \tag{3.26}$$

and assuming that (3.25) holds for the considered wavelet basis $\{\Psi_\nu\}_{\nabla^D}$, for $u \in \mathrm{H}^{s,1}_{\mathrm{mix}}(\mathbb{R}; D)$ we obtain

$$\inf_{u_j \in \operatorname{span}\{\Psi_\lambda\}_{\lambda \in \hat{\Lambda}_j}} \|u_j - u\|_{\mathrm{H}^1(\mathbb{R}^D)} \lesssim \biggl(\sum_{|\lambda_1| + \ldots + |\lambda_D| > j} \Bigl(\sum_{i=1}^{D} 2^{2|\lambda_i|} \Bigr) |\langle u, \Psi_\lambda \rangle|^2 \biggr)^{\frac{1}{2}} \lesssim 2^{-sj} \|u\|_{\mathrm{H}^{s,1}_{\mathrm{mix}}(\mathbb{R};D)} \,.$$

In combination with suitable decay properties of u, this enables the construction of approximations u_j for which the scaling of the number of unknowns with respect to j for a given accuracy is very close to the one-dimensional case. To give a specific example, let in addition u be compactly supported, and let $\Lambda_u := \{\nu \in \nabla^D \colon \langle u, \Psi_\nu \rangle \neq 0\}$, then one obtains

$$\#(\hat{\Lambda}_j \cap \Lambda_u) \sim j^{D-1} 2^j \,.$$

Thus one obtains an almost – up to a logarithmic factor – dimension-independent convergence rate. For functions that are not compactly supported but decay exponentially, such as electronic Schrödinger eigenfunctions, approximations of this type will be considered in Section 4.1.1. For certain combinations of mixed regularity and approximation norm, such sparse grid constructions can be modified so as to remove the dimension-dependent logarithmic factor j^{D-1} and to yield a dimension-independent convergence rate, cf. [21].

For Besov spaces in higher dimensions, there exist wavelet characterizations similar to Theorem 3.9. For the further discussion, we need two dimensional parameters $d, D \in \mathbb{N}$, where the total space dimension is dD. For the standard Besov spaces $\mathrm{B}^s_{p,p}(\mathbb{R}^{dD})$, under assumptions similar to those of Theorem 3.9, as a further special case of [29, Theorem 3.7.7] one obtains

$$\|f\|_{\mathrm{B}^s_{p,p}(\mathbb{R}^{dD})} \;\sim\; \Bigl\| \bigl(2^{(s + \frac{dD}{2} - \frac{dD}{p})|\nu|} \langle f, \psi_\nu \rangle \bigr)_{\nu \in \nabla^{(dD)}} \Bigr\|_{\ell_p(\nabla^{(dD)})} \tag{3.27}$$

for a certain range of parameters including the case $p^{-1} = \frac{s-1}{dD} + \frac{1}{2}$. Consequently, $u \in \mathrm{B}^s_{p,p}(\mathbb{R}^{dD})$ implies

$$\bigl(2^{|\nu|} \langle u, \Psi_\nu \rangle \bigr)_{\nu \in \nabla^{(dD)}} \in \mathcal{A}^{s/(dD)}_\infty \,, \quad p^{-1} = \frac{s-1}{dD} + \frac{1}{2} \,,$$

and thus $u \in \mathcal{A}^{s/(dD)}_\infty(\mathrm{H}^1(\mathbb{R}^{dD}))$ with respect to sufficiently regular wavelet bases $\{\Psi_\nu\}_{\nu \in \nabla^{(dD)}}$. In the case of adaptive approximation by such isotropic wavelet bases, we obtain convergence of order $N^{-\frac{s}{dD}}$. The deterioration of the convergence rate with increasing dimension is therefore the same as in the case of Sobolev regularity and uniform refinement. In other words, adaptive approximation with basis functions of isotropic support reduces the regularity requirements for achieving a certain rate in comparison to linear approximation, but does not improve the dependence on space dimension.

The situation is different, however, in the case of nonlinear approximation by *anisotropic* tensor product bases $\{\Psi_\nu\}_{\nu\in(\nabla^{(d)})^D}$. The rates of best N-term approximation by such bases are governed by tensor product Besov spaces, which have been studied in [116, 131, 77].

Here we shall only consider those tensor product Besov spaces relevant for nonlinear approximation in $\mathrm{H}^1(\mathbb{R}^{dD})$, which we denote by $\tilde{\mathrm{B}}^s_p(\mathbb{R}^d;D)$. These spaces can be characterized as intersections of tensor products of lower-dimensional standard Besov spaces,

$$\tilde{\mathrm{B}}^s_p(\mathbb{R}^d;D) = \mathrm{B}^{s+1}_{p,p}(\mathbb{R}^d)\otimes \mathrm{B}^s_{p,p}(\mathbb{R}^d)\otimes\cdots\otimes \mathrm{B}^s_{p,p}(\mathbb{R}^d)\ \cap\ \dots$$
$$\cap\ \mathrm{B}^s_{p,p}(\mathbb{R}^d)\otimes\cdots\otimes \mathrm{B}^s_{p,p}(\mathbb{R}^d)\otimes \mathrm{B}^{s+1}_{p,p}(\mathbb{R}^d)\,,\quad p^{-1}=\frac{s}{d}+\frac{1}{2}\,. \tag{3.28}$$

These spaces thus provide an analogue to the Sobolev spaces $\mathrm{H}^{s,1}_{\mathrm{mix}}(\mathbb{R}^d;D)$. In the case $0<p<1$, (3.28) requires an appropriate notion of tensor product, cf. [116].

It can be shown that for elements of $\tilde{\mathrm{B}}^s_p(\mathbb{R}^d;D)$ one obtains rates $N^{-\frac{s}{d}}$ for best N-term approximation in $\mathrm{H}^1(\mathbb{R}^{dD})$ by the tensor product basis $\{\Psi_\nu\}_{\nu\in(\nabla^{(d)})^D}$, that is, a convergence rate independent of D.

We shall later use the families of spaces $\tilde{\mathrm{B}}^s_p(\mathbb{R};2)$ with $p=(s+\frac12)^{-1}$ and $\tilde{\mathrm{B}}^s_p(\mathbb{R}^3;2)$ with $p=(\frac{s}{3}+\frac12)^{-1}$, for which – again assuming the tensor product basis is constructed from a sufficiently regular univariate wavelet – one obtains the following norm equivalences analogous to (3.11), (3.27).

Proposition 3.18. *Let φ be a compactly supported, continuous, and L_2–orthonormal scaling function of a multiresolution analysis, let $\{\psi_\nu\}_{\nu\in\nabla}$ be a corresponding wavelet basis, and let $s>0$. Let $\varphi\in\mathrm{B}^t_{p,p}$ for a $t>s+1$, and let ψ have at least $\lfloor s+1\rfloor+1$ vanishing moments.*

(i) Let $p=(s+\frac12)^{-1}$, then for $u\in\tilde{\mathrm{B}}^s_p(\mathbb{R};2)$,

$$\|u\|_{\tilde{\mathrm{B}}^s_p(\mathbb{R};2)}\sim\big\|(2^{\max|\nu|}\langle u,\Psi_\nu\rangle)_{\nu\in\nabla^2}\big\|_{\ell_p}\,, \tag{3.29}$$

and thus $\tilde{\mathrm{B}}^s_p(\mathbb{R};2)\subset\mathcal{A}^s_\infty(\mathrm{H}^1(\mathbb{R}^2))$ with respect to the tensor product basis $\{\Psi_\nu\}_{\nu\in\nabla^2}$.

(ii) Let $p=(\frac{s}{3}+\frac12)^{-1}$, then for $u\in\tilde{\mathrm{B}}^s_p(\mathbb{R}^3;2)$,

$$\|u\|_{\tilde{\mathrm{B}}^s_p(\mathbb{R}^3;2)}\sim\big\|(2^{\max|\nu|}\langle u,\Psi_\nu\rangle)_{\nu\in(\nabla^{(3)})^2}\big\|_{\ell_p}\,, \tag{3.30}$$

and hence $\tilde{\mathrm{B}}^s_p(\mathbb{R}^3;2)\subset\mathcal{A}^{s/3}_\infty(\mathrm{H}^1(\mathbb{R}^6))$ with respect to the tensor product basis $\{\Psi_\nu\}_{\nu\in(\nabla^{(3)})^2}$.

For details, we refer to [147, 116, 131]; note that the particular norm equivalence (3.30) also plays a central role in [51].

Whereas the standard Besov spaces $\mathrm{B}^s_{p,p}$ are invariant under coordinate rotations, this is not the case for the tensor product spaces $\tilde{\mathrm{B}}^s_p$. In other words, the measure of regularity that governs the approximation rates achievable by anisotropic tensor product wavelets depends on the choice of coordinates.

Note that even if a dimension-independent *convergence rate* can be achieved in certain cases, by the constructions outlined above one generally does not obtain dimension-independent *complexity*: even if the convergence rate remains unchanged, the constants in the estimates can blow up with increasing dimension. This problem actually does arise in basic examples of the adaptive solution of constant-coefficient elliptic partial differential equations on higher-dimensional product domains, cf. [44]. It is therefore to be expected that in order to keep the complexity of approximations in higher dimensions in check, it will in general be necessary to exploit further structural properties of the concrete problem at hand. In Section 4.3 we study examples where such problem-specific structure – here, approximability by separable functions – can be used to reduce the approximation complexity.

3.5 Wavelet Representation of Operators

The approximations of wave functions by wavelet expansions in which we shall eventually be interested are not given explicitly, but need to be found as approximate solutions of eigenvalue problems for the corresponding Hamiltonian operators.

We have seen that under certain conditions on a wavelet basis, wavelet approximations to a given function can be found by solving simpler approximation problems in sequence spaces for the corresponding wavelet coefficients. A similar strategy can be followed for solving operator equations on Hilbert spaces. Using Riesz bases for these Hilbert spaces, the original problems can be reformulated as infinite matrix equations on ℓ_2–spaces. Some basic facts are summarized in the following proposition. For a proof, we refer to [34].

Proposition 3.19. *Let $\mathcal{H}$ be a Hilbert space and let $\{\gamma_\nu\}_{\nu\in\mathcal{I}}$ be a Riesz basis of $\mathcal{H}$ with bounds $C_\Gamma \geq c_\gamma > 0$.*

(a) If $A\colon \mathcal{H} \to \mathcal{H}'$ is bounded, then

$$\mathbf{A} := (\langle A\gamma_\mu, \gamma_\nu\rangle)_{\nu,\mu\in\mathcal{I}} \tag{3.31}$$

defines a bounded operator on $\ell_2(\mathcal{I})$ with $\|\mathbf{A}\| \leq C_\Gamma^2\|A\|$.

(b) If in addition A is invertible, then $\mathbf{A}$ is invertible on $\ell_2(\mathcal{I})$ with $\|\mathbf{A}^{-1}\| \leq c_\Gamma^{-2}\|A^{-1}\|$.

(c) If A is $\mathcal{H}$–elliptic, i.e., $\langle Av, v\rangle \geq c_A\|v\|_{\mathcal{H}}^2$ for all $v \in \mathcal{H}$ for a $c_A > 0$, then $\mathbf{A}$ is $\ell_2(\mathcal{I})$–elliptic with $\langle \mathbf{Av}, \mathbf{v}\rangle \geq c_\Gamma^2 c_A\|\mathbf{v}\|_{\ell_2(\mathcal{I})}$ for all $\mathbf{v} \in \ell_2(\mathcal{I})$.

The matrix representation $\mathbf{A}$ in (3.31) of an operator A as in Proposition 3.19 thus inherits the boundedness, invertibility, and ellipticity properties of A, where the respective constants depend only on A and on the bounds of the Riesz basis.

We shall consider second-order differential operators $A\colon \mathrm{H}^1(\mathbb{R}^d) \to \mathrm{H}^{-1}(\mathbb{R}^d)$ in dimension $d \in \mathbb{N}$, and anisotropic tensor product wavelets indexed by ∇^d. Recall that if $\{\psi_\nu\}_{\nu\in\nabla}$ is a sufficiently regular orthonormal wavelet basis of $\mathrm{L}_2(\mathbb{R})$, as a consequence of (3.22) we obtain that $\{\bar{\Psi}_\nu\}_{\nu\in\nabla^d}$ with

$$\bar{\Psi}_\nu := \left(2^{2|\nu_1|} + \ldots + 2^{2|\nu_d|}\right)^{-\frac{1}{2}}\Psi_\nu\,, \quad \nu \in \nabla^d \tag{3.32}$$

is a Riesz basis of $\mathrm{H}^1(\mathbb{R}^d)$. As noted in Remark 3.17, as a consequence of the orthonormality of the underlying univariate wavelets, the condition number of this Riesz basis is then bounded uniformly with respect to the space dimension d.

For an operator equation $Au = f$ with $f \in \mathrm{H}^{-1}(\mathbb{R}^d)$ for $u \in \mathrm{H}^1(\mathbb{R}^d)$, we obtain the equivalent infinite linear system $\mathbf{Au} = \mathbf{f}$ with

$$\mathbf{A} = \big(\langle A\bar{\Psi}_\mu, \bar{\Psi}_\nu\rangle\big)_{\nu,\mu\in\nabla^d}\,, \quad \mathbf{f} = \big(\langle f, \bar{\Psi}_\nu\rangle\big)_{\nu\in\nabla^d}$$

for the coefficient vector of the solution u,

$$\mathbf{u} = \big(\langle u, \bar{\Psi}_\nu\rangle\big)_{\nu\in\nabla^d} = \big((2^{2|\nu_1|} + \ldots + 2^{2|\nu_d|})^{\frac{1}{2}}\langle u, \Psi_\nu\rangle\big)_{\nu\in\nabla^d} \in \ell_2(\nabla^d)\,.$$

The eigenvalue problem for A in weak formulation becomes

$$\mathbf{Au} = \lambda\mathbf{Mu}\,, \quad \text{where} \quad \mathbf{M} = \big(\langle\bar{\Psi}_\mu, \bar{\Psi}_\nu\rangle\big)_{\nu,\mu\in\nabla^d} = \big((2^{2|\nu_1|} + \ldots + 2^{2|\nu_d|})^{-1}\delta_{\nu,\mu}\big)_{\nu,\mu\in\nabla^d}\,.$$

Note that $\mathbf{M}$ is bounded, but not continuously invertible on $\ell_2(\nabla^d)$.

Wavelet-Galerkin discretizations are the most common way of extracting approximations with finitely many basis coefficients from these infinite systems. Here, one chooses a suitable finite $\Lambda \subset \nabla^d$ and solves the problem

$$(\mathbf{A}|_{\Lambda\times\Lambda})\mathbf{u}_\Lambda = \lambda(\mathbf{M}|_{\Lambda\times\Lambda})\mathbf{u}_\Lambda \tag{3.33}$$

for the Galerkin solution $\mathbf{u}_\Lambda \in \ell_2(\Lambda)$. Solving the (generally large-scale) matrix eigenvalue problem for the finite sections $\mathbf{A}|_{\Lambda\times\Lambda}$, $\mathbf{M}|_{\Lambda\times\Lambda}$ is a problem of numerical linear algebra; for employing iterative solvers, the sole requirement is some means of evaluating the corresponding matrix-vector products.

Recall from the previous section that if index sets Λ are chosen as suitable subsets $\Lambda \subset \hat{\Lambda}_j$, with $\hat{\Lambda}_j = \{\nu \colon \sum_i |\nu_i| \leq j\}$ as in (3.26), and assuming certain mixed regularity properties of the exact solution u, for the approximation of u one can obtain (almost) dimension-independent convergence rates. Discretizations based on such index sets are usually referred to as *sparse grid* discretizations.

Classical sparse grid methods, as reviewed in [21], are typically based on the hierarchical, piecewise linear Faber-Schauder basis, which is not a Riesz basis of H^1. Consequently, preconditioning the resulting linear systems is in general a nontrivial task. In this regard, sufficiently regular wavelet bases are advantageous: As a consequence of Proposition 3.19, for elliptic operators A the condition numbers of sections $\mathbf{A}|_{\Lambda\times\Lambda}$ remain uniformly bounded independently of Λ. Hence in this case, optimal preconditioning in the sense of a discretization-independent condition number can be achieved by a simple rescaling as in (3.32).

Due to the anisotropic support of such tensor product basis functions, one is facing the further problem that even if A is a local operator, the matrices $\mathbf{A}_{\Lambda\times\Lambda}$ are generally not sparse, but almost fully populated. Applying these matrices to vectors at a cost close to $\mathcal{O}(\#\Lambda)$ therefore involves some further complications, but is possible under certain conditions.

For instance, for operators that have a tensor product structure, efficient schemes for applying discretization matrices can be obtained by exploiting this product structure for certain blocks of the matrices corresponding to different combinations of levels, and operating along single dimensions in an appropriate order. For schemes that accomplish this, see [130, 78] and [20, 4]. For a review of different schemes and a unified complexity analysis, see [155].

A further option for computing matrix-vector products efficiently in this setting are operator compression schemes based on the vanishing moment properties of wavelets. We shall consider such methods in the context of inexact application of operators in adaptive schemes, but they are also applicable to sparse grid-type wavelet-Galerkin discretizations [129, 44].

3.6 Adaptive Solvers

A first possible construction of adaptive wavelet schemes, similar in spirit to adaptive finite element methods, is based on solving sequences of Galerkin discretizations on successively refined index sets [30]. A second approach, which we will mainly focus on, are adaptive wavelet schemes based on performing iterative methods for the infinite-dimensional problem approximately, using only finitely supported iterates. This type of method was introduced and analyzed in detail for linear operator equations in [31], and extended to nonlinear operator equations in [32]. An adaptive wavelet method for eigenvalue problems following the same strategy has been studied in [36]. Here, one no longer considers discretizations based on fixed sets of wavelet indices, but the index set is updated dynamically so as to stay sufficiently close to the ideal iterative method on the infinite-dimensional sequence space. We review this second class of methods here as the basis for schemes that additionally take advantage of the low-rank structure of solutions, which will be the subject of Chapter 5.

3.6.1 Iterative Schemes for Linear Operator Equations

We first consider an adaptive method introduced in [31] for linear operator equations $\mathbf{A}\mathbf{u} = \mathbf{f}$, where we assume $\mathbf{A}$ to be bounded and elliptic on ℓ_2 with

$$\langle \mathbf{A}\mathbf{v}, \mathbf{v}\rangle_{\ell_2} \geq c_{\mathbf{A}} \|\mathbf{v}\|_{\ell_2}^2 , \quad \|\mathbf{A}\mathbf{v}\|_{\ell_2} \leq C_{\mathbf{A}} \|\mathbf{v}\|_{\ell_2} ,$$

and $\mathbf{f} \in \ell_2$. The scheme can be regarded as a perturbation of a simple Richardson iteration,

$$\mathbf{v}_{i+1} := \mathbf{v}_i - \alpha(\mathbf{A}\mathbf{v}_i - \mathbf{f})\,, \tag{3.34}$$

which is applicable to both symmetric and nonsymmetric elliptic $\mathbf{A}$, provided that the parameter $\alpha > 0$ is chosen appropriately.

We assume the availability of functions apply and rhs such that for $\eta > 0$ and finitely supported $\mathbf{v}$, we have

$$\|\mathsf{apply}(\mathbf{v};\eta) - \mathbf{A}\mathbf{v}\| \le \eta \tag{3.35}$$

as well as

$$\|\mathsf{rhs}(\eta) - \mathbf{f}\| \le \eta\,, \tag{3.36}$$

where both $\mathsf{apply}(\mathbf{v};\eta)$ and $\mathsf{rhs}(\eta)$ are finitely supported and can be evaluated in a finite number of operations. In addition, for finitely supported $\mathbf{v}$, we assume that $\mathsf{coarsen}(\mathbf{v};\eta)$ produces an approximation to $\mathbf{v}$ such that

$$\|\mathsf{coarsen}(\mathbf{v};\eta) - \mathbf{v}\| \le \eta \tag{3.37}$$

holds.

Algorithm 3.1 $\mathbf{u}_\varepsilon = \mathsf{solve}(\mathbf{A}, \mathbf{f}; \varepsilon)$

```
input   $\alpha > 0$ and $\rho \in (0,1)$ such that $\|\mathrm{I} - \alpha\mathbf{A}\| \le \rho$, and $\theta, \kappa \in (0,1)$.
output  $\mathbf{u}_\varepsilon$ satisfying $\|\mathbf{u}_\varepsilon - \mathbf{u}\| \le \varepsilon$.
$\mathbf{u}_0 := 0$, $\delta := c_{\mathbf{A}}^{-1}\|\mathbf{f}\|$
$i := 0$, $K := \min\{k\colon \rho^k(1 + \alpha k) \le \kappa\theta\}$
while $\theta^i\delta > \varepsilon$
    $\mathbf{w}_0 \leftarrow \mathbf{u}_i$
    repeat
        $\eta_j \leftarrow \rho^{j+1}\theta^i\delta$
        $\mathbf{r}_j \leftarrow \mathsf{apply}(\mathbf{w}_j; \frac{1}{2}\eta_j) - \mathsf{rhs}(\frac{1}{2}\eta_j)$
        $\mathbf{w}_{j+1} \leftarrow \mathbf{w}_j - \alpha\mathbf{r}_j$
        $j \leftarrow j + 1$.
    until $(j \ge K \quad \vee \quad c_{\mathbf{A}}^{-1}\rho\|\mathbf{r}_{j-1}\| + (c_{\mathbf{A}}^{-1}\rho + \alpha)\eta_{j-1} \le \kappa\theta^{i+1}\delta)$
    $\mathbf{u}_{i+1} := \mathsf{coarsen}(\mathbf{w}_j; (1-\kappa)\theta^{i+1}\delta)$
    $i \leftarrow i + 1$
end while
$\mathbf{u}_\varepsilon := \mathbf{u}_i$
```

The adaptive scheme of [31] is given in Algorithm 3.1. We first recapitulate a simple result concerning the convergence of this iteration.

Proposition 3.20 ([31])**.** *Let the step size $\alpha > 0$ in Algorithm 5.5 satisfy $\|\mathrm{I} - \alpha\mathbf{A}\| \le \rho < 1$. Then the intermediate steps $\mathbf{u}_i$ of Algorithm 3.1 satisfy $\|\mathbf{u}_i - \mathbf{u}\| \le \theta^i\delta$, and in particular, for the result $\mathbf{u}_\varepsilon$ we have $\|\mathbf{u}_\varepsilon - \mathbf{u}\| \le \varepsilon$.*

Proof. It suffices to show that for any i, after the termination of the inner loop the error bound

$$\|\mathbf{w}_j - \mathbf{u}\| \le \kappa\theta^{i+1}\delta \tag{3.38}$$

holds. By the choice of α, we have

$$\begin{aligned}\|\mathbf{w}_{j+1} - \mathbf{u}\| &\le \|(\mathrm{I} - \alpha\mathbf{A})(\mathbf{w}_j - \mathbf{u})\| + \alpha\|(\mathbf{A}\mathbf{w}_j - f) - \mathbf{r}_j\| \\ &\le \rho\|\mathbf{w}_j - \mathbf{u}\| + \alpha\eta_j\,,\end{aligned}$$

and recursive application of this estimate yields

$$\|\mathbf{w}_j - \mathbf{u}\| \leq \rho^j \|\mathbf{w}_0 - \mathbf{u}\| + \alpha \sum_{k=0}^{j-1} \rho^{j-1-k} \eta_k \leq \rho^j \bigl(1 + j\alpha\bigr)\theta^i \delta\,.$$

Thus on the one hand, if the inner loop exits with the first condition in line 10, then (3.38) holds by definition of K. On the other hand, if the second condition is met, then (3.38) holds because

$$\|\mathbf{w}_j - \mathbf{u}\| \leq \rho \|\mathbf{w}_{j-1} - \mathbf{u}\| + \alpha\eta_{j-1} \leq \rho c_{\mathbf{A}}^{-1}(\|\mathbf{r}_{j-1}\| + \eta_{j-1}) + \alpha\eta_{j-1} \leq \kappa\theta^{i+1}\delta\,. \qquad \square$$

The following complexity estimate for Algorithm 3.1 shown in [31] states that under certain assumptions on the involved subroutines, and if for the exact solution we have $\mathbf{u} \in \mathcal{A}^s_\infty$, then the computation of an approximation $\mathbf{u}_\varepsilon$ with $\|\mathbf{u} - \mathbf{u}_\varepsilon\| \leq \varepsilon$ requires a number of operations and memory locations proportional to $\varepsilon^{-1/s}$ – that is, of the same order as the number of terms in the best N-term approximation of accuracy ε. Under these conditions, the scheme is thus *asymptotically optimal.*

Theorem 3.21 ([31])**.** *Let $s > 0$, let $\mathbf{u} \in \mathcal{A}^s_\infty$, let $\mathbf{f} \in \mathcal{A}^s_\infty$, and let* (3.36) *hold for* rhs*, where in addition*

$$\|\mathsf{rhs}(\eta)\|_{\mathcal{A}^s_\infty} \lesssim \|\mathbf{f}\|_{\mathcal{A}^s_\infty}\,, \quad \#\operatorname{supp}\mathsf{rhs}(\eta) \lesssim \eta^{-\frac{1}{s}} \|\mathbf{f}\|^{\frac{1}{s}}_{\mathcal{A}^s_\infty}\,.$$

For finitely supported $\mathbf{v}$, let $\mathbf{w}_\eta := \mathsf{apply}(\mathbf{v};\eta)$ satisfy (3.35) *and*

$$\|\mathbf{w}_\eta\|_{\mathcal{A}^s_\infty} \lesssim \|\mathbf{v}\|_{\mathcal{A}^s_\infty}\,, \quad \#\operatorname{supp}\mathbf{w}_\eta \lesssim \eta^{-\frac{1}{s}} \|\mathbf{v}\|^{\frac{1}{s}}_{\mathcal{A}^s_\infty}\,,$$

where the number of arithmetic operations required for the evaluation of $\mathbf{w}_\eta$ is of order

$$\mathcal{O}(\eta^{-1/s}\|\mathbf{v}\|^{1/s}_{\mathcal{A}^s_\infty} + \#\operatorname{supp}\mathbf{v})\,.$$

Let $\mathsf{coarsen}$ *satisfy* (3.37) *and*

$$\#\operatorname{supp}\mathsf{coarsen}(\mathbf{v};\eta) \lesssim \eta^{-\frac{1}{s}} \|\mathbf{v}\|^{\frac{1}{s}}_{\mathcal{A}^s_\infty}\,,$$

requiring $\mathcal{O}(\#\operatorname{supp}\mathbf{v})$ operations. Then Algorithm 3.2 requires $\mathcal{O}(\varepsilon^{-1/s}\|\mathbf{u}\|^{1/s}_{\mathcal{A}^s_\infty})$ operations, with constant dependent on s, but independent of ε and $\mathbf{u}$.

For the proof, see [31]. Note that the requirements on $\mathsf{coarsen}$ are slightly weakened here in that the produced approximation is not required to have minimal support. For further details on this modification of $\mathsf{coarsen}$ suggested in [7, 110], see the discussion of the assumptions of Theorem 3.21 in Subsection 3.6.3.

Remark 3.22. *An alternative would be the mentioned class of adaptive wavelet schemes based on approximately solving a sequence of Galerkin discretizations, as proposed originally in [30]. In [57], it has been shown that such methods do not require a coarsening step for asymptotic optimality if the iteration parameters are chosen appropriately. This type of method has also been applied to Poisson-type high-dimensional problems on product domains in [44], and to problems on unbounded domains in [90]. Such an approach can be quantitatively advantageous compared to methods based on direct iteration as considered in this section. The latter, however, is applicable to a larger class of problems, and will form the basis of our further developments in Chapter 5.*

The broader applicability of Algorithm 3.1 in comparison to adaptive schemes based on Galerkin discretizations concerns in particular the case of nonsymmetric elliptic operators. This is relevant for the explicitly correlated formulation (2.11)*, where due to the compressibility properties of the involved operators (see also Subsection 6.4.3), we need to avoid solving normal equations. Although it has been shown in [56] that under certain conditions, directly treating nonsymmetric problems by*

Galerkin-based adaptive methods as in [30, 57] without passing to the normal equations is possible, this involves a requirement on an initial refinement of the basis that is too expensive in the higher-dimensional case. Algorithm 3.1, however, can be applied to nonsymmetric elliptic problems without further restrictions.

3.6.2 Iterative Schemes for Eigenvalue Problems

We next consider an adaptive method for elliptic eigenvalue problems based on the method introduced in [36]. This scheme is applicable to self-adjoint operators; we shall comment on the case of eigenvalue problems for nonsymmetric operators in Remark 3.28 below.

For this subsection, let $\mathbf{M}$ be an infinite diagonal matrix defining a bounded operator on ℓ_2, and let $\mathbf{A}$ be symmetric as well as bounded and elliptic on ℓ_2. Note that these assumptions correspond to the observations made in Section 3.5. Furthermore, let

$$\lambda(\mathbf{v}) := \frac{\langle \mathbf{A}\mathbf{v}, \mathbf{v}\rangle}{\langle \mathbf{M}\mathbf{v}, \mathbf{v}\rangle}$$

and

$$\lambda_0 = \inf_{\mathbf{v}\neq 0} \lambda(\mathbf{v})\,,$$

where we assume that $V_0 := \ker(\mathbf{A} - \lambda_0\mathbf{M})$ is one-dimensional and $\mathbf{A} - \lambda_0\mathbf{M}$ is elliptic on $V_0^\perp$. Let $\mathbf{u}_0$ be such that $V_0 = \operatorname{span}\{\mathbf{u}_0\}$ and $\|\mathbf{u}_0\| = 1$, and let $\mathbf{P}_0$ be the orthogonal projector onto V_0, that is, $\mathbf{P}_0 = \langle \cdot, \mathbf{u}_0\rangle \mathbf{u}_0$. For $\mathbf{v} \in \ell_2$, we define

$$e_\perp(\mathbf{v}) := (\mathrm{I} - \mathbf{P}_0)(\mathbf{v} - \mathbf{u}_0)\,,$$

which means that if $\|\mathbf{v}\| = 1$, then $\|e_\perp(\mathbf{v})\|$ equals the sine of the angle between V_0 and $\mathbf{v}$. This provides an adequate measure for the error in the eigenfunction. As part (ii) of Lemma 3.23 below shows, this quantity controls the error in the eigenvalue as well.

For finding approximations to λ_0 and to a normalized element of V_0, we consider a basic Richardson-type method,

$$\hat{\mathbf{v}}_{i+1} := \mathbf{v}_i - \alpha\big(\mathbf{A}\mathbf{v}_i - \lambda(\mathbf{v}_i)\mathbf{M}\mathbf{v}_i\big)\,, \quad \mathbf{v}_{i+1} := \frac{\hat{\mathbf{v}}_{i+1}}{\|\hat{\mathbf{v}}_{i+1}\|}\,, \tag{3.39}$$

which amounts to a gradient descent scheme for the Rayleigh quotient, and can also be regarded as a special case of preconditioned inverse iteration. A convergence analysis has been given in [36]. Based on the same arguments, in what follows we obtain a slightly modified analysis with a different choice of iteration parameters.

Lemma 3.23 summarizes some prerequisites for the convergence analysis, following closely the treatment in [36].

Lemma 3.23. *Under the above assumptions on* $\mathbf{A}$ *and* $\mathbf{M}$*, where we set* $\mathbf{R}_0 := \mathbf{A} - \lambda_0\mathbf{M}$*, the following hold:*

(i) *There exists an* $\alpha > 0$ *such that for* $\mathbf{T}_\alpha := \mathrm{I} - \alpha\mathbf{R}_0$ *we have*

$$\|(\mathrm{I} - \mathbf{P}_0)\mathbf{T}_\alpha\| =: \rho < 1\,.$$

(ii) *There exists* $E > 0$ *such that for any* $\mathbf{v} \in \ell_2$*, we have*

$$\lambda(\mathbf{v}) - \lambda_0 \le E\lambda(\mathbf{v})\|e_\perp(\mathbf{v})\|^2\,.$$

In particular, if $\|e_\perp(\mathbf{v})\| \le E^{-1/2}$*, then*

$$\lambda(\mathbf{v}) \le \big(1 - E\|e_\perp(\mathbf{v})\|^2\big)^{-1}\lambda_0\,.$$

(iii) *Let* $C_0 := \|\mathbf{R}_0^{-1}\|_{V_0^\perp \to V_0^\perp}$ *and* $C_1 := \frac{C_0\|\mathbf{M}\|}{2(1+C_0\|\mathbf{M}\|)}$. *Provided that*

$$\|e_\perp(\mathbf{v})\| < \min\bigl\{E^{-1/2}, (1+C_1^2)^{1/2} - C_1\bigr\}\,,$$

with

$$R(\mathbf{v}) := C_0\biggl(1 - \frac{C_0\|\mathbf{M}\|E(1+\|e_\perp(\mathbf{v})\|)\|e_\perp(\mathbf{v})\|}{1 - E\|e_\perp(\mathbf{v})\|^2}\biggr)^{-1} \tag{3.40}$$

we have

$$\|e_\perp(\mathbf{v})\| \le R(\mathbf{v})\,\|(\mathbf{A} - \lambda(\mathbf{v})\mathbf{M})\mathbf{v}\|\,.$$

Proof. See [36], Lemmas 4, 5, and 6; the constants involved in the estimates as given here can be extracted from the corresponding proofs. ☐

The scheme is given in Algorithm 3.2, where we assume the availability of a routine apply as before, and additionally a procedure rayleigh such that for $\mathbf{v} \neq 0$, we have

$$|\mathsf{rayleigh}(\mathbf{v};\eta) - \lambda(\mathbf{v})| \le \eta\,.$$

Note that since $\mathbf{M}$ is assumed to be diagonal, $\mathbf{Mv}$ can be evaluated exactly for any finitely supported $\mathbf{v}$.

Algorithm 3.2 $\mathbf{u}_\varepsilon = \mathsf{evpsolve}(\mathbf{A}, \mathbf{v}_0; \varepsilon)$

input α, ρ, E, C_1 as in Lemma 3.23, and R as in (3.40); $\mathbf{v}_0$ with $\|\mathbf{v}_0\| = 1$ such that $\|e_\perp(\mathbf{v}_0)\| \le \delta$ with δ as in (3.41); $\theta, \kappa \in (0,1)$.

output $\mathbf{u}_\varepsilon$ with $\|\mathbf{u}_\varepsilon\| = 1$ and $\|e_\perp(\mathbf{u}_\varepsilon)\| \le \varepsilon$.

```
$i := 0$, $\varepsilon_0 := \delta$
while $\varepsilon_i > \varepsilon$
    $\mathbf{w}_0 \leftarrow \mathbf{v}_i$
    $\xi_i := \rho + \alpha\|\mathbf{M}\|(1 - E\varepsilon_i^2)^{-1}E\varepsilon_i$
    $\tilde\eta_i := \alpha^{-1}(1+\varepsilon_i)^{-1}\varepsilon_i(1-\xi_i)$
    $\varepsilon_{i+1} := \theta\varepsilon_i$
    $K_i := \min\bigl\{k\colon \bigl(\prod_{l=0}^{k-1}(1 - \xi_i^{l+1}\alpha\tilde\eta_i)\bigr)^{-1}\xi_i^k(\varepsilon_i + k\alpha\tilde\eta_i) \le \kappa\varepsilon_{i+1}\bigr\}$
    $j \leftarrow 0$
    repeat
        $\eta_j \leftarrow \xi_i^{j+1}\,\tilde\eta_i$
        $\mathbf{r}_j \leftarrow \mathsf{apply}(\mathbf{w}_j; \frac{1}{2}\eta_j) - \mathsf{rayleigh}(\mathbf{w}_j; \frac{1}{2}\|\mathbf{M}\|^{-1}\eta_j)\,\mathbf{M}\mathbf{w}_j$
        $\hat{\mathbf{w}}_{j+1} \leftarrow \mathbf{w}_j - \alpha\mathbf{r}_j$
        $\mathbf{w}_{j+1} \leftarrow \|\hat{\mathbf{w}}_{j+1}\|^{-1}\,\hat{\mathbf{w}}_{j+1}$
        $j \leftarrow j+1$
    until $(j \ge K_i \quad \vee \quad (1 - \alpha\eta_{j-1})^{-1}(\xi_i R(\mathbf{w}_{j-1})\|\mathbf{r}_{j-1}\| + (\alpha + \xi_i R(\mathbf{w}_{j-1}))\eta_{j-1}) \le \kappa\varepsilon_{i+1})$
    $\tau_{i+1} := (1+\varepsilon_{i+1}^2)^{-1}\bigl[\bigl(\kappa^2 + (1-\kappa^2)(1+\varepsilon_{i+1}^2)\bigr)^{1/2} - \kappa\bigr]$
    $\hat{\mathbf{v}}_{i+1} := \mathsf{coarsen}(\mathbf{w}_j;\, \tau_{i+1}\,\varepsilon_{i+1})$
    $\mathbf{v}_{i+1} := \|\hat{\mathbf{v}}_{i+1}\|^{-1}\hat{\mathbf{v}}_{i+1}$
    $i \leftarrow i+1$
end while
$\mathbf{u}_\varepsilon := \mathbf{v}_i$
```

Proposition 3.24. *Let* α, ρ, E, C_1 *be chosen as in Lemma 3.23, and let* $\mathbf{v}_0 \in \ell_2$ *with* $\|\mathbf{v}_0\| = 1$ *such that* $\|e_\perp(\mathbf{v}_0)\| \le \delta$, *where with* $C_2 := \frac{1}{2}(1-\rho)^{-1}\|\mathbf{M}\|$ *we have*

$$0 < \delta < \min\bigl\{(1+C_1^2)^{1/2} - C_1, (E^{-1} + (C_2\alpha)^2)^{1/2} - (C_2\alpha)\bigr\}\,. \tag{3.41}$$

Then the iterates $\mathbf{v}_i$ in Algorithm 3.2 satisfy $\|e_\perp(\mathbf{v}_i)\| \leq \theta^i\delta$ with $\|\mathbf{v}_i\| = 1$, and in particular, we have $\|e_\perp(\mathbf{u}_\varepsilon)\| \leq \varepsilon$ with $\|\mathbf{u}_\varepsilon\| = 1$.

Proof. Note first that the assumption on δ implies that $\delta < E^{-1/2}$, and hence the hypothesis of part (iii) of Lemma 3.23 is satisfied.

We consider the first outer iteration, i.e., $i = 0$. With $\mathbf{T}_\alpha$ as in Lemma 3.23, for any j we have

$$\hat{\mathbf{w}}_{j+1} - \mathbf{u}_0 = \mathbf{T}_\alpha(\mathbf{w}_j - \mathbf{u}_0) + \alpha\bigl(\lambda(\mathbf{w}_j) - \lambda_0\bigr)\mathbf{M}\mathbf{w}_j + \alpha\bigl((\mathbf{A} - \lambda(\mathbf{w}_j)\mathbf{M}\mathbf{w}_j) - \mathbf{r}_j\bigr)\,.$$

If $\|e_\perp(\mathbf{w}_j)\| \leq \delta$, from this we obtain

$$\begin{aligned}\|e_\perp(\hat{\mathbf{w}}_{j+1})\| &\leq \rho\|e_\perp(\mathbf{w}_j)\| + \alpha\|\mathbf{M}\|E\left(1 - E\|e_\perp(\mathbf{w}_j)\|^2\right)^{-1}\|e_\perp(\mathbf{w}_j)\|^2 + \alpha\eta_j \\ &\leq \left(\rho + \frac{\alpha\|\mathbf{M}\|E\delta}{1 - E\delta^2}\right)\|e_\perp(\mathbf{w}_j)\| + \alpha\eta_j \\ &= \xi_0\|e_\perp(\mathbf{w}_j)\| + \alpha\eta_j\,.\end{aligned}$$

On the other hand, because $\langle\mathbf{w}_j, (\mathbf{A} - \lambda(\mathbf{w}_j)\mathbf{M})\mathbf{w}_j\rangle = 0$ and $\|\mathbf{w}_j\| = 1$, we have

$$\begin{aligned}\|\hat{\mathbf{w}}_{j+1}\| = \|\mathbf{w}_j - \alpha\mathbf{r}_j\| &= \bigl\|\mathbf{w}_j - \alpha(\mathbf{A} - \lambda(\mathbf{w}_j)\mathbf{M})\mathbf{w}_j + \alpha\bigl((\mathbf{A} - \lambda(\mathbf{w}_j)\mathbf{M})\mathbf{w}_j - \mathbf{r}_j\bigr)\bigr\| \\ &\geq 1 - \alpha\eta_j\,.\end{aligned}$$

Since by definition of η_j, we have $\eta_j < \tilde{\eta}_i < \alpha^{-1}$, it follows that if $\|e_\perp(\mathbf{w}_j)\| \leq \delta$, then

$$\|e_\perp(\mathbf{w}_{j+1})\| = \frac{\|e_\perp(\hat{\mathbf{w}}_{j+1})\|}{\|\hat{\mathbf{w}}_{j+1}\|} \leq \frac{\xi_0\|e_\perp(\mathbf{w}_j)\| + \alpha\eta_j}{1 - \alpha\eta_j}\,. \tag{3.42}$$

By induction, the choice of $\tilde{\eta}_i$ now ensures that $\|e_\perp(\mathbf{w}_j)\| \leq \delta$ for all j, and thus in particular, (3.42) holds for all j.

Using the estimate (3.42) recursively, on the one hand we obtain

$$\|e_\perp(\mathbf{w}_j)\| \leq \frac{\xi_0^j\,\varepsilon_0}{\prod_{l=0}^{j-1}(1 - \alpha\eta_l)} + \sum_{k=0}^{j-1}\frac{\xi_0^{j-1-k}\alpha\eta_k}{\prod_{l=k}^{j-1}(1 - \alpha\eta_l)} \leq \Bigl(\prod_{l=0}^{j-1}(1 - \alpha\xi_0^{l+1}\tilde{\eta}_i)\Bigr)^{-1}\xi_0^j(\varepsilon_0 + j\alpha\tilde{\eta}_i)\,. \tag{3.43}$$

If $j \geq K_i$ holds at line 15, we thus have $\|e_\perp(\mathbf{w}_j)\| \leq \kappa\varepsilon_1$. On the other hand,

$$\begin{aligned}\|e_\perp(\mathbf{w}_j)\| &\leq \frac{\xi_0\|e_\perp(\mathbf{w}_{j-1})\| + \alpha\eta_{j-1}}{1 - \alpha\eta_{j-1}} \leq \frac{\xi_0 R(\mathbf{w}_{j-1})\|(\mathbf{A} - \lambda(\mathbf{w}_{j-1})\mathbf{M})\mathbf{w}_{j-1}\| + \alpha\eta_{j-1}}{1 - \alpha\eta_{j-1}} \\ &\leq (1 - \alpha\eta_{j-1})^{-1}\bigl(\xi_0 R(\mathbf{w}_{j-1})\|r_{j-1}\| + (\alpha + \xi_0 R(\mathbf{w}_{j-1}))\eta_{j-1}\bigr)\,,\end{aligned}$$

and thus $\|e_\perp(\mathbf{w}_j)\| \leq \kappa\varepsilon_1$ holds as well if the inner loop terminates with the second criterion in line 15.

It remains to show that there exists a uniform bound for K_i, which ensures that the inner loop finishes after a finite, uniformly bounded number of steps. To this end, note that

$$\ln\prod_{l=0}^{j-1}(1 - \alpha\eta_l)^{-1} = -\sum_{l=1}^{j}\ln(1 - \xi_0^l\alpha\tilde{\eta}_0) \leq -\sum_{l=1}^{\infty}\ln(1 - \xi_0^l\alpha\tilde{\eta}_0)\,,$$

and because

$$\lim_{l\to\infty}\frac{\ln(1 - \xi_0^{l+1}\alpha\tilde{\eta}_0)}{\ln(1 - \xi_0^l\alpha\tilde{\eta}_0)} = \lim_{x\to 0^+}\frac{\ln(1 - \xi_0 x)}{\ln(1 - x)} = \xi_0 < 1\,,$$

the infinite sum on the right hand side converges, which implies

$$\prod_{l=0}^{j-1}(1-\alpha\eta_l)^{-1} < \prod_{l=0}^{\infty}(1-\xi_0^l\alpha\tilde{\eta}_0)^{-1} \leq C < \infty\,,$$

and hence by monotonicity of ξ_i and $\tilde{\eta}_i$ we obtain that for given problem parameters, K_i is uniformly bounded with respect to i.

By definition of $\hat{\mathbf{v}}_1$, we have $\|\mathbf{w}_j - \hat{\mathbf{v}}_1\| \leq \tau_1\varepsilon_1$ as well as $\|\hat{\mathbf{v}}_1\|^2 \geq 1-(\tau_1\varepsilon_1)^2$, and as a consequence

$$\|e_\perp(\hat{\mathbf{v}}_1)\| \leq \|e_\perp(\mathbf{w}_j)\| + \|(\mathbf{I}-\mathbf{P}_0)(\mathbf{w}_j - \hat{\mathbf{v}}_1)\| = \kappa\varepsilon_1 + \tau_1\varepsilon_1\,.$$

For the normalized iterate $\mathbf{v}_1$, we thus obtain

$$\|e_\perp(\mathbf{v}_1)\| = \frac{\|e_\perp(\hat{\mathbf{v}}_1)\|}{\|\hat{\mathbf{v}}_1\|} \leq \frac{\kappa+\tau_1}{\sqrt{1-(\tau_1\varepsilon_1)^2}}\,\varepsilon_1\,,$$

and with our choice of τ_1, it follows that $\|e_\perp(\mathbf{v}_1)\| \leq \varepsilon_1$.

As the above steps can be repeated for general i, the statement follows by induction. □

In [36], a complexity estimate similar to Theorem 3.21 is shown for the eigenvalue solver. The modifications we have made to the constants in the iterative scheme do not affect this result, which is summarized in the following theorem.

Theorem 3.25. *Let $s > 0$, $\mathbf{u}_0 \in \mathcal{A}^s_\infty$, let $\mathbf{w}_\eta := \mathsf{apply}(\mathbf{v};\eta)$ satisfy*

$$\|\mathbf{w}_\eta\|_{\mathcal{A}^s_\infty} \lesssim \|\mathbf{v}\|_{\mathcal{A}^s_\infty}\,, \quad \#\operatorname{supp}\mathbf{w}_\eta \lesssim \eta^{-\frac{1}{s}}\|\mathbf{v}\|^{\frac{1}{s}}_{\mathcal{A}^s_\infty}\,,$$

where the order of arithmetic operations required for the evaluation of $\mathbf{w}_\eta$ and of $\mathsf{rayleigh}(\mathbf{v};\eta)$ are both of order $\mathcal{O}(\eta^{-\frac{1}{s}}\|\mathbf{v}\|^{\frac{1}{s}}_{\mathcal{A}^s_\infty} + \#\operatorname{supp}\mathbf{v})$, and let $\mathsf{coarsen}$ be as in Theorem 3.21. Then Algorithm 3.2 requires $\mathcal{O}(\varepsilon^{-\frac{1}{s}}\|\mathbf{u}_0\|^{\frac{1}{s}}_{\mathcal{A}^s_\infty})$ operations, and the result $\mathbf{u}_\varepsilon$ satisfies

$$\#\operatorname{supp}\mathbf{u}_\varepsilon \lesssim \varepsilon^{-\frac{1}{s}}\|\mathbf{u}_0\|^{\frac{1}{s}}_{\mathcal{A}^s_\infty}\,, \quad \|\mathbf{u}_\varepsilon\|_{\mathcal{A}^s_\infty} \lesssim \|\mathbf{u}_0\|_{\mathcal{A}^s_\infty}$$

with constants independent of ε and $\mathbf{u}_0$.

Proof. The result follows with the same arguments as in the proof of [36, Theorem 3]. □

Remark 3.26. *On the basis of a suitable routine* apply*, one can obtain a procedure* rayleigh *with the required properties by setting*

$$\mathsf{rayleigh}(\mathbf{v};\eta) := \frac{\langle \mathsf{apply}(\mathbf{v};\langle\mathbf{M}\mathbf{v},\mathbf{v}\rangle\eta),\mathbf{v}\rangle}{\langle\mathbf{M}\mathbf{v},\mathbf{v}\rangle}\,.$$

In this manner, the evaluation of apply *required in each step of the iteration can also be used for the approximation of the Rayleigh quotient. However, different constructions of a procedure* rayleigh *that lead to better complexity are possible, see [36, Section 4.3.1].*

Remark 3.27. *Further results along these lines for preconditioned inverse iteration with more general preconditioners have been obtained in [127]. In [156] it has been shown that inexact inverse iteration, which in the present setting can be realized by an iteration of the form*

$$\hat{\mathbf{v}}_{i+1} := \mathsf{solve}(\mathbf{A},\mathbf{v}_i,\varepsilon_i)\,, \quad \mathbf{v}_{i+1} := \frac{\hat{\mathbf{v}}_{i+1}}{\|\hat{\mathbf{v}}_{i+1}\|}\,,$$

shares the optimality properties as in Theorem 3.25 of the scheme considered above, provided that the tolerances ε_i are chosen appropriately.

Remark 3.28. *The convergence analysis for the eigenvalue solvers mentioned thus far has been carried out in the case of self-adjoint operators. For nonsymmetric problems, as in the case of the explicitly correlated formulation* (2.11) *of the electronic Schrödinger equation, preconditioned inverse iteration can generally not be expected to converge, but inexact inverse iteration as outlined in Remark 3.27 may serve as the basis of an adaptive solver.*

3.6.3 Prerequisites for Asymptotic Optimality

The complexity estimates of Theorems 3.21 and 3.25 require, as a first basic assumption, that the coefficient sequence representing the exact solution is in $\mathcal{A}^s_\infty$ for some $s > 0$. In view of the norm equivalences (3.11), (3.27), (3.29), and (3.30), this can be inferred from Besov regularity properties of the solution. In this section, we discuss the further requirements on the components of Algorithms 3.1 and 3.2 for these schemes to be asymptotically optimal with respect to the best N-term approximation of the exact solution. This concerns the procedure for the coarsening of vectors as well as the approximation of right hand sides and of the action of operators.

A routine coarsen whose output satisfies the properties required by Theorems 3.21 and 3.25 can be obtained by simply sorting entries of $\mathbf{v}$ by their absolute value; however, the sorting operation requires $\mathcal{O}(\#\operatorname{supp}\mathbf{v}\log\#\operatorname{supp}\mathbf{v})$ operations.

The additional logarithmic factor can be avoided by instead only ordering the entries approximately, which in this context was introduced in [7, 110]. The essential requirement on such an approximate ordering is that if $\mathbf{v} \in \mathcal{A}^s_\infty$ for some $s > 0$, and if $\mathbf{v}^\diamond := (v^\diamond_n)_{n\in\mathbb{N}}$ is the vector of correspondingly reordered entries of $\mathbf{v}$, then

$$\|\mathbf{v}^\diamond - (\mathbf{v}^\diamond|_{\{1,\dots,N\}})\| \lesssim N^{-s}\|\mathbf{v}\|_{\mathcal{A}^s_\infty} \tag{3.44}$$

with a constant independent of $\mathbf{v}$. If $\mathbf{v}^\diamond = \mathbf{v}^*$, that is, $\mathbf{v}^\diamond$ is determined by the mentioned exact sorting of coefficients by nonincreasing absolute value, the corresponding rearrangement satisfies (3.44) because $\mathbf{v} \in \mathcal{A}^s_\infty$, and restriction to the first N entries actually yields the best N-term approximation to $\mathbf{v}$.

However, a rearrangement that satisfies (3.44) with a different uniform constant can be obtained by a simplified ordering procedure known as *binary binning*. Let $M := \max_\nu |v_\nu|$, then sorting entries into the bins

$$[M, 2^{-\frac{1}{2}}M)\,,\ [2^{-\frac{1}{2}}M, 2^{-1}M)\,,\dots$$

according to their absolute values, but picking the entries from each bin in any order in the construction of $\mathbf{v}^\diamond$, one still obtains a rearrangement with the required properties. This approach only requires $\mathcal{O}(\#\operatorname{supp}\mathbf{v})$ operations.

For the approximation of a given right hand side vector $\mathbf{f}$, a routine rhs can be realized based on a priori estimates for the individual entries of $\mathbf{f}$, and an approximate ordering of these estimates for determining which entries actually need to be evaluated.

For the procedure apply approximating the action of $\mathbf{A}$ on a given vector, there exists a generic construction based on the following notion of s^*-*compressibility* introduced in [30].

Definition 3.29. Let Λ be a countable index set and let $s^* > 0$. An operator $\mathbf{B}\colon \ell_2(\Lambda) \to \ell_2(\Lambda)$ is called s^*-*compressible* if for any $0 < s < s^*$, there exist summable positive sequences $(\alpha_j)_{j\geq 0}$, $(\beta_j)_{j\geq 0}$ and for each $j \geq 0$, there exists $\mathbf{B}_j$ with at most $\alpha_j 2^j$ nonzero entries per row and column, such that $\|\mathbf{B} - \mathbf{B}_j\| \leq 2^{-sj}\beta_j$. We call $\mathbf{B}$ s^*-*computable* [58] if in addition, there exists a $C > 0$ such that the computation of the nonzero entries of $\mathbf{B}_j$ takes at most $C\alpha_j 2^j$ operations per column.

In [30], the property of s^*-compressibility has been investigated for isotropic wavelet bases and corresponding discretization matrices arising from a general class of operators whose entries satisfy a certain decay condition. In this construction of compressed matrices, the attainable value of s^* is constrained by the global Sobolev regularity of the wavelets. In [135], s^*-compressibility is investigated in the particular case of (piecewise smooth) spline wavelets, and it is shown that this constraint can be removed, that is, the value of s^* is limited only by the properties of the operator and the number of vanishing moments of the wavelets. For the particular case of the Laplacian, see Section 6.2.

The s^*-compressibility and s^*-computability of differential operators with constant or with sufficiently smooth coefficients with respect to tensor product spline wavelet bases have been studied in [115] and [129], respectively. Compressibility properties of the potential operators arising in the Hartree-Fock problem of quantum chemistry have been investigated in [52].

For s^*-compressible matrices, a scheme for the adaptive application of operators that has the properties required by Theorems 3.21 and 3.25 is given in [30]. The construction is summarized in the following proposition.

Proposition 3.30 ([30, Proposition 3.8])**.** *Let* $\mathbf{B}$ *be* s^**-compressible, then for each* $s > 0$ *with* $s < s^*$, $\mathbf{B}$ *maps* $\mathcal{A}^s_\infty$ *boundedly to itself, and for each finitely supported* $\mathbf{v}$ *and* $\eta > 0$, *an* $\mathbf{w}_\eta$ *such that*

$$\|\mathbf{B}\mathbf{v} - \mathbf{w}_\eta\| \leq \eta\,, \quad \#\operatorname{supp}\mathbf{w}_\eta \lesssim \eta^{-\frac{1}{s}}\|\mathbf{v}\|^{\frac{1}{s}}_{\mathcal{A}^s_\infty}$$

can be computed with $\mathcal{O}(\eta^{-\frac{1}{s}}\|\mathbf{v}\|^{\frac{1}{s}}_{\mathcal{A}^s_\infty})$ *operations, where the constants are independent of* η *and* $\mathbf{v}$*.*

Proof. For given $\mathbf{v} \in \mathcal{A}^s_\infty$, let $\mathbf{v}^\diamond := (v^\diamond_n)_{n\in\mathbb{N}}$ be a vector of rearranged entries of $\mathbf{v}$, ordered approximately by descending absolute value, such that $\mathbf{v}_{[j]} := \mathbf{v}^\diamond|_{\{1,\ldots,2^j\}}$ for $j \in \mathbb{N}_0$ satisfy

$$\|\mathbf{v} - \mathbf{v}_{[j]}\| \lesssim 2^{-sj}\|\mathbf{v}\|_{\mathcal{A}^s_\infty}\,.$$

Thus we assume $\mathbf{v}_{[j]}$ to be almost best 2^j-term approximations, up to an additional constant factor, to $\mathbf{v}$ in ℓ_2. If $\mathbf{v}$ has finite support, such an approximate sorting can be performed by binary binning in $\mathcal{O}(\#\operatorname{supp}\mathbf{v})$ operations; as for coarsen, this is a modification of the original algorithm given in [30], which is instead based on an exact ordering requiring $\mathcal{O}(\#\operatorname{supp}\mathbf{v}\log\#\operatorname{supp}\mathbf{v})$ operations.

For $j \in \mathbb{N}_0$, let

$$\mathbf{w}_j := \mathbf{B}_j\mathbf{v}_{[0]} + \mathbf{B}_{j-1}(\mathbf{v}_{[1]} - \mathbf{v}_{[0]}) + \ldots + \mathbf{B}_0(\mathbf{v}_{[j]} - \mathbf{v}_{[j-1]})\,,$$

then

$$\begin{aligned}\|\mathbf{B}\mathbf{v} - \mathbf{w}_j\| &\lesssim \|\mathbf{B}\|\|\mathbf{v} - \mathbf{v}_{[j]}\| + \|\mathbf{B} - \mathbf{B}_0\|\|\mathbf{v}_{[j]} - \mathbf{v}_{[j-1]}\| + \ldots + \|\mathbf{B} - \mathbf{B}_j\|\|\mathbf{v}_{[0]}\| \\ &\lesssim \|\mathbf{B}\|\|\mathbf{v}\|_{\mathcal{A}^s_\infty}2^{-sj} + \beta_0\|\mathbf{v}\|_{\mathcal{A}^s_\infty}2^{-s(j-1)} + \ldots + 2^{-sj}\beta_j\|\mathbf{v}_{[0]}\| \\ &\lesssim 2^{-sj}\|\mathbf{v}\|_{\mathcal{A}^s_\infty}\end{aligned}$$

and $\#\operatorname{supp}\mathbf{w}_j \leq \alpha_j 2^j + 2\alpha_{j-1}2^{j-1} + \ldots + 2^j\alpha_0 \lesssim 2^j$. Choosing the minimal j such that $2^{-sj}\|\mathbf{v}\|_{\mathcal{A}^s_\infty} \leq \eta$, the statement follows. □

Note that the explicit construction of the sought approximation in the proof of Proposition 3.30 directly leads to a numerical procedure for computing such approximations, see [30, Section 6.4].

Remark 3.31. *The algorithms considered in this work do not require the application of the adjoint* $\mathbf{B}^*$*, and therefore the assumption of* s^**-compressibility can be weakened for our purposes. The construction of Proposition 3.30 still works if the approximate operators* $\mathbf{B}_j$ *in Definition 3.29 are only assumed to have at most* $\alpha_j 2^j$ *entries per column, without restriction on the number of entries per row.*

Remark 3.32. *It is interesting to note that when the operators of interest in our context are applied approximately as in Proposition 3.30, the problem of almost dense discretization matrices requiring* *special algorithms, as encountered in standard Galerkin discretizations based on anisotropic tensor product bases, essentially disappears. For the combinations of wavelet levels that dominate the complexity in the direct application of discretization matrices without compression, in a compressed application of the corresponding operators of interest one obtains entries that are sufficiently small to be neglected. These compressibility properties have been investigated for tensor product spline wavelet bases and a general class of operators with sufficiently smooth coefficients in [129].*

4 Wavelet Approximation of Electronic Wave Functions

This chapter is devoted to the approximability properties of electronic wave functions, where we pay particular attention to the two-electron case. Here the relevant measure for approximation errors is the H^1–norm, since the approximation errors in H^1 for the eigenfunctions also determine the errors in the corresponding eigenvalues.

We consider three types of approximation: First, linear approximation by sparse grid-type bases, which in a wavelet context are also referred to as hyperbolic wavelet bases; here, convergence and complexity estimates can be obtained via integrability properties of mixed derivatives. We review existing results for electronic Schrödinger wave functions and consider in detail the explicitly correlated formulation of Section 2.2 in the two-electron case. In addition, we review results for the ground states of hydrogenic systems and of hookium, where explicit solutions permit a more detailed analysis, and also transfer the corresponding result for hookium to the explicitly correlated formulation.

Second, we consider best N-term approximation by tensor product wavelet bases, where one considers the error in keeping the N largest coefficients of the function to be approximated with respect to such a basis. Since the active basis elements depend on the approximand, this is an instance of nonlinear approximation; in this case, complexity estimates can be obtained using regularity estimates in a certain scale of Besov spaces. To the author's knowledge, such estimates are currently not known for solutions for the electronic Schrödinger equation for more than one electron. We therefore restrict our discussion to the above mentioned model systems, where we again review existing estimates and obtain an additional result for the explicitly correlated formulation for hookium.

Third, we consider decompositions of wave functions into sums of separable functions, which in our setting amount to wavelet approximations with nonlinearly parametrized wavelet coefficients, or can also be interpreted as choosing problem-adapted basis functions that are in turn represented in a wavelet basis. This general type of approximation is sometimes also referred to as highly nonlinear approximation. Here we obtain new complexity estimates for approximations of this type of the ground states of hydrogenic systems and hookium, the latter also for the explicitly correlated formulation.

4.1 Regularity of Electronic Schrödinger Wave Functions

In [150], it is shown that electronic wave functions, i.e., eigenfunctions u of (2.3) for a fixed spin configuration, one has $u \in \mathrm{H}^{1/2,1}_{\mathrm{mix}}(\mathbb{R}^3; n)$. This result strongly relies on the partial antisymmetry property (2.4); in the particular case that all spins are equal, and hence u is completely antisymmetric, the proof yields the stronger result $u \in \mathrm{H}^{1,1}_{\mathrm{mix}}(\mathbb{R}^3; n)$.

Using similar arguments, in addition to the exponential decay in $\mathrm{L}_2(\mathbb{R}^{3n})$ of u and $\mathrm{D}u$ as in Theorem 2.2, it is established in [152] that those mixed weak derivatives of u that are ensured to be square integrable by the mentioned regularity proof decay exponentially in the L_2-sense as well.

In [103], the regularity result is sharpened to $u \in \mathrm{H}^{s,1}_{\mathrm{mix}}(\mathbb{R}^3; n)$ for any $s < \frac{3}{4}$. Considerations for the hookium model system (2.17) given there show that, unless u is completely antisymmetric, one cannot expect $u \in \mathrm{H}^{s,1}_{\mathrm{mix}}(\mathbb{R}^3; n)$ for any $s \geq \frac{3}{4}$. The proof in [103] relies on interpolation theory and on a further result from [153] concerning higher regularity of solutions of an explicitly correlated formulation, similar to the one considered in Section 2.2. In the following subsection, we discuss results of the latter type in more detail.

4.1.1 Regularity for an Explicitly Correlated Formulation

In this section, we consider regularity properties relevant for sparse tensor product approximation of the modified eigenfunctions w as in Proposition 2.3.

The following is shown in [153] using a more general class of correlation factors, and corresponding explicitly correlated formulations of the electronic Schrödinger equation: Let u be an eigenfunction of (2.3), and let

$$w(x) = \exp\bigl(-\tfrac{1}{2}\textstyle\sum_{i<j}\phi(|x_i - x_j|)\bigr)u(x)\,, \tag{4.1}$$

where $\phi\colon [0,\infty) \to \mathbb{R}$ is infinitely differentiable with $\phi'(0) = 1$ and $\phi(t) \geq 0$, $|\phi'(t)| \lesssim 1$, $|\phi''(t)| \lesssim t^{-1}$, $|\phi^{(3)}(t)| \lesssim t^{-1}$ for $t \in [0,\infty)$; then $w \in \mathrm{H}^{1,1}_{\mathrm{mix}}(\mathbb{R}^3; n)$.

We restrict our attention to the two-electron case in which we will mainly be interested. We consider the specific ansatz $u = e^{\frac{1}{2}|x_1 - x_2|}w$, corresponding to the unbounded correlation factor e^F with F as in (2.10). Recall the definition of the nuclear Coulomb potential term V_{ne} in (2.5).

Theorem 4.1. *Let $u \in \mathrm{H}^1(\mathbb{R}^6)$ solve the electronic Schrödinger equation*

$$-\frac{1}{2}\Delta u + V_{\mathrm{ne}}u + \frac{1}{|x_1 - x_2|}u = \lambda u\,, \tag{4.2}$$

then $w := \exp(-\frac{1}{2}|x_1 - x_2|)u$ solves the modified problem

$$Tw := -\frac{1}{2}\Delta w + V_{\mathrm{ne}}\, w - \frac{1}{2}\frac{x_1 - x_2}{|x_1 - x_2|} \cdot (\mathrm{D}_{x_1} - \mathrm{D}_{x_2})w - \frac{1}{4}w = \lambda w \tag{4.3}$$

where $w \in \mathrm{H}^{1,1}_{\mathrm{mix}}(\mathbb{R}^3; 2)$.

Theorem 4.1 follows as a special case of the results in [153]. A simplified proof for the specific setting of Theorem 4.1, which also follows basic strategy of [150], is given in [3].

Remark 4.2. *In [152, Chapter 5.1], it is shown that also the mixed derivatives of electronic Schrödinger wave functions decay exponentially. This is demonstrated in [153] to hold also for general explicitly correlated wave functions w as in* (4.1)*. In the two-electron case as in Theorem 4.1 this can be phrased as follows: there exists $\bar\gamma > 0$ such that $\exp\bigl(\gamma(|x_1| + |x_2|)\bigr)w \in \mathrm{H}^{1,1}_{\mathrm{mix}}(\mathbb{R}^3; 2)$ for any γ, $0 < \gamma < \bar\gamma$.*

Remark 4.3. *The result of Theorem 4.1 cannot be expected to be sharp; the considerations for model problems in Section 4.2 support the conjecture that $w \in \mathrm{H}^{s,1}_{\mathrm{mix}}$ for $s < \frac{3}{2}$. Here, the nuclear cusps would become an additional limiting factor for the regularity.*

As to be expected in view of Proposition 2.4, the proof of Theorem 4.1 does not carry over to the adjoint problem (2.13)*, that is, for $w^* = e^F u$ one does not obtain higher regularity than for u.*

4.1.2 Linear Approximation by Wavelets

We define two families of hyperbolic wavelet bases with discretization parameter $L \in \mathbb{Z}$ by the index sets

$$\Lambda^{(3,n)}_L := \Bigl\{\lambda \in (\nabla^{(3)})^n \colon |\lambda_1|+\ldots+|\lambda_n| \leq L\Bigr\}\,, \quad \Lambda^{(1,3n)}_L := \Bigl\{\lambda \in \nabla^{3n} \colon |\lambda_1|+\ldots+|\lambda_{3n}| \leq L\Bigr\}\,, \tag{4.4}$$

which are nonempty for $L \geq nj_0$ and $L \geq 3nj_0$, respectively.

Following the basic concept outlined in Section 3.4, the regularity estimate of Theorem 4.1 and the exponential decay of Theorem 2.2 can be combined to a simple approximation result for eigenfunctions of (4.3). It is not the best possible, but is included here rather for illustrative purposes. A more detailed analysis can be found in [157], see Remark 4.5 below. In the following, we restrict the approximation to a subset Λ of indices of the hyperbolic wavelet bases $\Lambda_L^{(3,2)}$ or $\Lambda_L^{(1,6)}$ that is confined to a region around the origin, and estimate separately the error due to truncation in space by Theorem 2.2 and the error due to truncation in level L by Theorem 4.1.

For eigenfunctions $w \in \mathrm{H}^{1,1}_{\mathrm{mix}}(\mathbb{R}^3;2)$ as in Theorem 4.1, which also satisfy (2.8), the following applies with $s = 1$. Here, we again assume the tensor product wavelets to be constructed from an L_2–orthonormal univariate scaling function φ.

Theorem 4.4. *Let $s > 0$, let $u \in \mathrm{H}^{s,1}_{\mathrm{mix}}(\mathbb{R}^3;2)$ satisfy a decay condition* (2.8) *with some $\delta > 0$, and let either $d = 3$, $D = 2$ or $d = 1$, $D = 6$. Let $\varphi \in \mathrm{H}^{\tau}(\mathbb{R})$ for a $\tau > 1+s$. Then there exists a $C > 0$ depending on s, δ, ψ and j_0 such that for each $L \geq Dj_0$ there exists a subset $\Lambda \subset \Lambda_L^{(d,D)}$ with*

$$\inf_{v\in\operatorname{span}\{\Psi_\lambda\colon\, \lambda\in\Lambda\}} \|u - v\|_1 \leq C 2^{-\frac{d}{3}sL}\|u\|_{s,1}\,, \quad \textit{where } \#\Lambda \lesssim L^{5+D}2^{dL}.$$

Sketch of proof. We restrict ourselves to a brief summary of the argument and refer to [3] for the complete proof. For $R > 0$, let $\Lambda_R = \{\lambda \in \bar{\Lambda}_L : \operatorname{supp}\Psi_\lambda \cap B_R(0) \neq \emptyset\}$. By the wavelet characterization (3.22), we obtain

$$\Big\| u - \sum_{\lambda\in\Lambda_R} \langle u, \Psi_\lambda\rangle \Psi_\lambda \Big\|_1^2 \lesssim \sum_{\lambda\notin\Lambda_L^{(d,D)}} \sum_{i=1}^{D} 2^{2|\lambda_i|}|\langle u, \Psi_\lambda\rangle|^2 + \sum_{\lambda\notin\Lambda_R} \sum_{i=1}^{D} 2^{2|\lambda_i|}|\langle u, \Psi_\lambda\rangle|^2\,.$$

Now on the one hand, by (3.25)

$$\sum_{\lambda\notin\Lambda_L^{(d,D)}} \sum_{i=1}^{D} 2^{2|\lambda_i|}|\langle u, \Psi_\lambda\rangle|^2 \leq 2^{-2\frac{d}{3}s(L+1)} \sum_{\lambda\notin\Lambda_L^{(d,D)}} 2^{2\frac{d}{3}s\sum_{i=1}^{D}|\lambda_i|} \sum_{i=1}^{D} 2^{2|\lambda_i|}|\langle u, \Psi_\lambda\rangle|^2 \lesssim 2^{-2\frac{d}{3}sL}\|u\|^2_{s,1}\,,$$

where we have used $\prod_{k=1}^{3} 2^{\frac{2ds}{3}j_k} \leq \frac{1}{3}\sum_{k=1}^{3} 2^{2dsj_k}$ for $j \in \mathbb{Z}^3$ in the case $d = 1$, $D = 6$. On the other hand,

$$\sum_{\lambda\notin\Lambda_R} \sum_{i=1}^{D} 2^{2|\lambda_i|}|\langle u, \Psi_\lambda\rangle|^2 \lesssim e^{-2\delta R}\int_{\mathbb{R}^6} e^{2\delta|x|}\big(|u|^2 + |\mathrm{D}u|^2\big)\,\mathrm{d}x \lesssim e^{-2\delta R}\,.$$

In summary, $\|u - u_{\Lambda_R}\|_1 \lesssim e^{-\delta R} + 2^{-s\frac{d}{3}L}\|u\|_{s,1}$, where we choose R proportionally to L to balance the two expressions on the right hand side. Counting the resulting number of degrees of freedom yields the assertion. ☐

Remark 4.5. *A deeper analysis has been carried out in [157]. There a construction of suitable wavelet index sets for n electrons is given that exploits not only exponential decay of u and $\mathrm{D}u$, but also of the mixed derivatives of u. In the specific case of two electrons considered here, on the basis of such additional decay assumptions on u, the construction from [157] yields Λ with*

$$\inf_{v\in\operatorname{span}\{\Psi_\lambda\colon\, \lambda\in\Lambda\}} \|u - v\|_1 \lesssim 2^{-\frac{d}{3}sL}\,, \quad \#\Lambda \lesssim L^{D-1}2^{dL}\,,$$

with $d = 3$, $D = 2$ or $d = 1$, $D = 6$, in other words, the asymptotic estimate for $\#\Lambda$ is improved, in comparison to Theorem 4.4, by a factor L^6. Concerning the case of n electrons, it is also shown in [157] that based on the improved construction and taking antisymmetry into account, convergence rates independent of n can be achieved.

Remark 4.6. *For $s = 1$, as for the solution w of the explicitly correlated formulation* (4.3), *Theorem 4.4 already leads to an error in H^1 that decays, up to logarithmic terms, like $(\#\Lambda)^{-1/3}$. For comparison, we can apply Theorem 4.4 to a direct hyperbolic wavelet discretization of the* *standard formulation (4.2). Using that* $u \in \mathrm{H}^{1/2,1}_{\mathrm{mix}}(\mathbb{R}^3; 2)$*, one obtains a convergence rate of almost* $(\#\Lambda)^{-1/6}$*, whereas using the sharpened result* $u \in \mathrm{H}^{s,1}_{\mathrm{mix}}(\mathbb{R}^3; 2)$ *for any* $s < \frac{3}{4}$*, one obtains almost* $(\#\Lambda)^{-1/4}$*.*

Remark 4.7. *Both choices* $\Lambda_L^{(3,2)}$ *and* $\Lambda_L^{(1,6)}$ *yield essentially the same convergence rate, with* $\Lambda_L^{(1,6)}$ *requiring more unknowns by a factor proportional to* L^4*. Although this seems to indicate a disadvantage of the fully anisotropic basis, it should be noted that this reflects the underlying regularity assumptions, and that the comparison may change when more general sets of wavelet indices are used, corresponding to regularity assumptions on* u *different from those in Theorem 4.4.*

Some crucial differences concerning computational methods between the fully and partially anisotropic constructions, in particular related to the approximation of operators, will become apparent in Section 4.3 and Chapter 6.

4.2 Regularity for Model Systems with Explicit Solutions

In this section, we consider the ground states of hydrogenic systems and of the hookium model problem, for which explicit solutions are available and hence a closer investigation of regularity properties is possible.

4.2.1 Hydrogen

As a first example, we consider hydrogenic ground state wave functions, whose regularity properties are representative of nuclear cusps, as discussed in Section 2.1.

To obtain Sobolev regularity estimates, we apply the following observation concerning the asymptotics of Fourier transforms of rotationally symmetric functions, which has also been used in [51, 103] for this purpose. For the proof, we follow the lines of [103, Lemma 6.1] to obtain a slightly more general version that will also be used in the following subsection.

Lemma 4.8. *Let* $k \in \mathbb{N}$*,* $f \in \mathrm{C}^{2k+1}(\mathbb{R}_0^+) \cap \mathrm{W}_1^{2k+1}(\mathbb{R}_0^+; x\,\mathrm{d}x)$ *and* $F(x) = f(|x|)$ *for* $x \in \mathbb{R}^3$*. Then for* $\xi \neq 0$*,*

$$\sqrt{\frac{\pi}{2}}\hat{F}(\xi) = \sum_{n=1}^{k} (-1)^n \frac{2n}{|\xi|^{2(n+1)}} f^{(2n-1)}(0) + \frac{(-1)^k}{|\xi|^{2(k+1)}} \int \bigl(r f^{(2k+1)}(r) + (2k+1) f^{(2k)}(r)\bigr) \cos(|\xi| r)\,\mathrm{d}r\,.$$

Proof. Using rotational symmetry,

$$\begin{aligned}\int_{\mathbb{R}^3} F(x) e^{-i\xi\cdot x}\,\mathrm{d}x &= \int_{\mathbb{R}^3} f(|x|) e^{-i|\xi| x_1}\,\mathrm{d}x = \int_{\mathbb{R}^3} f(|x|)\cos(|\xi| x_1)\,\mathrm{d}x \\ &= 2\pi \int_0^\infty s \int_{-\infty}^{\infty} f\bigl(\sqrt{s^2+r^2}\bigr)\cos(|\xi| r)\,\mathrm{d}r\,\mathrm{d}s = \frac{4\pi}{|\xi|}\int_0^\infty r f(r)\sin(|\xi| r)\,\mathrm{d}r\,.\end{aligned}$$

Note that $\mathrm{D}^m(r f(r)) = r f^{(m)}(r) + m f^{(m-1)}(r)$, $m \in \mathbb{N}$, and

$$\begin{aligned}\int_0^\infty r f(r)\sin(|\xi| r)\,\mathrm{d}r &= -\frac{2f'(0)}{|\xi|^3} - \frac{1}{|\xi|^3}\int_0^\infty \mathrm{D}^3(r f(r))\cos(|\xi| r)\,\mathrm{d}r \\ &= -\frac{2f'(0)}{|\xi|^3} + \frac{1}{|\xi|^4}\int_0^\infty \mathrm{D}^4(r f(r))\sin(|\xi| r)\,\mathrm{d}r\,.\end{aligned}$$

The assertion thus follows by repeated integration by parts. □

The following regularity result for hydrogenic ground state eigenfunctions is also contained as a special case in the discussion of the regularity of general hydrogenic eigenfunctions given in [151].

Proposition 4.9. *For $\gamma > 0$, the hydrogen-type wave function* $\exp(-\gamma|x|)$, $x \in \mathbb{R}^3$, *is in* $\mathrm{H}^s(\mathbb{R}^3)$ *if and only if* $s < \frac{5}{2}$.

Proof. Let $F(x) := \exp(-\gamma|x|)$ and $f(r) = \exp(-\gamma r)$, then by the Riemann-Lebesgue Lemma, $\hat{F}$ is uniformly continuous, and since $f'(0) = -\gamma$, Lemma 4.8 yields the asymptotic decay $|\hat{F}(\xi)| = \mathcal{O}(|\xi|^{-4})$ for $|\xi| \to \infty$. Thus $\int_{\mathbb{R}^3}(1+|\xi|^2)^s|\hat{F}(\xi)|^2\,\mathrm{d}\xi < \infty$ if and only if

$$\int_1^\infty (1+r^2)^s(r^{-4})^2 r^2\,\mathrm{d}r < \infty\,,$$

which in turn holds if and only if $2s-6<-1$, i.e., $s < \frac{5}{2}$. □

Whereas the above Sobolev regularity estimates govern the rates possible for linear approximation, estimates in certain Besov norms yield rates for best N-term approximation. The following theorem is a direct consequence of the results in [50].

Theorem 4.10 ([50])**.** *For $\gamma > 0$, the function $u(x) = \exp(-\gamma|x|)$, $x \in \mathbb{R}^3$ satisfies*

$$u \in \mathrm{B}^s_{p,p}(\mathbb{R}^3) \quad \text{with} \quad p^{-1} = \frac{s-1}{3} + \frac{1}{2}\,, \qquad\qquad u \in \tilde{\mathrm{B}}^s_p(\mathbb{R};3) \quad \text{with} \quad p^{-1} = s + \frac{1}{2}$$

for any $s > 0$.

The result is shown in [50] for more general functions on a bounded $\Omega \subset \mathbb{R}^3$, but in our setting carries over to $\mathbb{R}^3$ by exponential decay of u.

As a consequence, when using basis functions of sufficiently high order, with adaptive approximation arbitrarily high convergence rates with respect to the number of terms can be achieved. For an orthonormal wavelet ψ with m vanishing moments, Theorem 4.10 yields best N-term rates for approximation in $\mathrm{H}^1(\mathbb{R}^3)$ of $N^{-\frac{m-1}{3}}$ for the corresponding basis $\{\Psi_\nu\}_{\nu\in\nabla^{(3)}}$, and $N^{-(m-1)}$ for the basis $\{\Psi_\nu\}_{\nu\in\nabla}$.

4.2.2 Hooke's Law Atom

The Sobolev and Besov smoothness of the ground state

$$u_0(x) = \bigl(1 + \tfrac{1}{2}|x_1 - x_2|\bigr)\exp\bigl(-\tfrac{1}{4}|x|^2\bigr)\,, \quad x \in (\mathbb{R}^3)^2 \tag{4.5}$$

of the model system (2.17) discussed in Section 2.3 have been investigated in [51, 103]. We review these results and compare to the analogous estimates for the explicitly correlated case, i.e., for the function

$$w_0(x) = \exp(-\tfrac{1}{2}|x_1 - x_2|)\,u_0(x)\,. \tag{4.6}$$

Regularity of u_0

Using asymptotics of the Fourier transform of u_0, it was shown in [51] that $u_0 \in \mathrm{H}^{s,1}_{\mathrm{mix}}(\mathbb{R}^3;2)$ for $0 < s < \frac{3}{4}$, and in [103] that this result is sharp in the sense that $u_0 \notin \mathrm{H}^{\frac{3}{4},1}_{\mathrm{mix}}(\mathbb{R}^3;2)$. We combine the two statements in the following proposition.

Proposition 4.11 ([51, 103])**.** *For u_0 as in* (4.5), $u_0 \in \mathrm{H}^{s,1}_{\mathrm{mix}}(\mathbb{R}^3;2)$ *if and only if* $s < \frac{3}{4}$.

Proof. By a rotation of coordinates, this can again be reduced to an application of Lemma 4.8.

For the Fourier transform $\hat{G}$ of $G(x) := g(|x_1 - x_2|)\exp(-\frac{1}{4}|x|^2)$ with $g(r) = 1 + \frac{1}{2}r$, we find

$$\begin{aligned}\hat{G}(\xi) &= (2\pi)^{-3}\int_{\mathbb{R}^6} g(|x_1 - x_2|)e^{-\frac{1}{4}|x|^2}e^{-i\xi\cdot x}\,\mathrm{d}x \\ &= (2\pi)^{-3}\int_{\mathbb{R}^3} e^{-\frac{1}{4}|x_2|^2}e^{-\frac{i}{\sqrt{2}}(\xi_1+\xi_2)\cdot\tilde{x}_2}\,\mathrm{d}x_2 \int_{\mathbb{R}^3} g(\sqrt{2}|x_1|)e^{-\frac{1}{4}|x_1|^2}e^{-\frac{i}{\sqrt{2}}(\xi_1-\xi_2)\cdot\tilde{x}_1}\,\mathrm{d}x_1 \\ &= 2^{-3}\pi^{-\frac{3}{2}}\,e^{-\frac{1}{16}|\frac{1}{\sqrt{2}}(\xi_1+\xi_2)|^2}\int_{\mathbb{R}^3} g(\sqrt{2}|x|)e^{-\frac{1}{4}|x|^2}e^{-i\frac{1}{\sqrt{2}}(\xi_1-\xi_2)\cdot x}\,\mathrm{d}x\,.\end{aligned}$$

Note furthermore that

$$\begin{aligned}&\int_{\mathbb{R}^6}\bigl(1+|\xi|^2\bigr)\bigl(1+|\xi_1|^{2s}|\xi_2|^{2s}\bigr)\,|\hat{G}(\xi)|^2\,\mathrm{d}\xi \;= \\ &2^{-3}\pi^{-\frac{3}{2}}\int_{\mathbb{R}^6}\bigl(1+|\xi|^2\bigr)\bigl(1+\bigl(\tfrac{1}{2}|\xi_1-\xi_2||\xi_1+\xi_2|\bigr)^{2s}\bigr)\,e^{-\frac{1}{16}|\xi_2|^2}\int_{\mathbb{R}^3} g(\sqrt{2}|x|)e^{-\frac{1}{4}|x|^2}e^{-i\xi\cdot x}\,\mathrm{d}x\,\mathrm{d}\xi \qquad (4.7)\end{aligned}$$

and $|\xi_1-\xi_2||\xi_1+\xi_2| \leq \frac{1}{2}\bigl(|\xi_1-\xi_2|^2+|\xi_1+\xi_2|^2\bigr) = |\xi|^2$. Lemma 4.8 applied to $F(x) := g(\sqrt{2}|x|)e^{-\frac{1}{4}|x|^2}$, i.e., $f(r) := (1+\frac{1}{\sqrt{2}}r)e^{-\frac{1}{4}r^2}$ with $f'(0) = \frac{1}{\sqrt{2}}$, yields $|\hat{F}(\xi)| = \mathcal{O}(|\xi|^{-4})$. Hence the integral in (4.7) converges provided that

$$\int_1^\infty r^{2+4s}r^{-8}r^2\,dr < \infty\,, \qquad (4.8)$$

which holds if and only if $s < \frac{3}{4}$. Moreover, since $|\xi_1-\xi_2||\xi_1+\xi_2| \geq ||\xi_1|^2 - |\xi_2|^2|$, the integral in (4.7) restricted to $\{|\xi_1| \geq 1,\, |\xi_2| \leq 1\} \subset \mathbb{R}^6$ cannot converge unless (4.8) holds, which shows that $u_0 \notin \mathrm{H}^{s,1}_{\mathrm{mix}}$ for $s \geq \frac{3}{4}$. □

Rates for adaptive approximation by tensor product wavelet bases of the form $\{\Psi_\nu\}_{\nu\in(\nabla^{(3)})^2}$ are related to the regularity in the scale of Besov spaces $\tilde{\mathrm{B}}^s_p(\mathbb{R}^3;2)$ as defined in (3.28). The following result is contained in [51].

Theorem 4.12 ([51])**.** *For u_0 as in* (4.5)*, we have $u_0 \in \tilde{\mathrm{B}}^s_p(\mathbb{R}^3;2)$ for $0 < s < \frac{3}{2}$, but not for $s = \frac{3}{2}$, where $p^{-1} = \frac{s}{3} + \frac{1}{2}$.*

This is proven in [51] for a more general class of functions on $\Omega \times \Omega$ with bounded $\Omega \subset \mathbb{R}^3$; taking the spatial decay of u_0 into account, the proof directly carries over to $\mathbb{R}^6$.

Theorem 4.12 yields convergence of order $N^{-\frac{1}{2}+\varepsilon}$ for best N-term approximation by $\{\Psi_\nu\}_{\nu\in(\nabla^{(3)})^2}$ in $\mathrm{H}^1(\mathbb{R}^6)$, as opposed to $N^{-\frac{1}{4}+\varepsilon}$, on the basis of Proposition 4.11, for sparse grid approximation. As noted in [51], one does not obtain a better result for the scale of spaces $\tilde{\mathrm{B}}^s_p(\mathbb{R};6)$ with $p^{-1} = s+\frac{1}{2}$, i.e., approximation by $\{\Psi_\nu\}_{\nu\in\nabla^6}$.

Regularity of w_0

Note that Theorem 4.1 can be applied to (2.17), which shows $w_0 \in \mathrm{H}^{1,1}_{\mathrm{mix}}(\mathbb{R}^3;2)$. In the following, the technique of Proposition 4.11 is adapted to the explicitly correlated case to show that in fact, $w_0 \in \mathrm{H}^{s,1}_{\mathrm{mix}}(\mathbb{R}^3;2)$ for $s < \frac{7}{4}$.

Proposition 4.13. *For w_0 as in* (4.6)*, $w_0 \in \mathrm{H}^{s,1}_{\mathrm{mix}}(\mathbb{R}^3;2)$ if and only if $s < \frac{7}{4}$.*

Proof. We proceed exactly as in the proof of Proposition 4.11, with the exception that we set $g(r) := e^{-\frac{1}{2}r}(1+\frac{1}{2}r)$ and accordingly apply Lemma 4.8 to $f(r) := e^{-\frac{1}{\sqrt{2}}r}(1+\frac{1}{\sqrt{2}}r)e^{-\frac{1}{4}r^2}$. As $f'(0) = 0$, $f^{(3)}(0) \neq 0$, in this case we obtain for $F(x) = f(|x|)$ the asymptotic behaviour $|\hat{F}(\xi)| = \mathcal{O}(|\xi|^{-6})$ as $|\xi| \to \infty$. □

The regularity obtained above for u_0 is essentially determined by the term $|x_1 - x_2|$. Note that by Taylor expansion,

$$e^{-\frac{1}{2}|x_1-x_2|}\Big(1+\frac{1}{2}|x_1-x_2|\Big) = 1-\frac{1}{2}|x_1-x_2|^2+\frac{1}{24}|x_1-x_2|^3-\frac{1}{128}|x_1-x_2|^4+\frac{1}{960}|x_1-x_2|^5-\dots\ , \quad (4.9)$$

which indicates that, since $|x_1 - x_2|^2$ is smooth, the regularity of w_0 should be the same as the local regularity of $|x_1 - x_2|^3$. Indeed, this can be confirmed by making the replacement $g(r) = r^3$ in the proof of Proposition 4.13.

For the Besov regularity of w_0, by simple modifications in the proof of Theorem 4.12 in [51], we obtain the following result.

Theorem 4.14. *For w_0 as in (4.5), we have $w_0 \in \tilde{\mathrm{B}}^s_p(\mathbb{R}^3; 2)$ for $0 < s < \frac{7}{2}$, but not for $s = \frac{7}{2}$, where $p^{-1} = \frac{s}{3} + \frac{1}{2}$.*

For the adaptation of the proof of Theorem 4.12 in [51] to Theorem 4.14, we refer to Appendix A.1.

We thus obtain rates $N^{-\frac{7}{12}+\varepsilon}$ for uniform sparse grid approximation, and $N^{-\frac{7}{6}+\varepsilon}$ for adaptive approximation. Note that uniform approximation of w_0 can therefore yield slightly better convergence than adaptive approximation of u_0.

4.3 Nonlinearly Parametrized Wavelet Expansions

For the model cases of the hydrogen and hookium ground states considered in the previous section, we will in what follows explicitly construct approximations by short sums of separable functions, and subsequently analyze the approximability of the lower-dimensional factors in these approximations by wavelets. We shall eventually show that in particular for approximation of the electron-electron cusp in the hookium ground state, by such an approach – which amounts to a nonlinear parametrization of wavelet coefficients – better convergence rates can be achieved than by a direct wavelet approximation as considered in the previous section.

Note that similar separable expansions, with lower-dimensional components approximated by wavelets, have been considered numerically for quantum-chemical model functions in [25, 26, 24, 27]. The approximability of lower-dimensional components in L_2–best approximations of given rank has been studied in [146, 27]. The new contribution here is an estimate for the total complexity of such an approximation, for prescribed error in H^1, where the rank is determined by the accuracy. The relations of our results in this section to the mentioned previous work will be discussed in Section 4.4.

The approximations by sums of separable functions that we construct in this section are based on exponential sum approximations. The results on the latter, summarized in the following subsection, which will also play an important part in Chapter 6.

4.3.1 Exponential Sums

We call a function $f\colon \mathbb{R}^+ \to \mathbb{R}$ an exponential sum if it can be written in the form

$$f(t) = \omega_0 + \sum_{k=1}^{N} \omega_k e^{-\alpha_k t}$$

with $N \in \mathbb{N}$, a constant term $\omega_0 \in \mathbb{R}$, and parameters $\omega_k, \alpha_k \neq 0$. This class of functions is relevant for our purposes because on the one hand, $f(|x|^2)$ with $x \in \mathbb{R}^d$ and $d \in \mathbb{N}$ is a sum of separable functions $\exp(-\alpha_k|x|^2) = \prod_{i=1}^d e^{-\alpha_k x_i^2}$, and on the other hand, certain functions can be approximated very efficiently by exponential sums. This holds true, for instance, for $t^{-1/2}$, which leads to a separable approximation of the Coulomb potential.

Concerning the latter case, the following estimate for best approximation by exponential sums is shown in [19].

Theorem 4.15. *Let $S > 1$, then for each $N \in \mathbb{N}$ there exist $\omega_{N,k}, \alpha_{N,k} > 0$, $k = 1, \ldots, N$, such that*

$$\sup_{t\in[1,S]} \Bigl| t^{-\frac{1}{2}} - \sum_{k=1}^{N} \omega_k \exp(-\alpha_k t) \Bigr| \leq \delta(N,S) := 8\sqrt{2}\exp\Bigl(-\frac{\pi^2 N}{\ln(8S)}\Bigr) . \tag{4.10}$$

Remark 4.16. *Note that for an error $\delta > 0$ in* (4.10)*, one has to choose $N \geq \frac{1}{\pi^2}\ln(8S)\ln(8\sqrt{2}\delta^{-1}) = \mathcal{O}(\ln S|\ln\delta|)$. An approximation satisfying the error estimate on $[1,\infty)$ can be obtained by choosing $S = \exp(\pi\sqrt{2N})/8$, cf. [19], which leads to $N = \mathcal{O}(|\ln\delta|^2)$. The best approximations as in Theorem 4.15 have been computed numerically for a large range of parameters by Hackbusch [70].*

We now consider a second construction of exponential sum approximations based on sinc quadrature that yields very similar results. Although the asymptotics of the number of terms for approximations on $[1,\infty)$ are the same for both constructions, the exponential sum approximations based on Theorem 4.15 turn out to be more efficient in practice. For analytical purposes, however, we shall later need certain estimates for the respective coefficients $\omega_{N,k}$, $\alpha_{N,k}$. To our knowledge, no suitable results are available for the coefficients in Theorem 4.15. In contrast, the advantage of the approach behind the following theorem is that it yields explicit expressions for the coefficients $\omega_{N,k}$, $\alpha_{N,k}$, which we subsequently use to derive the mentioned estimates. Note also that here, one directly obtains approximation on $[1,\infty)$.

Theorem 4.17 ([73, 71])**.** *There exists $C > 0$ such that for each $\delta > 0$, there exist $N \in \mathbb{N}$ and $\omega_{N,k}, \alpha_{N,k} > 0$, $k = 1, \ldots, N$ with*

$$\sup_{t\in[1,\infty)} \Bigl| t^{-\frac{1}{2}} - \sum_{k=1}^{N} \omega_{N,k} \exp(-\alpha_{N,k} t) \Bigr| \leq \delta , \tag{4.11}$$

where $N \leq C|\ln\delta|^2$.

For the error analysis, we need the following definition from [134].

Definition 4.18. For $d > 0$, let $\mathcal{D}_d = \{z \in \mathbb{C} \colon\ |\operatorname{Im} z| < d\}$ and for $0 < \varepsilon < 1$,

$$\mathcal{D}_d(\varepsilon) = \{z \in \mathbb{C} \colon\ |\operatorname{Re} z| < \varepsilon^{-1},\ |\operatorname{Im} z| < d(1-\varepsilon)\} .$$

For u analytic in $\mathcal{D}_d$ let

$$N_1(u, \mathcal{D}_d) = \lim_{\varepsilon\to 0} \int_{\partial\mathcal{D}_d(\varepsilon)} |u(z)|\,|dz| .$$

The proof of Theorem 4.17 relies on the following theorem; we refer to [134] for a proof.

Theorem 4.19 ([134], Theorem 3.2.1)**.** *Let u be analytic in $\mathcal{D}_d$ with $N_1(u,\mathcal{D}_d) < \infty$, then*

$$\Bigl| \int_{\mathbb{R}} u(x)\,dx - h\sum_{k\in\mathbb{Z}} u(kh) \Bigr| \leq \frac{e^{-\pi d/h}}{2\sinh(\pi d/h)} N_1(u,\mathcal{D}_d) . \tag{4.12}$$

Proof of Theorem 4.17. Starting from the identity

$$\frac{1}{\sqrt{t}} = \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-ts^2}\,ds , \quad t > 0 ,$$

we obtain, by substituting $s = \ln(1+e^x)$,

$$\frac{1}{\sqrt{t}} = \frac{2}{\sqrt{\pi}} \int_{\mathbb{R}} \frac{e^{-t\ln^2(1+e^x)}}{1+e^{-x}}\,dx , \quad t > 0 . \tag{4.13}$$

Let $f(x) := (1+e^{-x})^{-1}e^{-t\ln^2(1+e^x)}$ and $\alpha(x) := \ln^2(1+e^x)$, $\omega(x) := 2\pi^{-1/2}(1+e^{-x})^{-1}$. As demonstrated in [71, Appendix D.4.3/D.4.4] (see also [73]), f is analytic in the strip $\mathcal{D}_d$ for $d \le \pi/2$ with $N_1(f,\mathcal{D}_d)$ bounded uniformly for $t \ge 1$. We can therefore use Theorem 4.19 to obtain

$$\left| \frac{1}{\sqrt{t}} - h\sum_{k\in\mathbb{Z}} \omega(kh)e^{-t\alpha(kh)} \right| \le C_a e^{-\pi^2/h}$$

with $C_a > 0$ independent of $t \ge 1$ and $h > 0$. Concerning the asymptotic decay on $\mathbb{R}$, we have

$$|f(x)| \le C_1 e^{-x^2}\,, \quad x > 0\,, \qquad |f(x)| \le C_2 e^{-|x|}\,, \quad x < 0$$

for all $t \ge 1$. As in [59, Lemma 2.4], we obtain

$$h\sum_{k>N^+} e^{-(kh)^2} \le \frac{e^{-(N^+h)^2}}{2N^+h}\,, \qquad h\sum_{k>N^-} e^{-kh} \le e^{-N^-h}\,.$$

Let $h = \pi^2/|\ln\delta|$, such that $e^{-\pi^2/h} = \delta$. We choose the minimal $N^+ \ge 1/(2h)$ such that

$$C_1(2N^+h)^{-1}e^{-(N^+h)^2} \le C_1 e^{-(N^+h)^2} \le \delta\,,$$

and the minimal N^- such that $C_2e^{-N^-h} \le \delta$. We thus obtain the assertion with $N := N^+ + N^- + 1$ and, for $k = 1,\dots,N$,

$$\omega_{N,k} := h\,\omega\big(h(k-N^- - 1)\big)\,, \quad \alpha_{N,k} := \alpha\big(h(k-N^- - 1)\big)\,. \qquad \square$$

Corollary 4.20. *The coefficients* $\alpha_{N,k}$, $\omega_{N,k}$ *in Theorem 4.17 satisfy*

$$\frac{\omega_{N,k}}{\sqrt{\alpha_{N,k}}} \le \pi^2|\ln\delta|^{-1}\,, \quad k = 1,\dots,N\,.$$

Proof. Using the definitions in the proof of Theorem 4.17, we have

$$\max_{k\in\{-N^-,\dots,N^+\}} \frac{h\,\omega(hk)}{\sqrt{\alpha(hk)}} \le \pi^2|\ln\delta|^{-1}\sup_{x\in\mathbb{R}}\big((1+e^{-x})\ln(1+e^x)\big)^{-1} \le \pi^2|\ln\delta|^{-1}\,. \qquad \square$$

Corollary 4.21. *The coefficients* $\alpha_{N,k}$, $\omega_{N,k}$, $k = 1,\dots,N$, *in Theorem 4.17 satisfy*

$$\max_k \omega_{N,k} \le c_1|\ln\delta|^{-1}\,, \tag{4.14}$$

$$\max_k \alpha_{N,k} \le c_2|\ln\delta|^{\frac{1}{2}}\,, \tag{4.15}$$

$$\max_k\Big(\frac{\omega_{N,k}}{\alpha_{N,k}}\Big) \le c_3\delta^{-1}|\ln\delta|^{-1}\,, \tag{4.16}$$

$$\sum_k \omega_{N,k} \le c_4|\ln\delta|^{\frac{1}{2}}\,. \tag{4.17}$$

Proof. We adopt the definitions of Theorem 4.17. For $x \ge 1/2$, we have $\ln(1+e^x) \lesssim x$. Since either $N^+ \le (2h)^{-1}+1$ or $C_1e^{-(N^+-1)^2h^2} \ge \delta$, we have $N^+ \lesssim |\ln\delta|^{3/2}$ and thus $\alpha(N^+h) \lesssim |\ln\delta|^{1/2}$, we obtain (4.15). Uniform boundedness of ω is clear, which together with $h = \pi^2/|\ln\delta|$ implies (4.14). Note that ω/α is uniformly bounded on $[0,\infty)$ and strictly decreasing on $(-\infty,0)$. Using $C_2\exp(-(N^- - 1)h) \ge \delta$, which yields $\ln(C_2\delta^{-1})/h \le N^- \le 1 + \ln(C_2\delta^{-1})/h$, we obtain

$$\frac{\omega(-N^-h)}{\alpha(-N^-h)} \le \frac{1}{(1+C_2\delta^{-1})\ln^2(1+e^hC_2^{-1}\delta)} \lesssim \delta^{-1}\,,$$

which we again combine with the definition of h. Concerning the estimate (4.17), note that ω is integrable on $(-\infty,0]$ and $\omega \leq 1$ on $[0,\infty)$, and that by the definition of N^+, we have $N^+ \lesssim |\ln\delta|^{3/2}$, and hence

$$\sum_k \omega_{N,k} \lesssim \int_{-\infty}^0 \omega \, \mathrm{d}x + N^+ h \lesssim 1 + |\ln\delta|^{-1} |\ln\delta|^{3/2} \lesssim |\ln\delta|^{1/2} . \qquad \square$$

Theorem 4.17 will be instrumental in the construction of separable approximations of the ground state of hookium. For the ground states of hydrogenic systems and the explicitly correlated formulation for hookium, we instead need the following theorem.

Theorem 4.22. *Let $\rho \in (0,\rho_0]$ for a $\rho_0 > 0$. There exists $C > 0$ that may depend on ρ_0 such that for each $\delta > 0$,*

(i) *there exist $N \in \mathbb{N}$ and $\omega_{N,k}, \alpha_{N,k} > 0$, $k = 1,\dots,N$ with*

$$\sup_{t\in[1,\infty)} \left| e^{-\rho\sqrt{t}} - \sum_{k=1}^N \omega_{N,k} \exp(-\alpha_{N,k} t) \right| \leq \rho^{-1}\delta ,$$

where $N \leq C|\ln\delta|^2$,

(ii) *there exist $N \in \mathbb{N}$ and $\omega_{N,k}, \alpha_{N,k} > 0$, $k = 1,\dots,N$ with*

$$\sup_{t\in[1,\infty)} \left| t^{-\frac{1}{2}} e^{-\rho\sqrt{t}} - \sum_{k=1}^N \omega_{N,k} \exp(-\alpha_{N,k} t) \right| \leq \delta ,$$

where $N \leq C|\ln\delta|^2$.

Proof. We first consider part (i). The inverse Laplace transform yields

$$e^{-\rho\sqrt{t}} = \int_0^\infty \frac{\rho e^{-\frac{\rho^2}{4}s^{-1}}}{2\sqrt{\pi} s^{3/2}} e^{-ts} \, \mathrm{d}s = \frac{1}{\sqrt{\pi}} \int_0^\infty \rho s^{-2} e^{-\frac{\rho^2}{4}s^{-2}} e^{-ts^2} \, \mathrm{d}s .$$

Substituting $s = \ln(1+e^x)$, we obtain the representation

$$e^{-\rho\sqrt{t}} = \frac{1}{\sqrt{\pi}} \int_{\mathbb{R}} \frac{\rho e^{-\frac{\rho^2}{4}\ln^{-2}(1+e^x)}}{\ln^2(1+e^x)} \frac{e^{-t\ln^2(1+e^x)}}{(1+e^{-x})} \, \mathrm{d}x . \tag{4.18}$$

Note that the integrands in (4.13) in the proof of Theorem 4.17 and in (4.18) differ only by the factor

$$g_\rho(x) := \rho \ln^{-2}(1+e^x) e^{-\frac{\rho^2}{4}\ln^{-2}(1+e^x)} .$$

We show that $|g_\rho| \leq C_{\rho_0,d}\rho^{-1}$, with a $C_{\rho_0,d} > 0$, in any strip $\mathcal{D}_d = \{z \in \mathbb{C} \colon |\operatorname{Im} z| < d\}$ with $d < \frac{\pi}{4}$, and can subsequently treat the remaining integrand exactly as in the proof of Theorem 4.17.

Note first that g_ρ is analytic on $\mathcal{D}_d$ because $\ln(1+e^z) \neq 0$ for all $z \in \mathcal{D}_d$. Let $y \in \mathbb{R}$ with $|y| < d$, then by the assumptions on d, we have $\cos^2 y - \sin^2 y > \cos^2 d - \sin^2 d$. For $x, y \in \mathbb{R}$ such that $x + iy \in \mathcal{D}_d$, let $a(x,y) := \operatorname{Re}\ln(1+e^{x+iy})$ and $b(x,y) := \operatorname{Im}\ln(1+e^{x+iy})$, then exponentiation yields $e^a(\cos b + i\sin b) = 1 + e^x\cos y + ie^x \sin y$ and thus

$$a(x,y) = \frac{1}{2}\ln(1+2e^x\cos y + e^{2x}) , \quad b(x,y) = \arctan\frac{\sin y}{e^{-x}+\cos y} . \tag{4.19}$$

Setting $h(x,y) := |g_\rho(x+iy)|$ for $x, y \in \mathbb{R}$, $|y| < d$, we have

$$h = \left|\rho(a+ib)^{-2} e^{-\frac{\rho^2}{4}(a+ib)^{-2}}\right| = \rho(a^2+b^2)^{-1} e^{-\frac{a^2-b^2}{4}\rho^2(a^2+b^2)^{-2}} . \tag{4.20}$$

We thus need to estimate the right hand side of (4.20). Since $d < \frac{\pi}{4}$, we have $\cos^2 d > \sin^2 d$ and can therefore choose $\varepsilon > 0$ with $\varepsilon < \frac{1}{2}(\cos^2 d - \sin^2 d)$. It follows from (4.19) by Taylor expansion of $\ln(1+\cdot)$ and of arctan at zero that there exists $x_d \in \mathbb{R}$ such that for all $x < x_d$ and y with $|y| \le d$, we have

$$(1-\varepsilon)e^x \cos y \le a(x,y) \le (1+\varepsilon)e^x \cos y\,, \qquad b(x,y) \le (1+\varepsilon)e^x \sin y\,.$$

For $x \ge x_d$, since $|b(x,y)| \le |y| < \frac{\pi}{4}$ for all x, we have the estimate

$$\rho\, h(x,y) \le \rho_0^2\, a^{-1}(x_d,d)\, e^{\frac{(\rho_0\pi)^2}{16} a^{-2}(x_d,d)}\,, \tag{4.21}$$

i.e., a uniform bound depending only on ρ_d and d. For $x < x_d$, noting that $\cos^2 y - \sin^2 y > \cos^2 d - \sin^2 d$ as a consequence of $|y| < d < \frac{\pi}{4}$, we obtain

$$\begin{aligned}\frac{a^2-b^2}{a^2+b^2} &\ge \frac{(1-\varepsilon)\cos^2 y - (1+\varepsilon)\sin^2 y}{(1+\varepsilon)\cos^2 y + (1+\varepsilon)\sin^2 y} \\ &= \frac{\cos^2 y - \sin^2 y - \varepsilon}{1+\varepsilon} > \frac{1}{4}(\cos^2 y - \sin^2 y) \ge \frac{1}{4}(\cos^2 d - \sin^2 d) =: \gamma_d > 0\,.\end{aligned}$$

Consequently, for $x < x_d$,

$$\rho h = \rho^2(a^2+b^2)^{-1} e^{-\frac{a^2-b^2}{4}\rho^2(a^2+b^2)^{-2}} \le \rho^2(a^2+b^2)^{-1} e^{-\frac{\gamma_d}{4}\rho^2(a^2+b^2)^{-1}} \le \frac{4}{\gamma_d}\,,$$

which combined with (4.21) yields $|g_\rho(x+iy)| = h(x,y) \le \rho^{-1} C_{\rho_0,d}$ for $x+iy \in \mathcal{D}_d$.

For part (ii), we again use the inverse Laplace transform to obtain the representation

$$\frac{e^{-\rho\sqrt{t}}}{\sqrt{t}} = \int_0^\infty \frac{e^{-\frac{\rho^2}{4}s^{-1}}}{\sqrt{\pi s}} e^{-ts}\,\mathrm{d}s = \frac{2}{\sqrt{\pi}} \int_{\mathbb{R}} e^{-\frac{\rho^2}{4}\ln^{-2}(1+e^x)} \frac{e^{-t\ln^2(1+e^x)}}{1+e^{-x}}\,\mathrm{d}x\,. \tag{4.22}$$

We proceed similarly to part (i) by establishing a uniform bound for $\tilde{h}(x,y) := \left|e^{-\frac{\rho^2}{4}\ln^{-2}(1+e^{x+iy})}\right|$ for $x+iy \in \mathcal{D}_d$, $d < \frac{\pi}{4}$. As in (4.20), we find

$$\tilde{h} \le e^{-\frac{a^2-b^2}{4}\rho^2(a^2+b^2)^{-2}} \le e^{\pi^{-2}\rho_0^2} =: \tilde{C}_{\rho_0}\,.$$

For both parts (i) and (ii), the remaining integrand $(1+e^{-x})^{-1}e^{-t\ln^2(1+e^x)}$ can now be treated exactly as in the proof of Theorem 4.17, which yields the statements (i) and (ii), again with the choice $h = \pi^2/|\ln\delta|$. □

Remark 4.23. *As can be seen from* (4.22)*, the statement of Corollary 4.21 also holds for* $\omega_{N,k}$*,* $\alpha_{N,k}$ *as in part (ii) of Theorem 4.22; in the same way, one also finds*

$$\max_{k=1,\dots,N}\left(\frac{\omega_{N,k}}{\alpha_{N,k}^2}\right) \le c_3\delta^{-3}|\ln\delta|^{-1}\,.$$

Similar estimates for the coefficients in part (i) are possible, but will not be required in what follows.

Remark 4.24. *There is a connection between the two types of exponential sum approximations in Theorem 4.15 and in Theorems 4.17, 4.22. The proof of Theorem 4.15 in [19] (see also [18]) relies on the assumption that the function* f *to be approximated, e.g.* $f(t) = t^{-\frac{1}{2}}$*,* is completely monotone, *that is,* $(-1)^k f^{(k)}(t) \ge 0$ *for all* $k \in \mathbb{N}_0$ *and* $t \in (0,\infty)$*. By the Bernstein-Widder theorem [23],* f

is completely monotone if and only if there exists a nonnegative measure μ *on* $[0,\infty)$ *such that*

$$f(t) = \int_0^\infty e^{-tx}\, d\mu(x)\,.$$

This provides the link to the existence of an inverse Laplace transform of f*, which forms the basis of the second approach based on sinc quadrature. In view of these very restrictive conditions on* f*, it is clear that results on approximation by exponential sums as considered in this section can be expected to hold only for very specific functions.*

4.3.2 Hydrogen

As a first example, we employ Theorem 4.22 to explicitly construct separable approximations for the ground state of hydrogen.

Theorem 4.25. *Let* $\gamma > 0$ *and* $u(x) = \exp(-\gamma|x|)$ *for* $x \in \mathbb{R}^3$*. Then for* $\varepsilon > 0$ *there exist* $N \lesssim |\ln \varepsilon|^2$ *and* $f_k \in \mathrm{C}_0^\infty(\mathbb{R})$*,* $k = 0, \ldots, N$*, such that*

$$\|u - \tilde u\|_{\mathrm{H}^1(\mathbb{R}^3)} \le \varepsilon\,, \qquad \tilde u(x) := \sum_{k=0}^{N} \prod_{i=1}^{3} f_k(x_i)\,, \quad x \in \mathbb{R}^3\,.$$

Note that as a consequence of the symmetries of the function to be approximated, we can take the univariate components f_k of each summand in the separable approximation $\tilde u$ to be the same for each coordinate direction, that is, each summand is the threefold tensor product of a single function.

Remark 4.26. *To enable estimates for the convergence rates that can be achieved by wavelet approximation of the* f_k*, we need to control the quantities* $\max_k \omega_k$*,* $\max_k \alpha_k$*,* $\max_k(\omega_k/\alpha_k)$*, and* $\sum_k \omega_k$ *in dependence on a prescribed error in the corresponding exponential sum approximation; we therefore use a separable approximation based on Theorem 4.17 rather than on Theorem 4.15.*

Proof of Theorem 4.25. Let $q(t) := e^{-\gamma\sqrt{t}}$, so that $q(|x|^2) = e^{-\gamma|x|}$. As our aim is to approximate u with respect to the H^1–norm, we construct a $\tilde q$ such that both $|q - \tilde q|$ and $|q' - \tilde q'|$ are sufficiently small on a certain interval. To achieve this, we first approximate q' by exponential sums and obtain an approximation to q by integration.

Since $q'(t) = -\gamma e^{-\gamma\sqrt{t}}/(2\sqrt{t})$, for any $r > 0$ and $\delta > 0$, Theorem 4.22 ensures the existence of ω_k, α_k, $k = 1, \ldots, N$ with $N \lesssim |\ln \delta|^2$, such that

$$\sup_{t\in[r^2,\infty)} |q'(t) - \tilde p(t)| \le \frac{\gamma}{2r}\delta\,, \quad \tilde p(t) := \sum_{k=1}^{N} \Bigl(\frac{\gamma}{2} r^{-1}\omega_k\Bigr) e^{-r^{-2}\alpha_k t}\,.$$

Let

$$\tilde q(t) := -\sum_{k=1}^{N} \frac{\gamma r \omega_k}{2\alpha_k}\, e^{-r^{-2}\alpha_k t} + \sum_{k=1}^{N} \frac{\gamma r\omega_k}{2\alpha_k} e^{-\alpha_k} + q(r^2)\,,$$

so that $\tilde q' = \tilde p$, and hence for $t \in [r^2, \infty)$,

$$\bigl|q(t) - \tilde q(t)\bigr| \le \left|\int_{r^2}^{t} q'(\tau) - \tilde q'(\tau)\,\mathrm{d}\tau\right| \le (t - r^2)\frac{\gamma}{2r}\,\delta\,. \tag{4.23}$$

For $t \in (0, r^2)$, by the mean value theorem and Remark 4.23, we have

$$|q(t) - \tilde q(t)| \le |q(t) - q(r^2)| + r\sum_k \frac{\gamma\omega_k}{2\alpha_k} |e^{-\alpha_k} - e^{-r^{-2}\alpha_k t}| \le \Bigl(\gamma + \frac{\gamma}{2}\sum_k \omega_k\Bigr) r \lesssim \gamma\bigl(1 + |\ln\delta|^{\frac12}\bigr) r$$

as well as

$$\sqrt{t}|q'(t) - \tilde{q}'(t)| \leq \frac{\gamma}{2} + \frac{\gamma}{2}\sum_k \omega_k \lesssim \gamma\bigl(1 + |\ln\delta|^{\frac{1}{2}}\bigr)\,.$$

As can be seen from (4.23), the family of functions $\tilde{q}$ we have thus obtained can be made to approximate q on any fixed bounded interval contained in $[r^2, \infty)$ to any accuracy, by choosing δ sufficiently small. However, $\tilde{q}(t)$ grows linearly as $t \to \infty$. To obtain the desired approximation to u on all of $\mathbb{R}^3$, we thus multiply $\tilde{q}(|x|^2)$ by a suitable separable cutoff function and use the exponential decay of u.

To this end, for $R > 0$, we define a family of cutoff functions $\theta_R \in \mathrm{C}_0^\infty(\mathbb{R})$ with $\operatorname{supp}\theta_R \subseteq (-R-1, R+1)$, $\theta_R \leq 1$ on $\mathbb{R}$ and $\theta_R \equiv 1$ on $[-R, R]$, and $\|\mathrm{D}^n\theta_R\|_\infty \leq c_n$ for $n \in \mathbb{N}$, with $c_n > 0$ independent of R.

Let $\hat{u}(x) := \tilde{q}(|x|^2)$ and $\tilde{u} := \hat{u}\,\Theta_R$, where $\Theta_R(x) := \prod_i \theta_R(x_i)$, and with $R > r$ to be determined. This amounts to the choice, for $k = 1, \ldots, N$,

$$f_0(x) := \Bigl(\sum_l \frac{\gamma r \omega_l}{2\alpha_l} e^{-\alpha_l} + q(r^2)\Bigr)^{\frac{1}{3}} \theta_R(x)\,, \quad f_k(x) := -\Bigl(\frac{\gamma r \omega_k}{2\alpha_k}\Bigr)^{\frac{1}{3}} \theta_R(x)\, e^{-r^{-2}\alpha_k x^2}\,. \tag{4.24}$$

Then on the one hand,

$$\begin{aligned}\int_{\{|x|\leq r\}} |u - \tilde{u}|^2 + |\mathrm{D}(u-\tilde{u})|^2 \,\mathrm{d}x &= \int_{\{|x|\leq r\}} \bigl|q(|x|^2) - \tilde{q}(|x|^2)\bigr|^2 + 4|x|^2\bigl|q'(|x|^2) - \tilde{q}'(|x|^2)\bigr|^2 \,\mathrm{d}x \\ &\lesssim \int_0^r \rho^2\bigl(\bigl|q(\rho^2) - \tilde{q}(\rho^2)\bigr|^2 + 4\rho^2\bigl|q'(\rho^2) - \tilde{q}'(\rho^2)\bigr|^2\bigr)\,\mathrm{d}\rho \\ &\lesssim \gamma^2\bigl(1 + |\ln\delta|^{\frac{1}{2}}\bigr)^2 r^3\,,\end{aligned}$$

and on the other hand

$$\begin{aligned}&\int_{\{|x|\geq r\}} |u - \Theta_R\hat{u}|^2 + |\mathrm{D}(u - \Theta_R\hat{u})|^2 \,\mathrm{d}x \\ &\qquad\lesssim \int_{\{|x|\geq r\}} |u - \Theta_R\hat{u}|^2 + |\mathrm{D}u - \Theta_R\mathrm{D}\hat{u}|^2 + |\mathrm{D}\Theta_R|^2(|u|^2 + |u - \hat{u}|^2)\,\mathrm{d}x\,.\end{aligned}$$

The latter expression can be estimated further by

$$\begin{aligned}\int_{\{|x|\geq r\}} |u - \Theta_R\hat{u}|^2 + |\mathrm{D}u - \Theta_R\mathrm{D}\hat{u}|^2 \,\mathrm{d}x &\leq \int_{\{r\leq|x|\leq\sqrt{3}(R+1)\}} |u - \hat{u}|^2 + |\mathrm{D}(u-\hat{u})|^2\,\mathrm{d}x \\ &\quad + \int_{\{|x|\geq R\}} |u|^2 + |\mathrm{D}u|^2\,\mathrm{d}x \\ &\lesssim (\gamma r^{-1}\delta)^2(R^7 + R^3) + (1+\gamma)R^2 e^{-2\gamma R}\end{aligned}$$

and by

$$\int_{\mathbb{R}^3} |\mathrm{D}\Theta_R|^2(|u| + |u - \hat{u}|^2)\,\mathrm{d}x \lesssim R^2 e^{-2\gamma R} + R^4(\gamma r^{-1}\delta)^2\,.$$

Thus in summary,

$$\|u - \tilde{u}\|_{\mathrm{H}^1(\mathbb{R}^3)} \lesssim \gamma\bigl(1 + |\ln\delta|^{\frac{1}{2}}\bigr)r^{\frac{3}{2}} + (R^{\frac{7}{2}} + R^{\frac{3}{2}})\gamma r^{-1}\delta + R\sqrt{1+\gamma}\,e^{-\gamma R}\,.$$

Accordingly, for given $\varepsilon > 0$ we choose $R \sim |\ln\varepsilon|$ and $r \sim (\varepsilon|\ln\varepsilon|^{-\frac{1}{2}})^{\frac{2}{3}}$, which yields $(R^{\frac{7}{2}} + R^{\frac{3}{2}})r^{-1} \lesssim \varepsilon^{-\frac{2}{3}}|\ln\varepsilon|^{\frac{23}{6}}$. Thus, choosing $\delta \sim \varepsilon^{\frac{5}{3}}|\ln\varepsilon|^{-\frac{23}{6}}$, we obtain $|\ln\delta| \lesssim |\ln\varepsilon|$ and hence the assertion. □

Remark 4.27. *As it involves cancellation of terms that are unbounded as $\varepsilon \to 0$, the particular separable approximation provided by Theorem 4.25 is numerically unstable. Gram-Schmidt orthog-*

onalization with respect to the L_2*-inner product, however, yields the representation*

$$\tilde{u}(x) = \sum_{k_1=0}^{N}\sum_{k_2=0}^{N}\sum_{k_3=0}^{N} a_{k_1,k_2,k_3}\, g_{k_1}(x_1)\, g_{k_2}(x_2)\, g_{k_3}(x_3) \tag{4.25}$$

with pairwise L_2*-orthogonal* g_k*, and* $\|\tilde{u}\|^2_{\mathrm{L}_2(\mathbb{R}^3)} = \sum_k |a_{k_1,k_2,k_3}|^2$*. This corresponds to the so-called Tucker tensor format, which will be discussed in more detail in Chapter 5.*

Theorem 4.25 provides an explicit construction of approximations to hydrogenic ground state eigenfunctions by sums of separable functions, which converge almost exponentially in H^1–norm with respect to the number of summands. It should be emphasized, however, that we do not have a direct numerical application of this type of construction in mind. The functions f_k we have obtained are rather unsuitable for such purposes due to the ill-conditioning of the expansion, as noted in Remark 4.27. Applying the orthogonalization leading to the representation (4.25) does not mitigate this problem, since the representation of the new tensor factors g_k in terms of the f_k will generally again be ill-conditioned.

The result of Theorem 4.25 is therefore of interest mainly in ensuring the existence of a separable expansion of a certain rank for each given error tolerance. For making use of this property numerically, our aim will eventually be to find univariate tensor factors that are finite linear combinations of functions from a reference basis with more favorable numerical properties. Specifically, for a suitable orthonormal wavelet basis $\{\psi_\nu\}_{\nu\in\nabla}$ on $\mathbb{R}$, in Chapter 5 we propose iterative schemes for directly computing coefficients (a_{k_1,k_2,k_3}) and $U^{(i)}_{k,\nu}$ with

$$u(x) \approx \sum_{k_1=0}^{N}\sum_{k_2=0}^{N}\sum_{k_3=0}^{N} a_{k_1,k_2,k_3} \prod_{i=1}^{3}\Bigl(\sum_{\nu\in\nabla} U^{(i)}_{k_i,\nu}\psi_\nu(x_i)\Bigr)\,, \tag{4.26}$$

where due to the symmetries of the function to be approximated, we can take $U^{(i)}_{k,\nu} = U_{k,\nu}$ for $i = 1,2,3$ with some $U_{k,\nu}$ independent of i. Note that the role that was played by the functions g_k in (4.25) is in (4.26) taken by the expansions $\sum_{\nu\in\Lambda_k\subset\nabla} U_{k,\nu}\psi_\nu$. We can also interpret (4.26) as a nonlinear parametrization of wavelet coefficients,

$$\langle u, \Psi_\nu\rangle \approx \sum_{k_1,k_2,k_3=0}^{N} a_{k_1,k_2,k_3} \prod_{i=1}^{3} U^{(i)}_{k_i,\nu_i}\,, \quad \nu = (\nu_1,\nu_2,\nu_3)\in\nabla^3\,.$$

The question we address next is the efficiency of approximations of the form (4.26) in terms of number of coefficients, that is, we ask for the asymptotic behaviour of the number of nonzero coefficients $\#\operatorname{supp} U^{(i)}_k$ required for a certain target error. We shall compare the results to the case of linearly parametrized wavelet expansions

$$u(x) \approx \sum_{\nu\in\Lambda\subset\nabla^3} u_\nu \prod_{i=1}^{3}\psi_{\nu_i}(x_i)\,,$$

which have been considered in Section 4.2.

We will obtain the desired results on $\#\operatorname{supp} U_{k,\nu}$, which are summarized in Theorem 4.29 below, by studying the approximability of the functions f_k provided by Theorem 4.25. These functions are smooth, but their derivatives depend on the exponents in the underlying exponential sum approximations, which in turn depend on the desired approximation error. The following lemma summarizes the scaling of relevant norms with respect to these exponents.

Lemma 4.28. *Let* $\gamma > 0$*, then for* $u(x) := e^{-\gamma x^2}$*,* $x \in \mathbb{R}$*, we have*

$$\|u\|_{\mathrm{L}_p(\mathbb{R})} = \Big(\frac{\pi}{\gamma p}\Big)^{\frac{1}{2p}}\,, \quad p > 0\,, \tag{4.27}$$

$$|u|_{\mathrm{H}^s(\mathbb{R})} \leq \sqrt{\Gamma(s+\tfrac{1}{2})}\,(2\gamma)^{\frac{s}{2}-\frac{1}{4}}\,, \quad s > 0\,, \tag{4.28}$$

and for $s \in \mathbb{R}^+$ *with* $s > 1$*,*

$$\|u\|_{\mathrm{B}^s_{p,p}} \leq C_s\big(1 + \gamma^{-\frac{1}{2}s+\frac{1}{4}} + \gamma^{\frac{1}{2}} + \gamma^{\frac{1}{2}+\tau}\big)\,, \quad p^{-1} = (s-1) + \frac{1}{2}\,, \tag{4.29}$$

where $\tau \in (0, \frac{1}{2}]$*. If in addition* $\kappa \in \mathrm{C}^\infty_0(\mathbb{R})$ *with* $\|\kappa\|_\infty \leq 1$*, then*

$$|\kappa u|_{\mathrm{H}^n(\mathbb{R})} \leq C_n c^*_n\big(\sqrt{|\operatorname{supp}\kappa|} + \gamma^{\frac{n}{2}-\frac{1}{4}}\big)\,, \quad n \in \mathbb{N}\,, \tag{4.30}$$

$$\|\kappa u\|_{\mathrm{B}^s_{p,p}(\mathbb{R})} \leq C_s C^*_\kappa(s)\,\big(1 + |\operatorname{supp}\kappa|^{s-\frac{1}{2}} + \gamma^{\frac{1}{2}} + \gamma^{\frac{1}{2}+\tau}\big)\,, \quad p^{-1} = (s-1) + \frac{1}{2}\,, \tag{4.31}$$

where $c^*_n := 1 + \max_{1\leq m\leq n}\|\mathrm{D}^m\kappa\|_\infty$ *and* $C^*_s := c^*_{\lfloor s+\frac{1}{2}\rfloor+1}$*, and* $\tau \in (0, \frac{1}{2}]$*.*

For the proof of Lemma 4.28, see Appendix A.2.

Theorem 4.29. *Let* $\gamma > 0$ *and* $u(x) = \exp(-\gamma|x|)$ *for* $x \in \mathbb{R}^3$*, and let* $\{\psi_\nu\}_{\nu\in\nabla}$ *be a wavelet basis for* $\mathrm{L}_2(\mathbb{R})$ *such that* $\{2^{-|\nu|}\psi_\nu\}$ *is a Riesz basis of* $\mathrm{H}^1(\mathbb{R})$*. Then for each* $\varepsilon > 0$*,* u *has an approximation* $\tilde{u}$ *with* $\|u - \tilde{u}\|_{\mathrm{H}^1(\mathbb{R}^3)} \lesssim \varepsilon$ *of the form*

$$\tilde{u} = \sum_{k_1=0}^{N}\sum_{k_2=0}^{N}\sum_{k_3=0}^{N} a_{k_1,k_2,k_3} \bigotimes_{i=1}^{3}\Big(\sum_{\nu_i\in\nabla} U_{k_i,\nu_i}\psi_{\nu_i}\Big)\,, \tag{4.32}$$

where $N \lesssim |\ln\varepsilon|^2$*,* $\langle U_{k,\cdot}, U_{l,\cdot}\rangle = \delta_{kl}$*, and* $\operatorname{supp} U_{k,\cdot} \subseteq \Lambda_k$ *for* $\Lambda_k \subset \nabla$*, where for* $\#\Lambda_k$ *the following holds:*

(i) (uniform approximation)
If $\{\psi_\nu\}$ *satisfies a direct estimate for* $\mathrm{H}^n(\mathbb{R})$ *with integer* $n > 1$*, and* Λ_k *are chosen as* $\Lambda_k := \Lambda_\varepsilon$*, where*

$$\Lambda_\varepsilon := \{\nu\colon\ \operatorname{supp}\psi_\nu \cap [-K_\varepsilon, K_\varepsilon] \neq \emptyset \text{ and } |\nu| \leq j_\varepsilon\} \tag{4.33}$$

with $K_\varepsilon > 0$*,* $K_\varepsilon \sim |\ln\varepsilon|$ *and* $j_\varepsilon \in \mathbb{Z}_{j_0}$ *chosen appropriately as specified in the proof, then* $\#\Lambda_\varepsilon \lesssim \varepsilon^{-\frac{2}{3}c_1(n)}|\ln\varepsilon|^{2c_2(n)}$ *where* $c_1(n), c_2(n) \downarrow 1$ *as* $n \to \infty$*.*

(ii) (adaptive approximation)
If $\{\psi_\nu\}$ *satisfies the norm equivalence* (3.11) *for* $\mathrm{B}^s_{p,p}(\mathbb{R})$ *with* $p^{-1} = (s-1) + \frac{1}{2}$*, then* Λ_k *can be chosen such that* $\#\Lambda_k \lesssim \varepsilon^{-c_3(s)}|\ln\varepsilon|^{2+c_4(s)}$*, where* $c_3(s), c_4(s) \downarrow 0$ *as* $s \to \infty$*.*

Note that the coefficients $U_{k,\nu}$ in the representation (4.32) are the same for all coordinate directions, which is a consequence of the symmetries of u and the approximations constructed in Theorem 4.25.

Proof. For $\varepsilon > 0$, let f_k for $k = 0, \dots, N$ be as in the statement of Theorem 4.25, i.e., as defined in (4.24), and let R and θ_R be chosen as in the corresponding proof. Each f_k is a multiple of $\theta_R\, e^{-\tilde{\alpha}|\cdot|^2}$ with $\tilde{\alpha} \geq 0$, where by the choice of r and $\{\alpha_k\}$ in the proof of Theorem 4.25, and by Remark 4.23,

$$\tilde{\alpha} \leq r^{-2} \max_{k=1,\dots,N} \alpha_k \lesssim \varepsilon^{-\frac{4}{3}}|\ln\varepsilon|^{\frac{7}{6}}\,. \tag{4.34}$$

With $K_\varepsilon := R + 1$, let Λ_ε be defined as in (4.33), with j_ε to be determined. Let $f_{k,\varepsilon}$ be defined as the projection of f_k onto $\operatorname{span}\{\psi_\nu\}_{\nu\in\Lambda_\varepsilon}$, then

$$\begin{aligned}\bigl\|\textstyle\bigotimes_{i=1}^3 f_k - \bigotimes_{i=1}^3 f_{k,\varepsilon}\bigr\|_{\mathrm{H}^1} \leq \|(f_k - f_{k,\varepsilon})\otimes f_k \otimes f_k\|_{\mathrm{H}^1} \\ + \|f_{k,\varepsilon}\otimes (f_k - f_{k,\varepsilon})\otimes f_k\|_{\mathrm{H}^1} + \|f_{k,\varepsilon}\otimes f_{k,\varepsilon}\otimes (f_k - f_{k,\varepsilon})\|_{\mathrm{H}^1}\end{aligned}$$

In view of Lemma 3.15, the right hand side can be estimated by

$$\begin{aligned}&\|f_k - f_{k,\varepsilon}\|_{\mathrm{H}^1}\|f_k\|_{\mathrm{L}_2}^2 + 2\|f_k - f_{k,\varepsilon}\|_{\mathrm{L}_2}\|f_k\|_{\mathrm{H}^1}\|f_k\|_{\mathrm{L}_2} \\ &\quad + \|f_k - f_{k,\varepsilon}\|_{\mathrm{H}^1}\|f_k\|_{\mathrm{L}_2}\|f_{k,\varepsilon}\|_{\mathrm{L}_2} + \|f_k - f_{k,\varepsilon}\|_{\mathrm{L}_2}(\|f_{k,\varepsilon}\|_{\mathrm{H}^1}\|f_k\|_{\mathrm{L}_2} + \|f_k\|_{\mathrm{H}^1}\|f_{k,\varepsilon}\|_{\mathrm{L}_2}) \\ &\qquad + \|f_k - f_{k,\varepsilon}\|_{\mathrm{H}^1}\|f_{k,\varepsilon}\|_{\mathrm{L}_2}^2 + 2\|f_k - f_{k,\varepsilon}\|_{\mathrm{L}_2}\|f_{k,\varepsilon}\|_{\mathrm{H}^1}\|f_{k,\varepsilon}\|_{\mathrm{L}_2}\,.\end{aligned}$$

Note that by the Riesz basis property for L_2 and H^1, we have $\|f_{k,\varepsilon}\|_{\mathrm{L}_2} \lesssim \|f_k\|_{\mathrm{L}_2}$ as well as $\|f_{k,\varepsilon}\|_{\mathrm{H}^1} \lesssim \|f_k\|_{\mathrm{H}^1}$. From the above, we thus obtain

$$\bigl\|\textstyle\bigotimes_{i=1}^3 f_k - \bigotimes_{i=1}^3 f_{k,\varepsilon}\bigr\|_{\mathrm{H}^1} \lesssim \|f_k\|_{\mathrm{L}_2}\|f_k\|_{\mathrm{H}^1}\|f_k - f_{k,\varepsilon}\|_{\mathrm{H}^1}\,. \tag{4.35}$$

We consider f_k for $k \geq 1$, where by (4.34), the choice of δ in the proof of Theorem 4.25, Remark 4.23, and (4.16) we find

$$\frac{r\omega_k}{\alpha_k} \lesssim \varepsilon^{\frac{2}{3}}|\ln\varepsilon|^{-\frac{1}{3}}\varepsilon^{-\frac{5}{3}}|\ln\varepsilon|^{\frac{23}{6}}|\ln\varepsilon|^{-1} = \varepsilon^{-1}|\ln\varepsilon|^{\frac{15}{6}}\,.$$

Combining this with Lemma 4.28, we obtain

$$\begin{aligned}\|f_k\|_{\mathrm{L}_2}\|f_k\|_{\mathrm{H}^1}\|f_k - f_{k,\varepsilon}\|_{\mathrm{H}^1} &\lesssim \varepsilon^{-1}|\ln\varepsilon|^{\frac{15}{6}}|\ln\varepsilon|^{\frac{1}{2}}\bigl(|\ln\varepsilon|^{\frac{1}{2}} + \varepsilon^{-\frac{1}{3}}|\ln\varepsilon|^{\frac{7}{24}}\bigr) \\ &\qquad \times 2^{-(n-1)j_\varepsilon}\bigl(|\ln\varepsilon|^{\frac{1}{2}} + \varepsilon^{-\frac{2}{3}n+\frac{1}{3}}|\ln\varepsilon|^{\frac{7}{12}n-\frac{7}{24}}\bigr) \\ &\lesssim 2^{-(n-1)j_\varepsilon}\varepsilon^{-\frac{2}{3}n-1}|\ln\varepsilon|^{\frac{7}{12}n+2}\,.\end{aligned} \tag{4.36}$$

Similarly,

$$\begin{aligned}\|f_0\|_{\mathrm{L}_2}\|f_0\|_{\mathrm{H}^1}\|f_0 - f_{0,\varepsilon}\|_{\mathrm{H}^1} &\lesssim \bigl(|\ln\varepsilon|^2\varepsilon^{-1}|\ln\varepsilon|^{\frac{15}{6}}\bigr)\bigl(|\ln\varepsilon|^{\frac{1}{2}}\bigr)^2 2^{-(n-1)j_\varepsilon}|\ln\varepsilon|^{\frac{1}{2}} \\ &\lesssim 2^{-(n-1)j_\varepsilon}\varepsilon^{-\frac{2}{3}n-1}|\ln\varepsilon|^{\frac{7}{12}n+2}\,,\end{aligned} \tag{4.37}$$

where in the last step we have used that $n > 1$. Since $N \lesssim |\ln\varepsilon|^2$, we conclude

$$\Bigl\|\sum_{k=0}^{N}\bigotimes_{i=1}^{3} f_k - \sum_{k=0}^{N}\bigotimes_{i=1}^{3} f_{k,\varepsilon}\Bigr\|_{\mathrm{H}^1} \lesssim 2^{-(n-1)j_\varepsilon}\varepsilon^{-\frac{2}{3}n-1}|\ln\varepsilon|^{\frac{7}{12}n+4}\,. \tag{4.38}$$

For the right hand side in (4.38) to be bounded by ε, we therefore choose

$$j_\varepsilon = \Bigl\lceil\Bigl(\frac{2}{3}\frac{n}{n-1} + \frac{2}{n-1}\Bigr)|\log_2\varepsilon| + \Bigl(\frac{7}{12}\frac{n}{n-1} + \frac{4}{n-1}\Bigr)\log_2|\ln\varepsilon|\Bigr\rceil\,, \tag{4.39}$$

and since $\#\Lambda_\varepsilon \lesssim 2^{j_\varepsilon}|\ln\varepsilon|$, by orthogonalization of $\{f_{k,\varepsilon}\}$ as described in Remark 4.27, we arrive at assertion (i).

For the proof of part (ii), let $f_{k,m}$ denote the best m-term approximation in H^1 of f_k; according to our assumptions, we have

$$\|f_k - f_{k,m}\|_{\mathrm{H}^1} \lesssim m^{-s}\|f_k\|_{\mathrm{B}^s_{p,p}}\,.$$

Thus by (4.35) and Lemma 4.28, for $k > 0$,

$$\begin{aligned}\bigl\|\bigotimes_{i=1}^3 f_k - \bigotimes_{i=1}^3 f_{k,m}\bigr\|_{\mathrm{H}^1} &\lesssim \varepsilon^{-1}|\ln\varepsilon|^{\frac{15}{6}}|\ln\varepsilon|^{\frac{1}{2}}\bigl(|\ln\varepsilon|^{\frac{1}{2}} + \varepsilon^{-\frac{1}{3}}|\ln\varepsilon|^{\frac{7}{24}}\bigr)m^{-s}\bigl(|\ln\varepsilon|^{s-\frac{1}{2}} + \varepsilon^{-\frac{4}{3}}|\ln\varepsilon|^{\frac{7}{6}}\bigr)\\ &\lesssim m^{-s}\varepsilon^{-\frac{8}{3}}|\ln\varepsilon|^{\frac{107}{24}}\,,\end{aligned}$$

and as for part (i), one obtains the same estimate for $k = 0$. Using $N \lesssim |\ln\varepsilon|^2$ we obtain

$$\Bigl\|\sum_{k=0}^N \bigotimes_{i=1}^3 f_k - \sum_{k=0}^N \bigotimes_{i=1}^3 f_{k,m}\Bigr\|_{\mathrm{H}^1} \lesssim m^{-s}\varepsilon^{-\frac{8}{3}}|\ln\varepsilon|^{\frac{155}{24}}\,.$$

The latter expression is bounded by ε if $m \geq \varepsilon^{-\frac{11}{3s}}|\ln\varepsilon|^{\frac{155}{24s}}$. Choosing for each f_k the minimum such permissible m and the corresponding best m-term approximation, we obtain the assertion by applying orthogonalization, which may in the worst case increase the resulting cardinality of Λ_k by a factor $N \lesssim |\ln\varepsilon|^2$. □

4.3.3 Hooke's Law Atom

We now return to the ground state u_0 of the hookium model system as in (4.5), and its explicitly correlated counterpart w_0 given by (4.6). The separable approximations we obtain are slightly different from the construction for hydrogen: in order to realize an efficient approximation of the diagonal electron-electron cusp, we expand into sums of products of functions on $\mathbb{R}^2$, i.e., pairs of two coordinates remain unseparated. This approach is related to Gaussian geminal basis functions in quantum chemistry mentioned in Section 2.1.

Before coming to the construction of separable approximations for u_0 and w_0, we obtain an error estimate that will be of use in both cases. For the function $\tilde{q}$ in the following lemma we will subsequently substitute appropriate exponential sum approximations.

Lemma 4.30. *Let $\gamma > 0$ and $q\colon \mathbb{R}^+ \to \mathbb{R}$ such that u defined by $u(x) := q(|x_1 - x_2|^2)\exp(-\gamma|x|^2)$ for $x = (x_1, x_2) \in (\mathbb{R}^3)^2$ is in $\mathrm{H}^1(\mathbb{R}^6)$. If for $r > 0$, the function $\tilde{q}\colon \mathbb{R}^+ \to \mathbb{R}$ satisfies, for some $\alpha \geq 0$,*

$$|q(t) - \tilde{q}(t)| \leq (t - r^2)^{\alpha+1}\varepsilon\,, \quad |q'(t) - \tilde{q}'(t)| \leq (t - r^2)^{\alpha}\varepsilon\,, \quad t \in [r^2, \infty)$$

and for some $\beta \geq 0$,

$$|q(t) - \tilde{q}(t)| \leq c_1 r^{2\beta}\,, \quad \sqrt{t}|q'(t) - \tilde{q}'(t)| \leq c_2 r^{2\beta}\,, \quad t \in (0, r^2)\,,$$

then

$$\|u - \tilde{u}\|_{\mathrm{H}^1(\mathbb{R}^6)} \lesssim (c_1 + c_2) r^{\frac{3}{2}+2\beta} + \varepsilon\,, \tag{4.40}$$

where $\tilde{u} := \tilde{q}(|x_1 - x_2|^2)\exp(-\gamma|x|^2)$.

Proof. A change of variables yields

$$\begin{aligned}&\int_{\mathbb{R}^6} |u - \tilde{u}|^2 + |\mathrm{D}_x(u - \tilde{u})|^2\,\mathrm{d}x\\ &\qquad = 2^{-3}\int_{\mathbb{R}^3} e^{-\gamma|y|^2}\,\mathrm{d}y \int_{\mathbb{R}^3} \bigl|q(|x|^2) - \tilde{q}(|x|^2)\bigr|^2 e^{-\gamma|x|^2} + \bigl|\mathrm{D}\bigl((q(|x|^2) - \tilde{q}(|x|^2))e^{-\frac{\gamma}{2}|x|^2}\bigr)\bigr|^2\,\mathrm{d}x\,.\end{aligned}$$

Since $\int_{\mathbb{R}^3} e^{-\gamma|y|^2}\,\mathrm{d}y = \sqrt{\gamma^{-3}\pi^3}$ and

$$\mathrm{D}\bigl((q(|x|^2) - \tilde{q}(|x|^2))e^{-\frac{\gamma}{2}|x|^2}\bigr) = x\bigl(2(q'(|x|^2) - \tilde{q}'(|x|^2)) - \gamma(q(|x|^2) - \tilde{q}(|x|^2))\bigr)e^{-\frac{\gamma}{2}|x|^2}\,,$$

we obtain

$$\|u-\tilde{u}\|^2_{\mathrm{H}^1(\mathbb{R}^6)} \leq 8^{-1}\sqrt{\gamma^{-3}\pi^3}\biggl(\int_{\mathbb{R}^3}\bigl((1+(\gamma^2+2\gamma)|x|^2)|q(|x|^2)-\tilde{q}(|x|^2)|^2 \\ + 2(2+\gamma)|q'(|x|^2)-\tilde{q}'(|x|^2)|^2|x|^2\bigr)e^{-\gamma|x|^2}\,\mathrm{d}x\biggr)\,.$$

Switching to polar coordinates, we conclude

$$\|u-\tilde{u}\|^2_{\mathrm{H}^1(\mathbb{R}^6)} \lesssim \int_0^r \rho^2\bigl(|q(\rho^2)-\tilde{q}(\rho^2)|^2+(\sqrt{\rho^2}|q'(\rho^2)-\tilde{q}'(\rho^2)|)^2\bigr)e^{-\gamma\rho^2}\,\mathrm{d}\rho \\ + \int_r^\infty \rho^2\bigl((1+\rho^2)|q(\rho^2)-\tilde{q}(\rho^2)|^2+\rho^2|q'(\rho^2)-\tilde{q}'(\rho^2)|)^2\bigr)e^{-\gamma\rho^2}\,\mathrm{d}\rho\,,$$

and using the assumptions on $\tilde{q}$, we obtain

$$\lesssim (c_1+c_2)^2\int_0^r \rho^2 r^{4\beta}\,\mathrm{d}\rho + \varepsilon^2\int_r^\infty (1+\rho^{8+4\alpha})e^{-\gamma\rho^2}\,\mathrm{d}\rho \lesssim (c_1+c_2)^2 r^{3+4\beta}+\varepsilon^2\,. \square$$

Direct Approximation of the Ground State

In conjunction with Lemma 4.30, the following result yields a separable approximation for u_0.

Lemma 4.31. *Let $q(t)=1+\frac{1}{2}\sqrt{t}$, $t\in\mathbb{R}^+$. For any $r>0$ and $\delta>0$, there exists an exponential sum approximation $\tilde{q}$ with $N\lesssim|\ln\delta|^2$ terms such that*

$$|q(t)-\tilde{q}(t)|\leq(t-r^2)4^{-1}r^{-1}\delta\,,\quad |q'(t)-\tilde{q}'(t)|\leq 4^{-1}r^{-1}\delta\,,\quad t\in[r^2,\infty)\,,$$
$$|q(t)-\tilde{q}(t)|\lesssim\bigl(1+|\ln\delta|^{\frac{1}{2}}\bigr)r\,,\quad \sqrt{t}|q'(t)-\tilde{q}'(t)|\lesssim\bigl(1+|\ln\delta|^{\frac{1}{2}}\bigr)\,,\quad t\in(0,r^2)\,.$$

Proof. As for Theorem 4.25, in order to obtain an approximation of both q and its derivative, we integrate an approximation of q'. We apply Theorem 4.17 and rescale the corresponding error estimate (4.11) to obtain

$$\sup_{t\in[r^2,\infty)}|4^{-1}t^{-\frac{1}{2}}-\tilde{p}(t)|\leq 4^{-1}r^{-1}\delta\,,\quad \tilde{p}(t):=\sum_{k=1}^N(4^{-1}r^{-1}\omega_k)e^{-r^{-2}\alpha_k t}\,.$$

Let

$$\tilde{q}(t):=-\sum_{k=1}^N\frac{r\omega_k}{4\alpha_k}e^{-r^{-2}\alpha_k t}+\sum_{k=1}^N\frac{r\omega_k}{4\alpha_k}e^{-\alpha_k}+q(r^2)\,, \tag{4.41}$$

so that in particular $\tilde{q}'=\tilde{p}$. Then for any $t\in[r^2,\infty)$, one has

$$\bigl|q(t)-\tilde{q}(t)\bigr|\leq\left|\int_{r^2}^t q'(\tau)-\tilde{q}'(\tau)\,\mathrm{d}\tau\right|\leq(t-r^2)4^{-1}r^{-1}\delta\,.$$

For $t\in(0,r^2)$, using the mean value theorem, we obtain

$$|q(t)-\tilde{q}(t)|\leq|q(t)-q(r^2)|+r\sum_k\frac{\omega_k}{4\alpha_k}|e^{-\alpha_k}-e^{-r^{-2}\alpha_k t}|\leq\left(\frac{1}{2}+\frac{1}{4}\sum_k\omega_k\right)r$$

and furthermore

$$\sqrt{t}|q'(t)-\tilde{q}'(t)|\leq\frac{1}{4}+\sum_k\omega_k\,,$$

hence an application of Corollary 4.21 concludes the proof. $\square$

It remains to choose the parameters in the above construction appropriately, which is summarized in the following theorem. As a consequence of the symmetries in u_0, each summand in the separable expansion is the threefold tensor product of a single bivariate function.

Theorem 4.32. *Let* $u_0(x) = \bigl(1 + \frac{1}{2}|x_1 - x_2|\bigr) \exp\bigl(-\frac{1}{4}|x|^2\bigr)$, $x \in (\mathbb{R}^3)^2$. *Then for* $\varepsilon > 0$ *there exist* $N \lesssim |\ln \varepsilon|^2$ *and* $f_k \in \mathrm{C}^\infty(\mathbb{R}^2)$, $k = 0, \dots, N$, *such that*

$$\|u_0 - \tilde{u}_0\|_{\mathrm{H}^1(\mathbb{R}^6)} \leq \varepsilon\,, \qquad \tilde{u}_0(x) := \sum_{k=0}^{N} \prod_{i=1}^{3} f_k(x_{1,i}, x_{2,i})\,, \quad x = (x_1, x_2) \in (\mathbb{R}^3)^2\,.$$

Proof. By Lemma 4.31, we can apply Lemma 4.30 with $\alpha = \beta = 0$ to obtain an approximation $\tilde{u}_0(x) := \tilde{q}(|x_1 - x_2|^2) \exp(-\frac{1}{4}|x|^2)$ of the desired form with $\tilde{q}$ as in (4.41). We thus have

$$\|u_0 - \tilde{u}_0\| \lesssim \bigl(1 + |\ln \delta|^{\frac{1}{2}}\bigr)\, r^{\frac{3}{2}} + r^{-1}\delta\,.$$

Choosing $r \sim \bigl(\varepsilon |\ln \varepsilon|^{-\frac{1}{2}}\bigr)^{\frac{2}{3}}$, $\delta \sim \varepsilon^{\frac{5}{3}} |\ln \varepsilon|^{-\frac{1}{3}}$, and noting that $|\ln \delta| \lesssim |\ln \varepsilon|$, we obtain the assertion.

Note that using the notation of the proof of Lemma 4.31, the definition of $\tilde{u}_0$ amounts to choosing

$$f_0(x) = \Bigl(1 + \frac{r}{2} + \sum_{l=1}^{N} \frac{r\omega_l}{4\alpha_l}\Bigr)^{\frac{1}{3}} e^{-\frac{1}{4}|x|^2}\,, \quad f_k(x) = -\Bigl(\frac{r\omega_k}{4\alpha_k}\Bigr)^{\frac{1}{3}} e^{-r^{-2}\alpha_k (x_1 - x_2)^2 - \frac{1}{4}|x|^2}\,, \quad x \in \mathbb{R}^2\,, \tag{4.42}$$

for $k = 1, \dots, N$, where $N \lesssim |\ln \delta|^2 \lesssim |\ln \varepsilon|^2$. □

Similarly as for hydrogenic ground states in Subsection 4.3.2, we proceed to consider approximations of the form

$$u_0(x) \approx \sum_{k_1=0}^{N} \sum_{k_2=0}^{N} \sum_{k_3=0}^{N} a_{k_1,k_2,k_3} \prod_{i=1}^{3} \Bigl(\sum_{\nu_i \in \nabla^2} U_{k_i,\nu_i} \Psi_{\nu_i}(x_{1,i}, x_{2,i}) \Bigr)\,, \quad x \in (\mathbb{R}^3)^2\,,$$

for which we need the following lemma.

Lemma 4.33. *Let* $\beta, \gamma > 0$, *then for* $u(x) := e^{-\beta(x_1 - x_2)^2 - \gamma |x|^2}$, $x \in \mathbb{R}^2$, *we have*

$$\|u\|_{\mathrm{L}_p(\mathbb{R}^2)} = \biggl(\frac{\pi}{p\sqrt{\gamma(\gamma + 2\beta)}}\biggr)^{\frac{1}{p}}\,, \quad p > 0\,, \tag{4.43}$$

$$|u|_{\mathrm{H}^s(\mathbb{R}^2)} \leq \pi^{\frac{1}{4}} \sqrt{\Gamma(s + \tfrac{1}{2})\, 2^s\, 2^{(s-1)_+}}\, \gamma^{-\frac{1}{4}} (\gamma + 2\beta)^{\frac{s}{2} - \frac{1}{4}}\,, \quad s > 0\,. \tag{4.44}$$

Furthermore, for $s \geq \frac{1}{2}$,

$$\|u\|_{\tilde{\mathrm{B}}^s_p(\mathbb{R};2)} \leq \tilde{C}_s \bigl(1 + \gamma^{-(s + \frac{1}{2})} + (\gamma + \beta)^{\frac{1}{2}} + \gamma^{-(\frac{s}{2} + \frac{1}{4})} (\gamma + \beta)^{\frac{s}{2} + \tau}\bigr)\,, \quad p^{-1} = s + \frac{1}{2}\,, \tag{4.45}$$

with $\tau \in (\frac{1}{2}, 1]$.

The proof of Lemma 4.33 is given in Appendix A.2.

Theorem 4.34. *Let* $u_0(x) = \bigl(1 + \frac{1}{2}|x_1 - x_2|\bigr) \exp\bigl(-\frac{1}{4}|x|^2\bigr)$ *for* $x \in (\mathbb{R}^3)^2$, *and let* $\{\psi_\nu\}_{\nu \in \nabla}$ *be a wavelet basis for* $\mathrm{L}_2(\mathbb{R})$ *such that* $\{2^{-|\nu|}\psi_\nu\}$ *is a Riesz basis of* $\mathrm{H}^1(\mathbb{R})$. *Then for each* $\varepsilon > 0$, u_0 *has an approximation* $\tilde{u}_0$ *with* $\|u_0 - \tilde{u}_0\|_{\mathrm{H}^1(\mathbb{R}^6)} \lesssim \varepsilon$ *of the form*

$$\tilde{u}_0(x) = \sum_{k_1=0}^{N} \sum_{k_2=0}^{N} \sum_{k_3=0}^{N} a_{k_1,k_2,k_3} \prod_{i=1}^{3} \Bigl(\sum_{\nu_i \in \nabla^2} U_{k_i,\nu_i} \Psi_{\nu_i}(x_{1,i}, x_{2,i}) \Bigr)\,, \quad x \in (\mathbb{R}^3)^2\,, \tag{4.46}$$

where $N \lesssim |\ln\varepsilon|^2$, $\langle U_{k,\cdot}, U_{l,\cdot}\rangle = \delta_{kl}$, *and* $\operatorname{supp} U_{k,\cdot} \subseteq \Lambda_k$ *for* $\Lambda_k \subset \nabla^2$, *where for* $\#\Lambda_k$ *the following holds:*

(i) (uniform approximation)
If $\{\psi_\nu\}$ *satisfies a direct estimate for* $\mathrm{H}^n(\mathbb{R})$ *with integer* $n > 1$, *and* Λ_k *are chosen as* $\Lambda_k := \Lambda_\varepsilon$, *where*

$$\Lambda_\varepsilon := \{\nu \in \nabla^2 \colon \operatorname{supp}\Psi_\nu \cap [-K_\varepsilon, K_\varepsilon]^2 \neq \emptyset \text{ and } \max|\nu| \leq j_\varepsilon\} \tag{4.47}$$

with $K_\varepsilon > 0$, $K_\varepsilon \sim |\ln\varepsilon|$ *and* $j_\varepsilon \in \mathbb{Z}_{j_0}$ *chosen appropriately as specified in the proof, then* $\#\Lambda_\varepsilon \lesssim \varepsilon^{-\frac{4}{3}c_1(n)}|\ln\varepsilon|^{c_2(n)}$ *where* $c_1(n), c_2(n) \downarrow 1$ *as* $n \to \infty$.

(ii) (adaptive approximation)
If $\{\Psi_\nu\}_{\nu\in\nabla^2}$ *satisfies the norm equivalence* (3.29) *for* $\tilde{\mathrm{B}}^s_p(\mathbb{R};2)$ *with* $s \geq \frac{1}{2}$ *and* $p^{-1} = s + \frac{1}{2}$, *then* Λ_k *can be chosen such that* $\#\Lambda_k \lesssim \varepsilon^{-\frac{2}{3}c_3(s)}|\ln\varepsilon|^{3c_4(s)}$, *where* $c_3(s), c_4(s) \downarrow 1$ *as* $s \to \infty$.

Proof. Similarly to the proof of Theorem 4.29, for the functions f_k, $k = 0, \dots, N$ provided by Theorem 4.32, defined in (4.42), we have $r^{-2}\alpha_k \lesssim \varepsilon^{-\frac{4}{3}}|\ln\varepsilon|^{\frac{7}{6}}$ for the exponents in the exponential sum and

$$\frac{r\omega_k}{\alpha_k} \lesssim \varepsilon^{-1}|\ln\varepsilon|^{-1}\,.$$

For part (i), with $f_{k,\varepsilon}$ defined as the projection onto $\{\Psi_\nu\}_{\nu\in\Lambda_\varepsilon}$, estimating differences of tensor products as in the proof of Theorem 4.29 and using Lemma 4.33, we thus arrive at

$$\Big\|\bigotimes_{i=1}^3 f_k - \bigotimes_{i=1}^3 f_{k,\varepsilon}\Big\|_{\mathrm{H}^1(\mathbb{R}^6)} \lesssim \|f_k\|_{\mathrm{L}_2}\|f_k\|_{\mathrm{H}^1}\|f_k - f_{k,\varepsilon}\|_{\mathrm{H}^1} \lesssim 2^{-(n-1)j_\varepsilon}\varepsilon^{-\frac{2}{3}n-\frac{2}{3}}|\ln\varepsilon|^{\frac{7}{12}n-\frac{31}{24}}\,. \tag{4.48}$$

The same estimates as for Theorem 4.29 lead to a choice of j_ε analogous to (4.39). We thus obtain part (i) with $\#\Lambda_\varepsilon \sim 2^{2j_\varepsilon}|\ln\varepsilon|^2$.

For part (ii), let $f_{k,m}$ denote the best m-term approximation in H^1 of f_k; according to our assumptions, we thus have

$$\|f_k - f_{k,m}\|_{\mathrm{H}^1} \lesssim m^{-s}\|f_k\|_{\tilde{\mathrm{B}}^s_p}\,.$$

Together with Lemma 4.33, analogously to (4.48) this leads to

$$\begin{aligned}\Big\|\bigotimes_{i=1}^3 f_k - \bigotimes_{i=1}^3 f_{k,m}\Big\|_{\mathrm{H}^1} &\lesssim \varepsilon^{-1}|\ln\varepsilon|^{-1}m^{-s}\varepsilon^{-\frac{2}{3}s-\frac{4}{3}}|\ln\varepsilon|^{\frac{7}{12}s+\frac{7}{6}}\\ &\lesssim m^{-s}\varepsilon^{-\frac{2}{3}s-\frac{7}{3}}|\ln\varepsilon|^{\frac{7}{12}s+\frac{1}{6}}\,.\end{aligned}$$

The latter estimate yields part (ii) by the same arguments as for Theorem 4.29, again with an additional factor $|\ln\varepsilon|^2$ entering the estimate due to the orthogonalization of the approximations of the f_k. □

Explicitly Correlated Case

In the following lemma, we construct a separable approximation for w_0.

Lemma 4.35. *Let* $q(t) = (1 + \frac{1}{2}\sqrt{t})e^{-\frac{1}{2}\sqrt{t}}$, $t \in \mathbb{R}^+$. *For any* $r > 0$ *and* $\delta > 0$, *there exists an exponential sum approximation* $\tilde{q}$ *with* $N \lesssim |\ln\delta|^2$ *terms such that*

$$\begin{gathered}|q(t) - \tilde{q}(t)| \leq (t - r^2)^2 64^{-1} r^{-1}\delta\,, \quad |q'(t) - \tilde{q}'(t)| \leq (t - r^2) 32^{-1} r^{-1}\delta\,, \quad t \in [r^2, \infty)\,,\\ |q(t) - \tilde{q}(t)| \lesssim \big(1 + r|\ln\delta|^{\frac{1}{2}}\big)r^2\,, \quad \sqrt{t}|q'(t) - \tilde{q}'(t)| \lesssim \big(1 + |\ln\delta|^{\frac{1}{2}}\big)r^2\,, \quad t \in [0, r^2)\,.\end{gathered}$$

Proof. In order to achieve the estimate on $[0, r^2)$, we need to approximate second derivatives of q as well. We thus proceed similarly to Lemma 4.31, but start from an approximation of q'' and integrate twice. Note first that

$$q'(t) = -\frac{1}{8}e^{-\frac{1}{2}\sqrt{t}}\,, \quad q''(t) = -\mathrm{D}_t\frac{1}{8}e^{-\frac{1}{2}\sqrt{t}} = \frac{1}{32\sqrt{t}}e^{-\frac{1}{2}\sqrt{t}}\,.$$

We now apply Theorem 4.22(ii) with $\rho = r/2$ to obtain

$$\sup_{t\in[r^2,\infty)} |q''(t) - \tilde{p}(t)| \leq 32^{-1}r^{-1}\delta\,, \quad \tilde{p}(t) := \sum_{k=1}^{N}(32^{-1}r^{-1}\omega_k)e^{-r^{-2}\alpha_k t}\,.$$

We define

$$\tilde{q}(t) := \sum_k \frac{r^3\omega_k}{32\alpha_k^2}\big(e^{-r^{-2}\alpha_k t} - e^{-\alpha_k}\big) + (t-r^2)\Big(\sum_k \frac{r\omega_k}{32\alpha_k}e^{-\alpha_k} + q'(r^2)\Big) + q(r^2)\,, \tag{4.49}$$

so that

$$\tilde{q}'(t) = -\sum_k \frac{r\omega_k}{32\alpha_k}(e^{-r^{-2}\alpha_k t} - e^{-\alpha_k}) + q'(r^2)\,, \quad \tilde{q}''(t) = \tilde{p}(t)\,.$$

The estimate for $|q'(t) - \tilde{q}'(t)|$, $t \in [r^2,\infty)$, now follows exactly as in the proof of Lemma 4.31, and as a consequence, for $t \in [r^2,\infty)$,

$$|q(t) - \tilde{q}(t)| = \left|\int_{r^2}^{t} q'(\tau) - \tilde{q}'(\tau)\,\mathrm{d}\tau\right| \leq 32^{-1}r^{-1}\delta\int_{r^2}^{t}(\tau - r^2)\,\mathrm{d}\tau = (t-r^2)^2 64^{-1}r^{-1}\delta\,.$$

Concerning the case $t \in [0,r^2)$, note that by the mean value theorem, for the first term in (4.49), we have

$$\sum_k \frac{r^3\omega_k}{32\alpha_k^2}\big(e^{-r^{-2}\alpha_k t} - e^{-\alpha_k}\big) = -(t-r^2)\sum_k \frac{r\omega_k}{32\alpha_k}e^{-r^{-2}\alpha_k\xi_k}$$

for some $\xi_k \in [t,r^2]$, and hence, using the mean value theorem once more,

$$\begin{aligned}|q(t) - \tilde{q}(t)| &\leq |q(t) - q(r^2)| + |t-r^2|\bigg(\Big|\sum_k \frac{r\,\omega_k}{32\alpha_k}(e^{-\alpha_k} - e^{-r^{-2}\alpha_k\xi})\Big| + |q(r^2)|\bigg)\\ &\leq 8^{-1}r^2 + 32^{-1}r^3\sum_k\omega_k + 8^{-1}r^2\,.\end{aligned}$$

Similarly, we find

$$|q'(t) - \tilde{q}'(t)| \leq \frac{1}{16}\Big(1 + \frac{1}{2}\sum_k\omega_k\Big)r\,.$$

Estimating $\sum_k \omega_k$ according to Remark 4.23, we obtain the assertion. □

Theorem 4.36. *Let* $w_0(x) = \exp(-\frac{1}{2}|x_1 - x_2|)\big(1 + \frac{1}{2}|x_1-x_2|\big)\exp\big(-\frac{1}{4}|x|^2\big)$*,* $x \in (\mathbb{R}^3)^2$*. Then for* $\varepsilon > 0$ *there exist* $N \lesssim |\ln\varepsilon|^2$ *and* $f_k^{(i)} \in \mathrm{C}^\infty(\mathbb{R}^2)$*, for* $k = 0,\dots,N+3$ *and* $i = 1,2,3$*, such that*

$$\|w_0 - \tilde{w}_0\|_{\mathrm{H}^1(\mathbb{R}^6)} \leq \varepsilon\,, \qquad \tilde{w}_0(x) := \sum_{k=0}^{N+3}\prod_{i=1}^{3} f_k^{(i)}(x_{1,i},x_{2,i})\,, \quad x = (x_1,x_2) \in (\mathbb{R}^3)^2\,.$$

Proof. By Lemma 4.35, we can apply Lemma 4.30 with $\alpha = \beta = 1$ to obtain an approximation $\tilde{w}_0(x) := \tilde{q}(|x_1-x_2|^2)\exp(-\frac{1}{4}|x|^2)$ of the desired form with $\tilde{q}$ as in (4.49) and

$$\|w_0 - \tilde{w}_0\|_{\mathrm{H}^1(\mathbb{R}^6)} \lesssim \big(1 + |\ln\delta|^{\frac{1}{2}}\big)r^{\frac{7}{2}} + r^{-1}\delta\,.$$

Choosing $r \sim \bigl(\varepsilon|\ln\varepsilon|^{-\frac{1}{2}}\bigr)^{\frac{2}{7}}$, $\delta \sim \varepsilon^{\frac{9}{7}}|\ln\varepsilon|^{-\frac{1}{7}}$, and noting that $|\ln\delta| \lesssim |\ln\varepsilon|$, we obtain the assertion.

With the coefficients α_l, ω_l for $l = 1,\dots,N$ as in the proof of Lemma 4.35, the functions $f_k^{(i)}$ for $i = 1,2,3$ and $k = 0,\dots,N+3$ read as follows: For $k = 0$, for all $i \in \{1,2,3\}$ we have the same function

$$f_0^{(i)}(x) = \Bigl(e^{-\frac{1}{2}r}\Bigl(1+\frac{r}{2}+\frac{r^2}{8}\Bigr) - \sum_{l=1}^{N}\frac{r^3\omega_l}{32\alpha_l}(1+\alpha_l^{-1})e^{-\alpha_l}\Bigr)^{\frac{1}{3}} e^{-\frac{1}{4}|x|^2}\,,\quad x\in\mathbb{R}^2\,; \tag{4.50}$$

for $k = 1,2,3$, the function for $i = k$ differs from those for $i \neq k$, that is,

$$f_k^{(k)}(x) = (x_1-x_2)^2\Bigl(\sum_{l=1}^{N}\frac{r\omega_l}{32\alpha_l}e^{-\alpha_l} - \frac{1}{8}e^{-\frac{1}{2}r}\Bigr)\,e^{-\frac{1}{4}|x|^2} \quad\text{and}\quad f_k^{(i)}(x) = e^{-\frac{1}{4}|x|^2}\,,\ i\neq k\,; \tag{4.51}$$

and for $k > 3$, we again have the same function for all i,

$$f_k^{(i)}(x) = \Bigl(\frac{r^3\omega_{k-3}}{32\alpha_{k-3}^2}\Bigr)^{\frac{1}{3}} e^{-r^{-2}\alpha_{k-3}\,(x_1-x_2)^2}e^{-\frac{1}{4}|x|^2}\,,\quad i=1,2,3\,,\quad x\in\mathbb{R}^2\,. \tag{4.52}$$

□

Note that in contrast to Theorems 4.25, 4.32, the summands for the indices $k = 1,2,3$ in the separable expansions provided by Theorem 4.36 are not threefold tensor products of single functions. In the representation (4.53) obtained in Theorem 4.37 below, however, the terms can be recombined so that one set of coefficients $U_{k,\nu}$ suffices. In other words, the resulting representation again shares the symmetry of those obtained in Theorems 4.29, 4.37.

Theorem 4.37. *Let* $w_0(x) = \exp\bigl(-\frac{1}{2}|x_1-x_2|\bigr)\bigl(1+\frac{1}{2}|x_1-x_2|\bigr)\exp\bigl(-\frac{1}{4}|x|^2\bigr)$ *for* $x\in(\mathbb{R}^3)^2$, *and let* $\{\psi_\nu\}_{\nu\in\nabla}$ *be a wavelet basis for* $\mathrm{L}_2(\mathbb{R})$ *such that* $\{2^{-|\nu|}\psi_\nu\}$ *is a Riesz basis of* $\mathrm{H}^1(\mathbb{R})$. *Then for each* $\varepsilon > 0$, w_0 *has an approximation* $\tilde{w}_0$ *with* $\|w_0-\tilde{w}_0\|_{\mathrm{H}^1(\mathbb{R}^6)} \lesssim \varepsilon$ *of the form*

$$\tilde{w}_0(x) = \sum_{k_1=0}^{N+1}\sum_{k_2=0}^{N+1}\sum_{k_3=0}^{N+1} a_{k_1,k_2,k_3}\prod_{i=1}^{3}\Bigl(\sum_{\nu_i\in\nabla^2}U_{k_i,\nu_i}\Psi_{\nu_i}(x_{1,i},x_{2,i})\Bigr)\,,\quad x\in(\mathbb{R}^3)^2\,, \tag{4.53}$$

where $N \lesssim |\ln\varepsilon|^2$, $\langle U_{k,\cdot},U_{l,\cdot}\rangle = \delta_{kl}$, *and* $\operatorname{supp}U_{k,\cdot}\subseteq\Lambda_k$ *for* $\Lambda_k\subset\nabla^2$, *where for* $\#\Lambda_k$ *the following holds:*

(i) (uniform approximation)
If $\{\psi_\nu\}$ *satisfies a direct estimate for* $\mathrm{H}^n(\mathbb{R})$ *with integer* $n > 1$, *and* Λ_k *are chosen as* $\Lambda_k := \Lambda_\varepsilon$, *where*

$$\Lambda_\varepsilon := \{\nu\in\nabla^2\colon\ \operatorname{supp}\Psi_\nu\cap[-K_\varepsilon,K_\varepsilon]^2\neq\emptyset \text{ and } \max|\nu|\leq j_\varepsilon\} \tag{4.54}$$

with $K_\varepsilon > 0$, $K_\varepsilon \sim |\ln\varepsilon|$ *and* $j_\varepsilon\in\mathbb{Z}_{j_0}$ *chosen appropriately as specified in the proof, then* $\#\Lambda_\varepsilon \lesssim \varepsilon^{-\frac{4}{7}c_1(n)}|\ln\varepsilon|^{c_2(n)}$ *where* $c_1(n)\downarrow 1$, $c_2(n)\to 1$ *as* $n\to\infty$.

(ii) (adaptive approximation)
If $\{\Psi_\nu\}_{\nu\in\nabla^2}$ *satisfies the norm equivalence* (3.29) *for* $\tilde{\mathrm{B}}^s_p(\mathbb{R};2)$ *with* $s\geq\frac{1}{2}$ *and* $p^{-1} = s+\frac{1}{2}$, *then* Λ_k *can be chosen such that* $\#\Lambda_k \lesssim \varepsilon^{-\frac{2}{7}c_3(s)}|\ln\varepsilon|^{3c_4(s)}$, *where* $c_3(s), c_4(s)\downarrow 1$ *as* $s\to\infty$.

Proof. We construct wavelet approximations for the functions $f_k^{(i)}$ provided by Theorem 4.36 for $\varepsilon > 0$, where $i = 1,2,3$ and $k = 0,\dots,N+3$. The definition of these functions in (4.50), (4.51), (4.52) involves parameters $\delta > 0$ with $|\ln\delta| \lesssim |\ln\varepsilon|$ and $r \sim (\varepsilon|\ln\varepsilon|^{-\frac{1}{2}})^{\frac{2}{7}}$, as well as the coefficients α_l, ω_l for $l = 1,\dots,N$. Since $\alpha_l \lesssim |\ln\varepsilon|^{1/2}$ by Corollary 4.21, we have

$$r^{-2}\alpha_l \lesssim \varepsilon^{-\frac{4}{7}}|\ln\varepsilon|^{\frac{9}{14}}\,.$$

Using Corollary 4.21 and Remark 4.23, furthermore we obtain

$$\frac{r\omega_l}{\alpha_l} \lesssim \varepsilon^{-1}|\ln\varepsilon|^{-1}\,, \quad \frac{r^3\omega_l}{\alpha_l^2} \lesssim \varepsilon^{-3}|\ln\varepsilon|^{-1}\,.$$

Note that the norms in $\tilde{\mathrm{B}}^s_p(\mathbb{R};2)$ of the functions $e^{-\frac{1}{4}|x|^2}$ and $(x_1-x_2)^2 e^{-\frac{1}{4}|x|^2}$ depend on s, but not on ε, and are thus treated as constants in what follows.

Proceeding as for Theorems 4.29, 4.34 with analogous definitions of $f^{(i)}_{k,\varepsilon}$ and $f^{(i)}_{k,m}$, we thus obtain

$$\big\|\bigotimes_{i=1}^3 f^{(i)}_k - \bigotimes_{i=1}^3 f^{(i)}_{k,\varepsilon}\big\|_{\mathrm{H}^1} \lesssim 2^{-(n-1)j_\varepsilon}\varepsilon^{-\frac{2}{7}n-\frac{20}{7}}|\ln\varepsilon|^{\frac{11}{28}n-\frac{67}{56}}$$

as well as

$$\big\|\bigotimes_{i=1}^3 f^{(i)}_k - \bigotimes_{i=1}^3 f^{(i)}_{k,m}\big\|_{\mathrm{H}^1} \lesssim m^{-s}\varepsilon^{-\frac{2}{7}s-\frac{25}{7}}|\ln\varepsilon|^{\frac{11}{28}s-\frac{3}{14}}\,.$$

Analogously to the proofs of Theorems 4.29, 4.34, we arrive at appropriate choices for j_ε and m. By the definition of $f^{(i)}_k$ for $k=0,\ldots,3$ in (4.50), (4.51), for $x=(x_1,x_2)\in\mathbb{R}^6$ we have

$$\sum_{k=0}^3\prod_{i=1}^3 f^{(i)}_k(x_{1,i},x_{2,i}) = \sum_{k_1=0}^1\sum_{k_2=0}^1\sum_{k_3=0}^1 c_{k_1,k_2,k_3}\prod_{i=1}^3 h_{k_i}(x_{1,i},x_{2,i})\,,$$

with $h_0(\hat{x}) = e^{-\frac{1}{4}|\hat{x}|^2}$, $h_1(\hat{x}) = (\hat{x}_1-\hat{x}_2)^2 e^{-\frac{1}{4}|\hat{x}|^2}$ for $\hat{x}\in\mathbb{R}^2$ and suitable $c_{k_1,k_2,k_3}\in\mathbb{R}$. The corresponding approximations $f^{(i)}_{k,\varepsilon}$ can therefore be chosen such that

$$\sum_{k=0}^3\prod_{i=1}^3 f^{(i)}_{k,\varepsilon}(x_{1,i},x_{2,i}) = \sum_{k_1=0}^1\sum_{k_2=0}^1\sum_{k_3=0}^1 \tilde{a}_{k_1,k_2,k_3}\prod_{i=1}^3\Big(\sum_{\nu_i\in\nabla^2}\tilde{U}_{k_i,\nu_i}\Psi_{\nu_i}(x_{1,i},x_{2,i})\Big) \tag{4.55}$$

for certain coefficients $\tilde{a}_{k_1,k_2,k_3}$, $k\in\{0,1\}^3$, and $\tilde{U}_{0,\nu}$, $\tilde{U}_{1,\nu}$, $\nu\in\nabla^2$, and we have an analogous representation for $f^{(i)}_{k,m}$ in the best m-term case. As in Theorems 4.29, 4.34, orthogonalization leads to the representation (4.53), where (4.55) yields a reduction in the range of summation from $N+3$, as in Theorem 4.36, to $N+1$. □

4.4 Discussion

We now briefly summarize the results obtained in this chapter, in order to obtain a comparison of the complexities of the different approximations. The relevant measure for this comparison is the number of coefficients required for an error of order ε in H^1–norm.

Based on the available mixed Sobolev regularity estimates, for electronic Schrödinger wave functions one obtains approximations which, using N coefficients, yield an approximation error slightly larger than $N^{-1/4}$. In the corresponding explicitly correlated formulation, this improves to almost $N^{-1/3}$, although it should be noted that the latter result is not necessarily sharp. This type of approximation has been studied in detail in [154].

In the model systems considered in Section 4.2, one can see clearly the advantage of nonlinear approximation. For the one-electron example of a hydrogenic ground state, in contrast to linear approximation, there is no limitation on the attainable order of convergence, which is determined only by the order of polynomial reproduction of the underlying wavelet basis. For the two-electron model system of the Hooke's law atom, there is still a limitation on the attainable convergence rate, but the limiting rate is twice as high as in the linear case, since with best N-term approximation one can come arbitrarily close to $N^{-1/2}$. A similar effect is observed for the solution of the corresponding explicitly correlated formulation for both linear and nonlinear approximation, where the limiting convergence rate, in comparison to the case without explicit correlation, is more than doubled: We have obtained a best N-term error for the explicitly correlated formulation that is almost of order $N^{-7/6}$.

In Section 4.3, we found that convergence rates for the nonlinearly parametrized wavelet expansions as in Section 4.3 in each case approach, for sufficiently high approximation orders, three times the convergence rate possible for direct wavelet approximation as in Section 4.2. This effect can be observed both for linear and for best N-term approximation of the corresponding lower-dimensional tensor components, and for both standard and explicitly correlated formulation of the two-electron model problem. In particular, with best N-term approximation of the lower-dimensional components, with a total number of N coefficients in the tensor decomposition, the error comes arbitrarily close to $N^{-3/2}$ in the standard formulation, and $N^{-7/2}$ in the explicitly correlated formulation.

As can be seen from the proofs of Theorems 4.29, 4.34 and 4.37, for wavelet approximation of the separable approximations we have constructed, fairly high wavelet orders are required to come close to the limiting convergence rate. This is, however, mostly a consequence of the ill-conditioning of the separable approximations of Theorems 4.25, 4.36, 4.36 due to the particular technique of integrating exponential sum approximations of derivatives we have used to obtain estimates in H^1–norm, and a different construction of separable approximations may lead to better convergence rates for lower-order wavelet approximation.

The estimates obtained in Section 4.3 have a strong connection to results in [146, 27] concerning lower-dimensional component functions in tensor approximations. There it is shown that, essentially, the component functions of the L_2–best approximation (for a prescribed number of summands, i.e., a prescribed rank, of the tensor approximation) inherit the order of regularity of the higher-dimensional approximand, which means that the components can be approximated at a higher rate. This result is applicable to a more general class of functions than the model problems discussed here, but it does not yield information on the number of summands required for a given error in H^1, and hence on the overall complexity of the approximation. Note that the corresponding complexity estimates for approximating the components that follow from this are approached by those obtained in Section 4.3 for increasing approximation order. The results in [146, 27] show in particular that the lower-dimensional component functions in L_2–best approximations of given rank can be approximated at precisely the rates that are approached by our explicit construction of H^1–approximations, which in each case correspond to three times the rate one obtains for the full higher-dimensional functions.

In [67] it was shown that when assuming only Sobolev regularity, the singular value decomposition of a bivariate function does not necessarily yield a more efficient approximation in terms of total number of coefficients than a sparse grid approximation. For an actual gain in efficiency, the error needs to decrease sufficiently rapidly with increasing number of summands in the singular value decomposition, in other words, the singular values need to have sufficiently fast decay. For the model problems we have considered, the results of Section 4.3 show that the expansion into separable functions has a sufficiently fast convergence to guarantee an advantage over a direct, linearly parametrized wavelet expansion.

It should be noted that the constants in the convergence estimates for wavelet approximation in this chapter depend on the wavelet basis, and in particular on the order of approximation. The different types of approximation also require quite different numerical schemes. The total complexity of obtaining the respective approximations as approximate solutions of eigenvalue problems is therefore a different matter. Computational schemes for direct wavelet discretization have been reviewed in Chapter 3; schemes that take advantage of separability by nonlinear parametrization of wavelet coefficients are the subject of Chapter 5.

5 Adaptive Wavelet Schemes for Low-Rank Tensor Representations of Coefficient Sequences

In Section 4.3, for the wavelet coefficients of the solutions of certain model problems we have constructed nonlinearly parametrized approximations that exploit both sparsity properties and low-rank structure of these coefficients. We have seen that by such an approach, in certain cases higher convergence rates can be achieved than by a direct linear parametrization of wavelets. The subject of this chapter are iterative solvers that represent wavelet coefficients directly in a low-rank tensor format. We shall apply these to the model problems analyzed in Section 4.3, as well as to the electronic Schrödinger equation for helium.

The most basic example of such structured representations is provided by low-rank matrices. If $M = (m_{ij}) \in \mathbb{R}^{m\times n}$ has matrix rank $r \leq \min\{m,n\}$, the singular value decomposition (SVD) gives a representation

$$m_{ij} = \sum_{k=1}^{r} u_{ki}\sigma_k v_{kj}\,, \qquad (u_{ki}), (v_{kj}) \text{ with orthonormal columns, } \sigma_k \geq \sigma_{k+1} \geq 0. \tag{5.1}$$

If M has full rank $r = \min\{m,n\}$, but many singular values σ_k are small, truncating the sum in (5.1) at some lower rank $\tilde r < r$ yields a low-rank approximation $\tilde M = (\tilde m_{ij})$ of M with the truncation error estimate

$$\sum_{i,j} (\tilde m_{ij} - m_{ij})^2 \leq \sum_{k=\tilde r+1}^{r} \sigma_k^2\,. \tag{5.2}$$

For tensors of order $d > 2$, there exist various different types of representation that can be regarded as generalizations of (5.1), and each of these tensor formats corresponds to a slightly different notion of tensor rank.

For the model problems under consideration here, we are dealing exclusively with tensors of order $d = 3$. In this case, the Tucker tensor format provides properties similar to those of the SVD, in particular an error estimate resembling (5.2); the complexity estimates for this format, however, deteriorate exponentially with d. Only recently, with the Hierarchical Tucker format [75, 64] and the special case of the Tensor Train format [121], tensor formats have been found that preserve reasonable complexity also for larger d, but still to some extent retain the favorable features of the SVD. As a comprehensive reference on such tensor formats, see [72].

A quite generally applicable strategy for using such representations in the numerical treatment of discretized operator equations is to perform standard iterative schemes, but with all intermediate steps carried out in the tensor format. Such iterations, however, cannot be performed exactly: in general, the tensor rank parameters will increase exponentially with the number of iterations. The addition of two matrices of rank r as in (5.1), for instance, in general gives a matrix of rank $2r$.

It is therefore necessary to perform perturbed iterative schemes, where intermediate results are replaced by approximations of lower rank. A general framework of this type has been proposed in [12, 13]. The basic approach has been pursued, based on different tensor formats, for the solution of linear operator equations and parametric problems, e.g., in [101, 5, 96, 140], and for eigenvalue problems in [92, 6, 74, 102, 95, 140].

The discretizations that such methods are based on are typically of finite difference or finite element type on a uniform grid, with tensor entries representing point values of functions. In our case, tensor entries represent wavelet coefficients, and instead of an a priori fixed discretization, the required wavelet coefficients are determined adaptively.

As outlined in Section 3.5, by a diagonal rescaling of the representation matrix of the second-order elliptic operator under consideration, we arrive at a uniformly well-conditioned problem on an ℓ_2–space. By the Riesz basis property, the ℓ_2–norms of wavelet coefficient sequences are then equivalent to the H^1–norms of the corresponding represented functions.

On the one hand, this rescaling provides asymptotically optimal preconditioning. On the other hand, for the tensor formats considered here, rank truncations with prescribed coefficient error in ℓ_2 can be performed by standard linear algebra routines. In the present setting, the rescaling thus has the second important benefit that we obtain explicit control over the H^1–error incurred by tensor approximation operations.

The price to pay is that the corresponding diagonal rescaling leads to a rank increase, similar to known preconditioners for low-rank schemes as considered in [93, 63]. In our context, the factor by which the rescaling may increase ranks turns out to be proportional to the maximum arising wavelet level, which can become particularly problematic for adaptive local refinements. This issue is addressed in detail in Section 5.2, leading to a modified tensor representation with an additional levelwise subdivision.

With this framework in place, we can follow the methodology of adaptive wavelet schemes as outlined in Section 3.6 by approximately applying iterative schemes for an infinite matrix formulation on ℓ_2 of the original problem to finitely supported iterates. Since all approximations required over the course of the iteration are done with respect to the appropriate norms, we obtain a rigorous convergence analysis and explicit choices of error tolerances for which the iteration is guaranteed to converge, where all arising constants depend only on the underlying infinite dimensional problem and on the wavelet basis, but not on a concrete discretization.

In this chapter, we restrict ourselves to the case of self-adjoint operators, and therefore do not consider the nonsymmetric explicitly correlated formulations at this point. Combined with iterative methods suitable for nonsymmetric problems, however, the basic construction is applicable to these cases as well.

5.1 Separable Representation of Operators

In addition to the low-rank structure of solutions, the methods developed in this chapter require a compatible separable structure of operators.

In the specific model cases under consideration, in the previous chapter we have obtained approximations to the eigenfunction of interest u_0 of the general form

$$u_0 \approx \sum_{k=1}^{N_f} f_k^{(1)}(x_1)\, f_k^{(2)}(x_2)\, f_k^{(3)}(x_3) \tag{5.3}$$

in the case of hydrogen, or

$$u_0 \approx \sum_{k=1}^{N_f} f_k^{(1)}(x_1 - y_1)\, f_k^{(2)}(x_2 - y_2)\, f_k^{(3)}(x_3 - y_3) \tag{5.4}$$

for the hookium test problem. These results lead us to the conjecture that an expansion of the form (5.4) can be expected to be efficient in the case of helium as well.

The three- and six-dimensional Laplacian terms arising in the Hamiltonian operators for these model systems can be written as

$$\Delta = \mathrm{D}^2_{x_1} \otimes \mathrm{I} \otimes \mathrm{I} + \mathrm{I} \otimes \mathrm{D}^2_{x_2} \otimes \mathrm{I} + \mathrm{I} \otimes \mathrm{I} \otimes \mathrm{D}^2_{x_3}$$

and

$$\Delta = (\mathrm{D}^2_{x_1} + \mathrm{D}^2_{y_1}) \otimes \mathrm{I} \otimes \mathrm{I} + \mathrm{I} \otimes (\mathrm{D}^2_{x_2} + \mathrm{D}^2_{y_2}) \otimes \mathrm{I} + \mathrm{I} \otimes \mathrm{I} \otimes (\mathrm{D}^2_{x_3} + \mathrm{D}^2_{y_3}) \,,$$

respectively, and thus have a tensor structure compatible with the representations of the solutions. The same holds true for the quadratic terms $|x|^2 + |y|^2$ arising in the Hamiltonian of the hookium eigenvalue problem.

The Coulomb potentials $|x|^{-1}$ and $|x-y|^{-1}$ do not have such a separable structure themselves. However, they can be replaced by efficient approximations of the form

$$\frac{1}{|x|} \approx \sum_{k=1}^{N_g} g_k(x_1)\, g_k(x_2)\, g_k(x_3)\,, \qquad \frac{1}{|x-y|} \approx \sum_{k=1}^{N_g} g_k(x_1 - y_1)\, g_k(x_2 - y_2)\, g_k(x_3 - y_3)\,, \tag{5.5}$$

which can be obtained based on exponential sum expansions. The number of terms N_g that needs to be dealt with thus depends on the required accuracy. A detailed study of such approximations and the wavelet representations of the resulting approximate operators is carried out in Chapter 6. There we also obtain analogous results for the nonsymmetric modified potential terms in the explicitly correlated formulation.

5.2 Tensor Structures for Wavelet Coordinates

For the model problems considered in Section 4.3, we have obtained approximations to the exact wavelet coefficients $\mathbf{u} = (u_\nu)_{\nu \in \nabla^d}$ of eigenfunctions of the form

$$u_\nu \approx \sum_{k_1=1}^{r_1} \sum_{k_2=1}^{r_2} \sum_{k_3=1}^{r_3} a_{k_1,k_2,k_3} U^{(1)}_{k_1,\nu_1} U^{(2)}_{k_2,\nu_2} U^{(3)}_{k_3,\nu_3}\,, \tag{5.6}$$

where $d = 3$ or $d = 6$ and $\nu = (\nu_1, \nu_2, \nu_3)$ with $\nu_i \in \nabla^{\hat d}$, $\hat d = \frac{d}{3}$, for $i \in \{1,2,3\}$. The representation in the form (5.6) corresponds to the Tucker tensor format that will be discussed in more detail in this section. Note that in the particular cases considered in Section 4.3, we have $\mathbf{U}^{(1)}_k = \mathbf{U}^{(2)}_k = \mathbf{U}^{(3)}_k$ for all k.

However, the functions we aim to approximate are given only implicitly as eigenfunctions of an operator $H\colon \mathrm{H}^1(\mathbb{R}^d) \to \mathrm{H}^{-1}(\mathbb{R}^d)$. The representation chosen for the wavelet coefficients therefore in addition needs to be suitable for the approximate application of H in the context of iterative eigensolvers. Concerning the latter point, the fact that the space H^1 in which such iterative methods need to be performed is not a tensor product space leads to some further complications; these issues will be discussed in this section as well, together with a further restriction on tensor representations that may yield slightly less efficient approximations, but enables a more efficient approximate application of operators.

The operator H is of the form $-\frac{1}{2}\Delta + V$ in the case of the self-adjoint electronic Schrödinger problem, or of the form $-\frac{1}{2}\Delta + W \cdot \mathrm{D} + \tilde V$ in the nonsymmetric transcorrelated formulation. In either case, by adding a suitable shift we can assume H to be H^1–elliptic, and the potential terms $V, W, \tilde V$ can be approximated by sums of separable functions as in (5.5).

Let us assume that for a wavelet basis $\{\Psi_\nu\}_{\nu \in \nabla^d}$ of $\mathrm{L}_2(\mathbb{R}^d)$, the rescaled basis functions $\{s_\nu \Psi_\nu\}_{\nu \in \nabla^d}$ are a Riesz basis for $\mathrm{H}^1(\mathbb{R}^d)$, where the entries of the sequence $\mathbf{s} = (s_\nu)_{\nu \in \nabla^d}$ are given by

$$s_\nu := \Bigl(\sum_{i=1}^{d} 2^{2|\nu_i|} \Bigr)^{-\frac{1}{2}}\,. \tag{5.7}$$

Then the infinite matrix

$$\mathbf{H} := \big(s_\nu \langle \Psi_\nu, H\Psi_\mu\rangle s_\mu\big)_{\mu,\nu\in\nabla^d} \tag{5.8}$$

defines an elliptic operator on $\ell_2(\nabla^d)$. We additionally assume the Ψ_ν to be L_2-orthonormal, and hence the corresponding eigenvalue problem reads

$$\sum_\mu \big(s_\nu \langle \Psi_\nu, H\Psi_\mu\rangle s_\mu\big)\, u_\mu = \lambda s_\nu^2\, u_\nu\,, \quad \nu \in \nabla^d\,, \tag{5.9}$$

where $\mathbf{u} = (u_\nu)_{\nu\in\nabla^d} = (s_\nu^{-1}\langle u, \Psi_\nu\rangle)_{\nu\in\nabla^d}$ for $u \in \mathrm{H}^1(\mathbb{R}^d)$, or briefly, $\mathbf{Hu} = \lambda \mathbf{s}^2\mathbf{u}$. Note that by the Riesz basis property, $\|u\|_{\mathrm{H}^1(\mathbb{R}^d)} \sim \|\mathbf{u}\|_{\ell_2(\nabla^d)}$.

5.2.1 Low-Rank Tensor Formats

Let us first consider low-rank approximation in the case of two-dimensional problems. Let $\mathbf{u} \in \ell_2(\Lambda_1 \times \Lambda_2)$ with finite $\Lambda_1, \Lambda_2 \subset \nabla$, then singular value decomposition yields a representation in the form

$$\mathbf{u} = \sum_{k=1}^{r} (\mathbf{U}_k^{(1)} \otimes \mathbf{U}_k^{(2)})\, \sigma_k\,, \tag{5.10}$$

where $\sigma_1 \geq \cdots \geq \sigma_r > 0$ and, for $i \in \{1,2\}$ and $k,l \in \{1,\ldots,r\}$, $\mathbf{U}_k^{(i)} = (U_{k,\nu}^{(i)})_{\nu\in\Lambda_i}$ with $\operatorname{supp}\mathbf{U}_k^{(i)} \in \Lambda_i$ and $\langle \mathbf{U}_k^{(i)}, \mathbf{U}_l^{(i)}\rangle = \delta_{kl}$.

Here r is the rank of the matrix $(u_{\nu_1,\nu_2})_{\nu_1\in\Lambda_1,\nu_2\in\Lambda_2}$, and the decomposition (5.10) also provides a means of computing the best approximation by an element of $\ell_2(\Lambda_1 \times \Lambda_2)$ with rank $\tilde r < r$: by the Eckart-Young theorem [47], the error

$$\Big\|\mathbf{u} - \sum_{k=1}^{\tilde r} (\mathbf{U}_k^{(1)} \otimes \mathbf{U}_k^{(2)})\sigma_k\Big\| = \Big(\sum_{k=\tilde r+1}^{r} |\sigma_k|^2\Big)^{\frac12} \tag{5.11}$$

is minimal among all rank-$\tilde r$ approximations of u.

This can be extended to $\mathbf{u} \in \ell_2(\nabla^2)$ without the restriction of finite support, in which case the singular value decomposition is replaced by the Hilbert-Schmidt decomposition of operators. For such a general $\mathbf{u}$, the infinite matrix $(u_{\nu_1,\nu_2})_{\nu_1\in\nabla,\nu_2\in\nabla}$ defines a Hilbert-Schmidt operator

$$T_{\mathbf{u}}\colon \ell_2(\nabla) \to \ell_2(\nabla)\,,\ \mathbf{c} \mapsto \Big(\sum_{\nu\in\nabla} u_{\tilde\nu,\nu} c_\nu\Big)_{\tilde\nu\in\nabla}\,,$$

and the spectral theorem yields a decomposition

$$\mathbf{u} = \sum_{k=1}^{\infty} (\mathbf{U}_k^{(1)} \otimes \mathbf{U}_k^{(2)})\, \sigma_k\,, \tag{5.12}$$

with a nonnegative nonincreasing sequence $(\sigma_k)_{k\in\mathbb{N}} \in \ell_2(\mathbb{N})$, and orthonormal bases $\{\mathbf{U}_k^{(i)}\}_{k\in\mathbb{N}}$ of $\ell_2(\nabla)$ for $i \in \{1,2\}$. The low-rank approximation property (5.11) carries over to this case, where in general $r = \infty$.

At first glance, a natural extension of (5.10) to the higher-dimensional case would be a representation of $\mathbf{u} \in \ell_2(\nabla^d)$ of the form

$$\mathbf{u} = \sum_{k=1}^{r} (\mathbf{U}_k^{(1)} \otimes \cdots \otimes \mathbf{U}_k^{(d)})\, a_k \tag{5.13}$$

with $\|\mathbf{U}_k^{(i)}\| = 1$ and $a_k \in \mathbb{R}$. This is typically referred to as *canonical format*, *canonical polyadic* *decomposition*, or *parallel factors*. The smallest $r \in \mathbb{N}_0 \cup \{\infty\}$ for which such a representation exists is referred to as the *canonical rank* of $\mathbf{u}$. For our purposes, the major problem with this type of representation is the lack of a sufficiently reliable recompression procedure. In fact, the problem of approximating a given $\mathbf{u}$ by an expansion (5.13) of specified rank is in general ill-posed [39], which additionally necessitates a suitable regularization. For such regularized problems, however, one still needs to rely on minimization procedures that generally cannot be guaranteed to converge to the global minimum.

In this regard, a representation in the form

$$\mathbf{u} = \sum_{k_1=1}^{r_1} \cdots \sum_{k_d=1}^{r_d} (\mathbf{U}^{(1)}_{k_1} \otimes \cdots \otimes \mathbf{U}^{(d)}_{k_d})\, a_{k_1,\ldots,k_d} \tag{5.14}$$

has substantially more favorable properties, and in this chapter we will be dealing with this format, and remark on generalizations with similar features. Here the order-d tensor $\mathbf{a}$ is referred to as *core tensor*, the matrix $\mathbf{U}^{(i)}$ with column vectors $\mathbf{U}^{(i)}_k \in \ell_2(\nabla)$, $k = 1, \ldots, r_i$, as the i-th *mode frame*. This is the so-called *Tucker format* [144, 145] or *subspace representation*. Note that for $\hat{d} \in \mathbb{N}$, we can also represent $\mathbf{u} \in \ell_2(\nabla^{\hat{d}d})$ in the form (5.14) with $\mathbf{U}^{(i)}_k \in \ell_2(\nabla^{\hat{d}})$. For the sake of simplicity, we consider the case $\hat{d} = 1$ in what follows, but one can proceed completely analogously for general $\hat{d}$.

Clearly, any compactly supported $\mathbf{u} \in \ell_2(\nabla^d)$ can be represented in the form (5.14) for some $r \in \mathbb{N}_0^d$. For general $\mathbf{u} \in \ell_2(\nabla^d)$, the sum in (5.14) may be infinite. We correspondingly define $\operatorname{rank}(\mathbf{u}) \in (\mathbb{N}_0 \cup \{\infty\})^d$ by

$$\operatorname{rank}(\mathbf{u})_i := \dim \operatorname{span}\{\mathbf{U}^{(i)}_k :\ k \in \mathbb{N}\}\,, \quad i = 1, \ldots, d\,. \tag{5.15}$$

This vector is referred to as the *multilinear rank* of $\mathbf{u}$. Note that in a representation of the form (5.14), one can always orthogonalize the columns of $\mathbf{U}^{(i)}$ to obtain $\langle \mathbf{U}^{(i)}_k, \mathbf{U}^{(i)}_l \rangle = \delta_{kl}$ for all i. We shall refer to $\mathbf{U}^{(i)}$ with the latter property as *orthonormal mode frames*.

Remark 5.1. *As we have seen in Section 4.3, when approximating the wavelet coefficients of hydrogenic ground states in the format* (5.14)*, one can achieve exponential decrease of the* H^1*-approximation error with respect to the multilinear ranks.*

In the case of helium or hookium, fast convergence of the representation with respect to the ranks can only be expected when – assuming single-electron coordinates $x, y \in \mathbb{R}^3$ *– the coordinate pairs* (x_i, y_i) *for* $i = 1, 2, 3$ *are not separated. We have shown for hookium in Section 4.3 that the corresponding wavelet coefficients* $\mathbf{u} \in \ell_2((\nabla^2)^3)$ *can be represented efficiently in the form* (5.14) *with* $d = 3$ *and* $\mathbf{U}^{(i)}_k \in \ell_2(\nabla^2)$*, where each* $\mathbf{U}^{(i)}$ *corresponds to a coordinate pair* (x_i, y_i)*.*

To simplify notation for the sums in (5.14), for $r \in \mathbb{N}_0^d$ we define

$$\mathcal{K}_d(r) := \bigtimes_{i=1}^{d} \{1, \ldots, r_i\} \quad \text{if } \min r > 0\,,$$

and $\mathcal{K}_d(r) := \emptyset$ if $\min r = 0$. For any $\nu \in \nabla^d$, $n \in \mathbb{N}_0^d$ and $i \in \{1, \ldots, d\}$, we define the notation

$$\check{\nu}_i := (\nu_1, \ldots, \nu_{i-1}, \nu_{i+1}, \ldots, \nu_d)\,, \quad \check{m}_i := (m_1, \ldots, m_{i-1}, m_{i+1}, \ldots, m_d) \tag{5.16}$$

for the corresponding vectors with entry i deleted. We shall also need the auxiliary quantities

$$a^{(i)}_{pq} := \sum_{k_1=1}^{r_1} \cdots \sum_{k_{i-1}=1}^{r_{i-1}} \sum_{k_{i+1}=1}^{r_{i+1}} \cdots \sum_{k_d=1}^{r_d} a_{k_1,\ldots,k_{i-1},p,k_{i+1},\ldots,k_d}\, a_{k_1,\ldots,k_{i-1},q,k_{i+1},\ldots,k_d}\,, \qquad \sigma^{(i)}_p := \sqrt{a^{(i)}_{pp}} \tag{5.17}$$

derived from the core tensor, where $i \in \{1, 2, 3\}$, $p, q \in \{1, \ldots, r_i\}$.

There exists an analogue of the singular value decomposition of matrices, the *higher-order singular value decomposition* [107], for the Tucker tensor format (5.14). In the following theorem, we summarize its properties in the more general case of sequence spaces, where the the singular value decomposition is replaced by the spectral theorem for compact operators.

Theorem 5.2. *For any* $\mathbf{u} \in \ell_2(\nabla^d)$ *there exist orthonormal mode frames* $\{\mathbf{U}^{(i)}_k\}_{k\in\mathbb{N}}$, $i = 1,\dots,d$, *with* $\mathbf{U}^{(i)}_k \in \ell_2(\nabla)$ *which uniquely determine a core tensor* $\mathbf{a} = (a_k)_{k\in\mathbb{N}^d} \in \ell_2(\mathbb{N}^d)$ *such that*

$$\mathbf{u} = \sum_{k\in\mathbb{N}^d} \bigl(\mathbf{U}^{(1)}_{k_1} \otimes \cdots \otimes \mathbf{U}^{(d)}_{k_d}\bigr)\, a_k\,,$$

and with $a^{(i)}_{pq}$ *and* $\sigma^{(i)}_p$ *as in* (5.17)*, the following holds:*

(i) *For all* $i \in \{1,\dots,d\}$ *we have* $(\sigma^{(i)}_k)_{k\in\mathbb{N}} \in \ell_2(\mathbb{N})$, *and* $\sigma^{(i)}_k \ge \sigma^{(i)}_{k+1} \ge 0$ *for all* $k \in \mathbb{N}$.

(ii) *For all* $i \in \{1,\dots,d\}$ *and all* $p,q \in \mathbb{N}$, *we have* $a^{(i)}_{pq} = \bigl|\sigma^{(i)}_p\bigr|^2\delta_{pq}$.

(iii) *For each* $r \in \mathbb{N}^d_0$, *we have*

$$\Bigl\|\mathbf{u} - \sum_{k\in\mathcal{K}_d(r)} (\mathbf{U}^{(1)}_{k_1} \otimes \cdots \otimes \mathbf{U}^{(d)}_{k_d})\, a_k\Bigr\| \le \Bigl(\sum_{i=1}^{d}\sum_{k=r_i+1}^{\infty} |\sigma^{(i)}_k|^2\Bigr)^{\frac12} \le \sqrt{d} \inf_{\operatorname{rank}(\mathbf{w})\le r} \|\mathbf{u}-\mathbf{w}\|\,. \tag{5.18}$$

If in addition $\operatorname{supp}\mathbf{u} \subseteq \Lambda_1 \times \cdots \times \Lambda_d \subset \nabla^d$ *for finite* $\Lambda_1,\dots,\Lambda_d \subset \nabla$, *then* $\operatorname{supp}\mathbf{U}^{(i)}_k \subseteq \Lambda_i$ *and we have* $\operatorname{supp}\mathbf{a} \subseteq \mathcal{K}_d(\bar r)$ *with* $\bar r \in \mathbb{N}^d_0$ *satisfying* $\bar r_i \le \#\Lambda_i$ *for* $i = 1,\dots,d$.

Proof. The following is essentially an adaptation of the arguments for the finite-dimensional case given in [107] to the infinite-dimensional sequence space $\ell_2(\nabla^d)$.

Let $\mathbf{u} = (u_\nu)_{\nu\in\nabla^d} \in \ell_2(\nabla^d)$. For each $i \in \{1,\dots,d\}$ we consider the mode-i matricization of $\mathbf{u}$, that is, the infinite matrix $(u^{(i)}_{\nu,\tilde\nu})_{\nu\in\nabla,\tilde\nu\in\nabla^{d-1}}$ with entries $u^{(i)}_{\nu_i,\check\nu_i} := u_\nu$ for $\nu \in \nabla^d$, which defines a Hilbert-Schmidt operator

$$T^{(i)} \colon \ell_2(\nabla^{d-1}) \to \ell_2(\nabla)\,,\ (c_{\tilde\nu})_{\tilde\nu\in\nabla^{d-1}} \mapsto \Bigl(\sum_{\tilde\nu\in\nabla^{d-1}} u^{(i)}_{\nu,\tilde\nu} c_{\tilde\nu}\Bigr)_{\nu\in\nabla}\,.$$

By the spectral theorem, for each i there exist a nonnegative real sequence $(\sigma^{(i)}_n)_{n\in\mathbb{N}}$, where $\sigma^{(i)}_n$ are the eigenvalues of $\bigl((T^{(i)})^*T^{(i)}\bigr)^{1/2}$, as well as orthonormal bases $\{\mathbf{U}^{(i)}_n\}_{n\in\mathbb{N}}$ for $\ell_2(\nabla)$ and $\{\mathbf{V}^{(i)}_n\}_{n\in\mathbb{N}}$ for $\ell_2(\nabla^{d-1})$, such that

$$T^{(i)} = \sum_{n\in\mathbb{N}} \sigma^{(i)}_n \langle \mathbf{V}^{(i)}_n, \cdot\rangle \mathbf{U}^{(i)}_n\,. \tag{5.19}$$

The representation (5.19) converges in the Hilbert-Schmidt norm, and as a consequence we have

$$\mathbf{u} = \Bigl(\sum_{n\in\mathbb{N}} \sigma^{(i)}_n \mathbf{U}^{(i)}_{n,\nu_i} \mathbf{V}^{(i)}_{n,\check\nu_i}\Bigr)_{\nu\in\nabla^d}\,, \tag{5.20}$$

where the series converges in $\ell_2(\nabla^d)$. By Theorem 3.14, $\{\bar{\mathbf{U}}_n\}_{n\in\mathbb{N}^d}$ with $\bar{\mathbf{U}}_n := \bigotimes_{j=1}^d \mathbf{U}^{(j)}_{n_j}$ is an orthonormal basis of $\ell_2(\nabla^d)$, and setting $a_n := \langle \bar{\mathbf{U}}_n, \mathbf{u}\rangle = \sum_{\nu\in\nabla^d} U^{(1)}_{n_1,\nu_1} \cdots U^{(d)}_{n_d,\nu_d} u_\nu$, we have $\mathbf{a} = (a_n) \in \ell_2(\mathbb{N}^d)$ and $\mathbf{u} = \sum_{n\in\mathbb{N}^d} a_n \bar{\mathbf{U}}_n$.

Property (i) is clear. For the proof of property (ii), for $\tilde n \in \mathbb{N}^{d-1}$ and $p \in \mathbb{N}$ we introduce the auxiliary notation $\hat{\mathbf{U}}^{(i)}_{\tilde n}(p) := \bar{\mathbf{U}}_m\big|_{m_i = p,\, \check m_i = \tilde n}$. By the definition (5.17), we obtain

$$a^{(i)}_{pq} = \sum_{k\in\mathbb{N}^{d-1}} \bigl\langle \hat{\mathbf{U}}^{(i)}_k(p), \mathbf{u}\bigr\rangle \bigl\langle \hat{\mathbf{U}}^{(i)}_k(q), \mathbf{u}\bigr\rangle\,,$$

and using the representation (5.20),

$$\begin{aligned}
&= \sum_{k\in\mathbb{N}^{d-1}} \Bigl(\sum_{\nu\in\nabla^d} (\hat{\mathbf{U}}^{(i)}_k(p))_\nu \sum_{l_1\in\mathbb{N}} \sigma^{(i)}_{l_1} \mathbf{U}^{(i)}_{l_1,\nu_i} \mathbf{V}^{(i)}_{l_1,\check{\nu}_i} \Bigr) \Bigl(\sum_{\mu\in\nabla^d} (\hat{\mathbf{U}}^{(i)}_k(q))_\mu \sum_{l_2\in\mathbb{N}} \sigma^{(i)}_{l_2} \mathbf{U}^{(i)}_{l_2,\mu_i} \mathbf{V}^{(i)}_{l_2,\check{\mu}_i} \Bigr) \\
&= \sum_{l_1,l_2} \sigma^{(i)}_{l_1} \sigma^{(i)}_{l_2} \sum_{k\in\mathbb{N}^{d-1}} \langle \mathbf{U}^{(i)}_p, \mathbf{U}^{(i)}_{l_1} \rangle \langle \mathbf{U}^{(i)}_q, \mathbf{U}^{(i)}_{l_2} \rangle \langle \bigotimes_{j\neq i} \mathbf{U}^{(j)}_{k_j}, \mathbf{V}^{(i)}_{l_1} \rangle \langle \bigotimes_{j\neq i} \mathbf{U}^{(j)}_{k_j}, \mathbf{V}^{(i)}_{l_2} \rangle ,
\end{aligned}$$

which by orthonormality of $\{\mathbf{U}^{(i)}_n\}_{n\in\mathbb{N}}$ yields

$$= \sigma^{(i)}_p \sigma^{(i)}_q \sum_{k\in\mathbb{N}^{d-1}} \langle \mathbf{V}^{(i)}_p, \bigotimes_{j\neq i} \mathbf{U}^{(j)}_{k_j} \rangle \langle \bigotimes_{j\neq i} \mathbf{U}^{(j)}_{k_j}, \mathbf{V}^{(i)}_q \rangle .$$

Noting that $\{\bigotimes_{j\neq i} \mathbf{U}^{(j)}_{k_j}\}_{k\in\mathbb{N}^{d-1}}$ is an orthonormal basis of $\ell_2(\nabla^{d-1})$, we obtain property (ii) by orthonormality of $\{\mathbf{V}^{(i)}_n\}_{n\in\mathbb{N}}$. Property (iii) follows with the observations

$$\|\mathbf{u} - \sum_{k\in\mathcal{K}_d(r)} a_k \bar{\mathbf{U}}_k\|^2 \leq \sum_{i=1}^{d} \| \sum_{\substack{k\in\mathbb{N}^d \\ k_i > r_i}} a_k \bar{\mathbf{U}}_k \|^2 = \sum_{i=1}^{d} \sum_{k=r_i+1}^{\infty} |\sigma^{(i)}_k|^2$$

and, for $i = 1,\dots,d$,

$$\sum_{k=r_i+1}^{\infty} |\sigma^{(i)}_k|^2 = \inf_{\operatorname{rank}(\mathbf{w})_i \leq r_i} \|\mathbf{u} - \mathbf{w}\|^2 \leq \inf_{\operatorname{rank}(\mathbf{w}) \leq r} \|\mathbf{u} - \mathbf{w}\|^2 .$$

The additional properties of the decomposition for finitely supported $\mathbf{u}$ are clear, since in this case the spectral decomposition reduces to a finite-dimensional singular value decomposition. ☐

Remark 5.3. *The result of Theorem 5.2 holds analogously for* $\mathbf{u} \in \ell_2(\nabla^{d\hat{d}})$ *and* $\mathbf{U}^{(i)}_k \in \ell_2(\nabla^{\hat{d}})$ *with* $d, \hat{d} \in \mathbb{N}$. *As noted in Remark 5.1, this is relevant for two-electron systems such as helium, where we use a decomposition with* $d = 3$ *and* $\hat{d} = 2$.

Note that by analogy to (5.10), the $\sigma^{(i)}_k$ are also referred to as mode-i singular values of $\mathbf{u}$. Property (iii) in Theorem 5.2 leads to a simple procedure for truncation to lower multilinear ranks with an explicit error estimate in terms of the mode-i singular values. In this manner, one does not necessarily obtain the best approximation for prescribed rank, but the approximation is quasi-optimal in the sense that the error is at most by a factor $\sqrt{d}$ larger than the error of best approximation with the same multilinear rank.

In principle, a representation as in Theorem 5.2 can be obtained for any $\mathbf{u} \in \ell_2(\nabla^d)$ by a combination of standard linear algebra procedures. For our purposes, the relevant task is to obtain such a representation for finitely supported $\mathbf{u}$ given in the form

$$\mathbf{u} = \sum_{k\in\mathcal{K}_d(\tilde{r})} \Bigl(\bigotimes_i \tilde{\mathbf{U}}^{(i)}_{k_i} \Bigr) \tilde{a}_k \tag{5.21}$$

without further assumptions on $\tilde{\mathbf{U}}^{(i)}$ and $\tilde{\mathbf{a}}$, where in particular the columns of the $\tilde{\mathbf{U}}^{(i)}$ may be linearly dependent. From the arguments in [107], one can extract the well-known procedure described in Algorithm 5.1 that yields a representation as in Theorem 5.2 for finitely supported $\mathbf{u}$.

Remark 5.4. *Assuming* $\operatorname{supp}\mathbf{u} \subseteq \Lambda_1 \times \dots \times \Lambda_d$, `hosvd` *as in Algorithm 5.1 can be performed in* $\mathcal{O}(|\tilde{r}|_\infty \prod_i \tilde{r}_i + \sum_i \tilde{r}_i^2 \#\Lambda_i)$ *operations, using only standard linear algebra operations.*

The procedure `hosvd` can be interpreted as the selection of basis functions, given by the columns of $\mathbf{U}^{(i)}$, which are adapted to a given $\mathbf{u}$. However, the tensor $\mathbf{a}$ containing the coefficients for

Algorithm 5.1 $[\{\mathbf{U}^{(i)}\},\mathbf{a}] = \mathsf{hosvd}(\{\tilde{\mathbf{U}}^{(i)}\},\tilde{\mathbf{a}})$

```
input   $\mathbf{u}$ in representation (5.21)
output  mode frames $\mathbf{U}^{(i)}$ and core tensor $\mathbf{a}$ as in Theorem 5.2
for all $i \in \{1,\dots,d\}$
    perform $QR$–factorization $\tilde{\mathbf{U}}^{(i)} = \mathbf{Q}^{(i)}\mathbf{R}^{(i)}$
        ▷ $\mathbf{Q}^{(i)} \in \mathbb{R}^{\Lambda^{(i)}\times\{1,\dots,r_i\}}$, $\mathbf{R}^{(i)} \in \mathbb{R}^{\{1,\dots,r_i\}\times\{1,\dots,\tilde r_i\}}$, where $r \le \tilde r$.
        ▷ columns of $\mathbf{Q}^{(i)}$ are orthonormal, $\mathbf{R}^{(i)}$ is right upper triangular
end for
$\hat a_k \leftarrow \sum_{l\in\mathcal{K}_d(\tilde r)} R^{(1)}_{k_1,l_1}\cdots R^{(d)}_{k_d,l_d}\,\tilde a_l$  for  $k \in \mathcal{K}_d(r)$
for all $i \in \{1,\dots,d\}$
    build matricization $\mathbf{T}^{(i)} \in \mathbb{R}^{\{1,\dots,r_i\}\times\mathcal{I}_i}$ with entries $T^{(i)}_{k_i,\check k_i} := \hat a_{k_1,\dots,k_d}$
        ▷ $\mathcal{I}_i = \{1,\dots,r_1\}\times\cdots\times\{1,\dots,r_{i-1}\}\times\{1,\dots,r_{i+1}\}\times\ldots\times\{1,\dots,r_d\}$
    perform singular value decomposition $\mathbf{T}^{(i)} = \mathbf{V}^{(i)}\mathbf{\Sigma}^{(i)}(\mathbf{W}^{(i)})^T$
    $\mathbf{U}^{(i)} \leftarrow \mathbf{Q}^{(i)}\mathbf{V}^{(i)}$
end for
$a_k \leftarrow \sum_{l\in\mathcal{K}_d(\mathbf{r})} V^{(1)}_{l_1,k_1}\cdots V^{(d)}_{l_d,k_d}\,\hat a_l$  for  $k \in \mathcal{K}_d(r)$
```

these basis functions has $\prod_i r_i$ components, which even for moderate multilinear ranks becomes too expensive for larger d.

A possible alternative for higher dimensions is the Hierarchical Tucker or $\mathcal{H}$–Tucker format [75]. It has similar features as the Tucker format, and there exists a scheme that parallels hosvd in its properties [64], but has storage and work complexity linear in d when applied to input tensors given in the appropriate $\mathcal{H}$–Tucker representation. This comes at the price of additional structural constraints on the tensors in the form of a modified notion of tensor ranks. For the model problems that we are considering in this chapter, the $\mathcal{H}$–Tucker format does not give an advantage over the Tucker format, and hence what follows will be formulated for the latter. The schemes developed here can, however, be applied to the $\mathcal{H}$–Tucker format without major modifications; we will come back to this point in Section 5.3.3.

5.2.2 The Problem with Diagonal Rescaling of Operators

As described briefly in the beginning of this chapter, using a sufficiently smooth wavelet basis, the eigenvalue problems under consideration can be reduced to well-posed problems on ℓ_2-spaces. On the basis of the higher-order SVD given in Algorithm 5.1 and the estimate for the trunctation error in ℓ_2 provided by Theorem 5.2, in this framework we can thus ensure the convergence of truncated iterative methods, with iterates represented in a tensor format as described in the previous section, by appropriately choosing the error tolerances in the tensor truncation steps. However, some fundamental additional difficulties arise the present context as a consequence of the diagonal rescaling of the operator.

Before turning to the application to higher-dimensional eigenvalue problems, we first discuss these fairly general issues at the example of a simpler model problem: we consider the following operator equation with low-rank structure on $\mathbb{R}^2$,

$$Au := -\Delta u + u = \big((-\mathrm{D}^2_{x_1})\otimes\mathrm{I} + \mathrm{I}\otimes(-\mathrm{D}^2_{x_2}) + \mathrm{I}\otimes\mathrm{I}\big)u = f_1\otimes f_2\,, \tag{5.22}$$

where $f_1, f_2 \in \mathrm{L}_2(\mathbb{R})$. It should be noted that even in this simple setting, the solution u does not necessarily have a representation as a finite sum of separable functions; our objective is to obtain approximations to u of this type that converge in the appropriate energy space, that is, in $\mathrm{H}^1(\mathbb{R}^2)$.

Let $\{\Psi_\nu\}_{\nu\in\nabla^2}$ with $\Psi_\nu = \psi_{\nu_1}\otimes\psi_{\nu_2}$ be an orthonormal tensor product wavelet basis on $\mathbb{R}^2$, then the coefficients of A and f read

$$\langle A\Psi_\nu, \Psi_\mu\rangle = \langle \psi'_{\mu_1}, \psi'_{\nu_1}\rangle \delta_{\mu_2\nu_2} + \langle \psi'_{\mu_2}, \psi'_{\nu_2}\rangle \delta_{\mu_1\nu_1} + \delta_{\mu_1\nu_1}\delta_{\mu_2\nu_2}\,, \quad \langle f, \Psi_\mu\rangle = \langle f_1, \psi_{\mu_1}\rangle\langle f_2, \psi_{\mu_2}\rangle\,.$$

Note that the matrix $(\langle A\Psi_\nu, \Psi_\mu\rangle)_{\nu,\mu\in\nabla^2}$, which corresponds to a discretization without preconditioning, is not continuously invertible on $\ell_2(\nabla^2)$. As we have seen in Section 3.3, however, assuming that $\psi \in \mathrm{H}^s(\mathbb{R})$ for some $s > 1$, the rescaled wavelet basis $\{s_\nu \Psi_\nu\}_{\nu\in\nabla^2}$ with

$$s_\nu = (2^{2|\nu_1|} + 2^{2|\nu_2|})^{-\frac{1}{2}}$$

as in (5.7) is a Riesz basis of $\mathrm{H}^1(\mathbb{R}^2)$, and as a consequence, the problem (5.22) is equivalent to

$$\sum_\nu \bigl(s_\nu \langle A\Psi_\nu, \Psi_\mu\rangle s_\mu\bigr)\bigl(s_\nu^{-1}\langle u, \Psi_\nu\rangle\bigr) = s_\mu \langle f, \Psi_\mu\rangle\,, \quad \mu \in \nabla^2\,.$$

This formulation has two main advantages for our purposes: the rescaled infinite matrix $\mathbf{A} := (s_\nu\langle A\Psi_\nu, \Psi_\mu\rangle s_\mu)$ is continuously invertible on $\ell_2(\nabla^2)$, and for any $v \in \mathrm{H}^1(\mathbb{R}^2)$ we have $\|v\|_{\mathrm{H}^1} \sim \|(s_\nu^{-1}\langle v, \Psi_\nu\rangle)_{\nu\in\nabla^2}\|_{\ell_2}$. Hence if we introduce an error of a certain ℓ_2–norm in the rescaled wavelet coefficients, we obtain a proportional error in the H^1-norm of the represented function. Our aim is to find an approximation $\tilde{\mathbf{u}} = (\tilde{u}_\nu)$ to the coefficient sequence $\mathbf{u} = (s_\nu^{-1}\langle u, \Psi_\nu\rangle)_{\nu\in\nabla^2}$ of the form[1]

$$\tilde{u}_\nu = \sum_{k\in\mathcal{K}_2(r)} a_{k_1,k_2} U^{(1)}_{k_1,\nu_1} U^{(2)}_{k_2,\nu_2} \tag{5.23}$$

with orthonormal mode frames $\mathbf{U}^{(i)}$. The crucial task in iterative methods, for instance Richardson iteration, for computing such $\tilde{\mathbf{u}}$ is the approximate application of $\mathbf{A}$ to the a low-rank representation as in (5.23) of a given previous iterate. For the following discussion, as an instance of such an iterate, let $\mathbf{v} = (v_\nu) \in \ell_2(\Lambda_1 \times \Lambda_2)$ with finite $\Lambda_1, \Lambda_2 \in \nabla$ and $\mathbf{v} = \sum_{k\in\mathcal{K}_2(r)} b_k \mathbf{V}^{(1)}_{k_1} \otimes \mathbf{V}^{(2)}_{k_1}$ for some $r \in \mathbb{N}^2$, and let $j_{\max}$ be the smallest integer such that $\operatorname{supp}\mathbf{v} \subset \nabla_{\max} := \{\nu \in \nabla^2\colon\, \max|\nu| \le j_{\max}\}$.

The problem we are facing at this point is that the sequence $\mathbf{s} = (s_\nu)_{\nu\in\nabla^2}$ does not have a representation as a finite sum of separable functions. Using the notation $\nabla_j = \{\nu \in \nabla\colon |\nu| = j\}$ for $j \in \mathbb{Z}$ introduced in (3.7), we do, however, have the expansion

$$\mathbf{s} = \bigl((2^{2|\nu_1|} + 2^{2|\nu_2|})^{-\frac{1}{2}}\bigr)_{\nu\in\nabla^2} = \sum_{n_1,n_2=0}^{\infty} (2^{2n_1} + 2^{2n_2})^{-\frac{1}{2}}\, \chi_{\nabla_{n_1}} \otimes \chi_{\nabla_{n_2}}\,,$$

where χ_{∇_n} is the characteristic function of ∇_n. Note first that as a consequence, the elementwise product of $\mathbf{v}$ and $\mathbf{s}$ has the tensor representation

$$\mathbf{v}\,\mathbf{s} = (v_\nu s_\nu)_{\nu\in\nabla^2} = \sum_{k_1=1}^{r_1}\sum_{n_1=0}^{j_{\max}}\sum_{k_2=1}^{r_2}\sum_{n_2=0}^{j_{\max}} b_k\,(2^{2n_1} + 2^{2n_2})^{-\frac{1}{2}}\,(\chi_{\nabla_{n_1}}\mathbf{V}^{(1)}_{k_1}) \otimes (\chi_{\nabla_{n_2}}\mathbf{V}^{(2)}_{k_2})\,.$$

Thus $\mathbf{v}\,\mathbf{s}$ again has a representation in the tensor format, but with a multilinear rank of up to $(j_{\max}+1)r \in \mathbb{N}^2$. In other words, multiplication by the scaling factor increases the multlinear rank of compactly supported vectors by a factor depending on the number of wavelet levels on which this vector does not vanish.

Concerning the application of the infinite matrix, the situation is similar. Note that

$$(\langle A\Psi_\nu, \Psi_\mu\rangle)_{\nu,\mu\in\nabla^2} = \sum_{i_1,i_2=0}^{1} c_i\, \mathbf{M}_{i_1} \otimes \mathbf{M}_{i_2}$$

---

[1] In the present two-dimensional case, we can always ensure $\mathbf{a}$ to be diagonal, but we use the more general form (5.23) corresponding to the Tucker format to achieve a closer analogy to the higher-dimensional case.

with

$$\mathbf{M}_0 := (\delta_{\nu,\mu})_{\nu,\mu\in\nabla}\,, \quad \mathbf{M}_1 := (\langle\psi'_\nu,\psi'_\mu\rangle)_{\nu,\mu\in\nabla}\,, \quad c_i = \begin{cases} 1\,, & i_1+i_2\leq 1\,,\\ 0\,, & \text{otherwise.}\end{cases}$$

An analogous representation also holds for the higher-dimensional Laplacian.

To simplify the further discussion, we restrict our considerations to the section $\mathbf{A}\mathbf{v}|_{\nabla_{\max}}$, which is relevant especially for Galerkin discretizations on index sets contained in $\nabla_{\max}$, and for which we have the representation

$$\begin{aligned}\mathbf{A}\mathbf{v}|_{\nabla_{\max}} = \sum_{i_1,i_2=0}^{1}\sum_{n_1,n_2=0}^{j_{\max}}\sum_{m_1,m_2=0}^{j_{\max}}\sum_{k\in\mathcal{K}_2(r)} & b_k\, c_i\,(2^{2n_1}+2^{2n_2})^{-\frac{1}{2}}(2^{2m_1}+2^{2m_2})^{-\frac{1}{2}}\\ & \times\big(\chi_{\nabla_{m_1}}\mathbf{M}_{i_1}\chi_{\nabla_{n_1}}\mathbf{V}^{(1)}_{k_1}\big)\otimes\big(\chi_{\nabla_{m_2}}\mathbf{M}_{i_2}\chi_{\nabla_{n_2}}\mathbf{V}^{(2)}_{k_2}\big)\end{aligned} \tag{5.24}$$

that formally has multilinear rank $2(j_{\max}+1)^2 r$. A subsequent recompression operation, which may reveal a lower effective multilinear rank, will therefore in the present two-dimensional example require up to

$$\mathcal{O}\big(j_{\max}^6|r|_\infty^3 + j_{\max}^4|r|_\infty^2 \max_{i=1,2}\#\Lambda_i\big) \tag{5.25}$$

operations. In the analogous three-dimensional problem, we instead obtain

$$\mathcal{O}\big(j_{\max}^8|r|_\infty^4 + j_{\max}^4|r|_\infty^2 \max_{i=1,2}\#\Lambda_i\big)\,.$$

Especially in view of our eventual aim of treating problems with nonsmooth solutions, where $j_{\max}$ is large in relation to the target accuracy, this is clearly problematic.

In general, we cannot expect to circumvent this problem entirely in the sense of completely eliminating the dependency on $j_{\max}$, but we next propose several measures for improving the above worst-case complexity estimate.

Note first that as a consequence of the wavelet compressibility properties discussed in Section 6.4, we have $\|\chi_{\nabla_m}\mathbf{M}_1\chi_{\nabla_n}\|_{\ell_2\to\ell_2}\lesssim 2^{-\sigma|n-m|}$ for some $\sigma>0$. Since $\mathbf{M}_0$ is diagonal, in this particular case we even have $\chi_{\nabla_m}\mathbf{M}_0\chi_{\nabla_n}=0$ if $m\neq n$. As we are only interested in applying operators approximately, on the basis of the properties of the wavelet representation of the operator we can therefore a priori discard summands in (5.24) that are negligibly small. What can be gained in this manner rather strongly depends on the specific operator under consideration, and we thus do not go into further detail at this point.

A second improvement that is easier to quantify can be achieved by a modification of the tensor representation of $\mathbf{v}$. Instead of decomposing and reassembling parts of the tensor representation corresponding to $\nabla_{n_1}\times\nabla_{n_2}\subset\nabla^2$ for applying operators as in (5.24), we can use a slightly different representation where these parts are kept separated,

$$\mathbf{v} = \sum_{n\in\{0,\ldots,j_{\max}\}^2}\sum_{k\in\mathcal{K}_2(r_n)} b_{n,k}\mathbf{V}^{(1)}_{n,k_1}\otimes\mathbf{V}^{(2)}_{n,k_2}\,, \tag{5.26}$$

with $r_n\leq r$ componentwise and $\mathbf{V}^{(i)}_{n,k}\subset\nabla_{n_i}$ for $i=1,2$. Note that the summands in the summation over n are ℓ_2–orthogonal due to their disjoint supports. Therefore, when representing $\mathbf{A}\mathbf{v}|_{\nabla_{\max}}$ in the same form (5.26), hosvd can be performed independently for each subset $\nabla_{n_1}\times\nabla_{n_2}$. Although the representation (5.26) is potentially more expensive concerning the number of coefficients, the total complexity of performing hosvd for all parts is only

$$\mathcal{O}\big(j_{\max}^2\times(j_{\max}^3|r|_\infty^3) + j_{\max}^2|r|_\infty^2(j_{\max}\times\max_{i=1,2}\#\Lambda_i)\big) \tag{5.27}$$

in the present two-dimensional example, and $\mathcal{O}(j_{\max}^3\times(j_{\max}^4|r|_\infty^4)+j_{\max}^2|r|_\infty^2(j_{\max}^2\times\max_{i=1,2}\#\Lambda_i))$ for the analogous three-dimensional problem; altogether, compared to (5.25), one thus obtains an

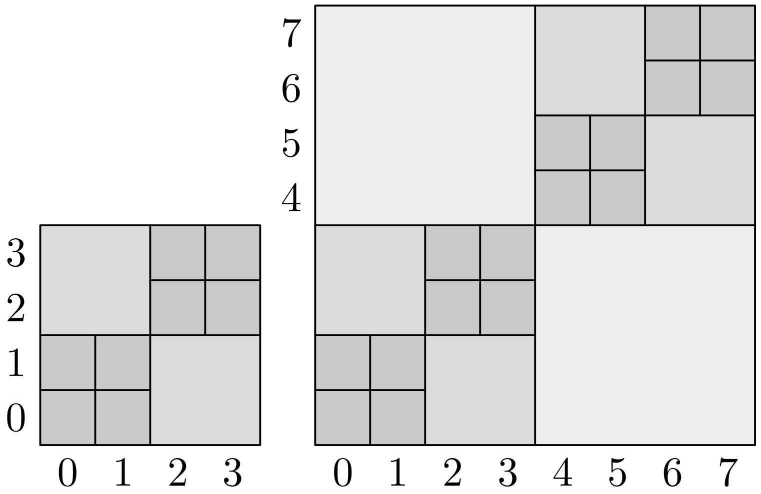

Figure 5.1. Structure of the partitions $\mathcal{J}^{(2)}_{\ell,\{1,2\}}$ for $\ell = 2, 3$; each square represents a subset in the partition.

improvement by a factor $j_{\max}$ in the leading order.

The type of subdivision underlying (5.26) is still rather unsatisfactory: we would ideally like to be able to use a similar approach combined with more involved tensor formats that are suitable also for higher dimensions, but the number of terms in a subdivision analogous to (5.26) in higher dimensions will generally grow too rapidly with $j_{\max}$.

We can do substantially better by making a third modification: we replace the sequence $\mathbf{s}$ by different scaling factors with a simpler structure, specifically, by $\bar{\mathbf{s}} := (2^{-\max|\nu|})_{\nu\in\nabla^2}$. Note that

$$2^{-\max|\nu|} \leq s_\nu \leq \sqrt{2}\, 2^{-\max|\nu|}\,, \quad \nu \in \nabla^2\,,$$

and as noted in Remark 3.17, $\{2^{-\max|\nu|}\Psi_\nu\}_{\nu\in\nabla^2}$ is a Riesz basis of $\mathrm{H}^1(\mathbb{R}^2)$ as well. As a consequence,

$$\bar{\mathbf{A}} := (2^{-\max|\nu|}\langle A\Psi_\nu, \Psi_\mu\rangle 2^{-\max|\mu|})_{\nu,\mu\in\nabla^2}$$

is an isomorphism on $\ell_2(\nabla^2)$ and $\|v\|_{\mathrm{H}^1} \sim \|(2^{\max|\nu|}\langle v, \Psi_\nu\rangle)\|_{\ell_2}$.

We now give a recursive definition of a tensor product decomposition of $\bar{\mathbf{s}}$. To this end, we define a notation that will also be used in the following subsection: let $k \in \mathbb{Z}^2$ and let $\mathcal{S}$ be a set of subsets of $\mathbb{Z}^2$, then

$$k + \mathcal{S} := \Bigl\{\{k + j \colon j \in S\} \colon S \in \mathcal{S}\Bigr\}\,. \tag{5.28}$$

For $\ell \in \mathbb{N}_0$, we set

$$\mathcal{J}^{(2)}_{\ell,\{\}} := \bigl\{\{0,\ldots,2^\ell - 1\} \times \{0,\ldots,2^\ell - 1\}\bigr\}\,.$$

The motivation for this particular choice of notation will become clearer in the following subsection. We successively build partitions $\mathcal{J}^{(2)}_{\ell,\{1,2\}}$ of $\{0,\ldots,2^\ell - 1\} \times \{0,\ldots,2^\ell - 1\}$ into Cartesian products for each $\ell \in \mathbb{N}_0$ by the recursion

$$\mathcal{J}^{(2)}_{0,\{1,2\}} := \mathcal{J}^{(2)}_{0,\{\}}\,, \tag{5.29a}$$

$$\mathcal{J}^{(2)}_{\ell+1,\{1,2\}} := \mathcal{J}^{(2)}_{\ell,\{1,2\}} \cup \bigl((2^\ell,0) + \mathcal{J}^{(2)}_{\ell,\{\}}\bigr) \cup \bigl((0,2^\ell) + \mathcal{J}^{(2)}_{\ell,\{\}}\bigr) \cup \bigl((2^\ell,2^\ell) + \mathcal{J}^{(2)}_{\ell,\{1,2\}}\bigr)\,. \tag{5.29b}$$

The resulting sets are illustrated in Figure 5.1. One easily checks that $\mathcal{J}^{(2)}_{\ell,\{1,2\}}$ has $3\cdot 2^\ell - 2$ elements. To obtain a partition of $\{0,\ldots,j_{\max}\} \times \{0,\ldots,j_{\max}\}$ for given $j_{\max} \in \mathbb{N}_0$ as above, we set $\mathcal{J}_{\max} := \mathcal{J}^{(2)}_{\lceil \log_2(j_{\max}+1)\rceil,\{1,2\}}$, which yields

$$\{0,\dots,j_{\max}\} \times \{0,\dots,j_{\max}\} \subseteq \bigcup_{S\in\mathcal{J}_{\max}} S$$

and $3j_{\max}+1 \leq \#\mathcal{J}_{\max} \leq 6j_{\max}+4$.

The decisive property of this construction is the following: for any ℓ and any $S \in \mathcal{J}^{(2)}_{\ell,\{1,2\}}$, we have $S = \{i_1,\dots,I_1\} \times \{i_2,\dots,I_2\}$ for some $i_1, I_1, i_2, I_2 \in \mathbb{N}_0$, and we have either $j_1 \geq j_2$ for all $j \in S$ or $j_1 \leq j_2$ for all $j \in S$. As a consequence, we have the representation

$$(2^{-\max|\nu|})\big|_{\{\nu\in\nabla^2\colon |\nu|\in S\}} = \begin{cases} \Big(\sum_{n=i_1}^{I_1} 2^{-n}\chi_{\{\nu\in\nabla\colon |\nu|=n\}}\Big) \otimes \chi_{\{\nu\in\nabla\colon i_2\leq|\nu|\leq I_2\}}\,, & i_1 \geq I_2\,, \\ \chi_{\{\nu\in\nabla\colon i_1\leq|\nu|\leq I_1\}} \otimes \Big(\sum_{n=i_2}^{I_2} 2^{-n}\chi_{\{\nu\in\nabla\colon |\nu|=n\}}\Big)\,, & i_2 \geq I_1\,, \end{cases}$$

and applying this on each $S \in \mathcal{J}_{\max}$, we obtain an expansion of $\bar{\mathbf{s}}|_{\nabla_{\max}}$ into $\mathcal{O}(j_{\max})$ separable terms with disjoint supports.

We again use a separate tensor representation for each section $\mathbf{v}|_S$ and $\bar{\mathbf{A}}\mathbf{v}|_S$, $S \in \mathcal{J}_{\max}$; note that the number of parts in this subdivision is of order $\mathcal{O}(j_{\max})$, as opposed to $\mathcal{O}(j_{\max}^2)$ as in (5.26). We thus find that the multilinear rank of each $\bar{\mathbf{A}}\mathbf{v}|_S$, $S \in \mathcal{J}_{\max}$, is of order $\mathcal{O}(j_{\max} r)$, and the complexity of applying hosvd for all S can be estimated by

$$\mathcal{O}\big(j_{\max} \times (j_{\max}^3 |r|_\infty^3) + j_{\max}^2 \log(j_{\max}) |r|_\infty^2 \max_{i=1,2} \#\Lambda_i\big)\,. \tag{5.30}$$

As we shall see, for the analogous three-dimensional problem, we can proceed similarly to obtain $\mathcal{O}((j_{\max}\log j_{\max}) \times (j_{\max}^4 \log^4 j_{\max}\, |r|_\infty^4) + j_{\max}^3 \log^2 j_{\max}\, |r|_\infty^2 \max_{i=1,2} \#\Lambda_i)$. More generally, we shall see in the following subsection that a construction analogous to (5.29) in d dimensions yields a subdivision into $\mathcal{O}(j_{\max}\log^{d-2} j_{\max})$ parts, as opposed to $\mathcal{O}(j_{\max}^d)$ in the higher-dimensional version of the subdivision in (5.26). Besides a further improvement in (5.30) by a factor $j_{\max}$ – up to the logarithmic terms – compared to (5.27), we thus also obtain a substantial reduction in the scaling of the number of subdivision elements with respect to the space dimension d.

It should be stressed that the simplified worst-case estimates considered in the preceding discussion will in general be very pessimistic. In particular, our previous considerations concerning possible further gains due to wavelet compressibility apply to the above construction based on $\bar{\mathbf{s}}$ as well. Furthermore, it will generally be useful to apply intermediate recompression steps to partial sums that need to be computed for $\bar{\mathbf{A}}\mathbf{v}|_S$, instead of applying hosvd only to the final result as described above for simplicity.

5.2.3 Partitioned Tensor Representations

For $d \in \mathbb{N}$, we define the operator $\mathbf{S}_d\colon \ell_2(\nabla^d) \to \ell_2(\nabla^d)$ by

$$\mathbf{S}_d\mathbf{v} := (2^{-\max|\nu|} v_\nu)_{\nu\in\nabla^d}\,, \quad \mathbf{v} \in \ell_2(\nabla^d)\,. \tag{5.31}$$

We now give a recursive characterization of a higher-dimensional generalization of the level partitions $\mathcal{J}^{(2)}_{\ell,\{1,2\}}$ described in the previous subsection. The resulting partitions $\mathcal{J}^{(d)}_{\ell,\{1,\dots,d\}}$ for $d > 2$ have the property that for an accordingly subdivided tensor representation of a vector $\mathbf{v}$, application of $\mathbf{S}_d$ leaves ranks unchanged, that is, we obtain the same ranks for $\mathbf{S}_d\mathbf{v}$ as for $\mathbf{v}$. We shall consider this point in more detail after discussing the definition of $\mathcal{J}^{(d)}_{\ell,\{1,\dots,d\}}$.

For $d \in \mathbb{N}$ and for any $D \subseteq \{1,\dots,d\}$, we define the binary vectors $b^{(d)}_D \in \{0,1\}^d$ by $b^{(d)}_{D,i} = 1$ if

$i \in D$, and $b^{(d)}_{D,i} = 0$ otherwise. For $\ell \in \mathbb{N}_0$, let

$$\mathcal{J}^{(d)}_{\ell,\{\}} := \bigl\{\{0,\dots,2^\ell - 1\}^d\bigr\}\,, \qquad d \geq 2\,. \tag{5.32}$$

For the case $d = 2$, in our present notation the subdivision defined in (5.29) reads

$$\begin{aligned} \mathcal{J}^{(2)}_{0,\{1,2\}} &:= \mathcal{J}^{(2)}_{0,\{\}}\,, \\ \mathcal{J}^{(2)}_{\ell+1,\{1,2\}} &:= \mathcal{J}^{(2)}_{\ell,\{1,2\}} \cup \bigl(2^\ell b^{(2)}_{\{1\}} + \mathcal{J}^{(2)}_{\ell,\{\}}\bigr) \cup \bigl(2^\ell b^{(2)}_{\{2\}} + \mathcal{J}^{(2)}_{\ell,\{\}}\bigr) \cup \bigl(2^\ell b^{(2)}_{\{1,2\}} + \mathcal{J}^{(2)}_{\ell,\{1,2\}}\bigr)\,. \end{aligned} \tag{5.33}$$

The definition of the higher-dimensional version of this subdivision is recursive both in d and in ℓ. For $d > 2$, we set

$$\begin{aligned} \mathcal{J}^{(d)}_{0,\{1,\dots,d\}} &:= \mathcal{J}^{(d)}_{0,\{\}}\,, \\ \mathcal{J}^{(d)}_{\ell+1,\{1,\dots,d\}} &:= \mathcal{J}^{(d)}_{\ell,\{1,\dots,d\}} \cup \Bigl(\bigcup_{k=1}^{d-1} \bigcup_{\substack{D\subset\{1,\dots,d\}\\ \#D=k}} \bigl(2^\ell b^{(d)}_D + \mathcal{J}^{(d)}_{\ell,D}\bigr)\Bigr) \cup \bigl(2^\ell b^{(d)}_{\{1,\dots,d\}} + \mathcal{J}^{(d)}_{\ell,\{1,\dots,d\}}\bigr)\,. \end{aligned} \tag{5.34}$$

To complete the definition (5.34), we still need to define $\mathcal{J}^{(d)}_{\ell,D}$ for all $D \subset \{1,\dots,d\}$ with $\#D \in \{1,\dots,d-1\}$ for $d > 2$. In the case $\#D = 1$, we set

$$\mathcal{J}^{(d)}_{\ell,\{i\}} := \mathcal{J}^{(d)}_{\ell,\{\}}\,, \quad i \in \{1,\dots,d\}\,. \tag{5.35}$$

In the case $\#D \in \{2,\dots,d-1\}$, a recursion with respect to d comes into play: we define

$$\begin{aligned} \mathcal{J}^{(d)}_{\ell,D} := \Bigl\{ \bigcap_{n\in D} \Bigl(\bigtimes_{i=1}^{n-1} \{0,\dots,2^\ell-1\} \times S_n \times \bigtimes_{i=n+1}^{d} \{0,\dots,2^\ell-1\}\Bigr) &: \\ S \in \mathcal{J}^{(\#D)}_{\ell,\{1,\dots,\#D\}}\,,\ S = \bigtimes_{n\in D} S_n \ \text{with}\ S_n \subset \mathbb{N}_0 \Bigr\}&. \end{aligned} \tag{5.36}$$

Note that for each ℓ, all elements of $\mathcal{J}^{(2)}_{\ell,\{1,2\}}$ can be written as Cartesian products, and since the recursion steps defined above preserve this property, each element of $\mathcal{J}^{(d)}_{\ell,\{1,\dots,d\}}$ can be written as a Cartesian product for $d > 2$ as well. This justifies the use of such a representation in (5.36).

Example 5.5. Expanding (5.34) in the case $d = 3$, we obtain

$$\begin{aligned} \mathcal{J}^{(3)}_{\ell+1,\{1,2,3\}} =& \mathcal{J}^{(3)}_{\ell,\{1,2,3\}} \\ & \cup \bigl((2^\ell,0,0) + \mathcal{J}^{(3)}_{\ell,\{\}}\bigr) \cup \bigl((0,2^\ell,0) + \mathcal{J}^{(3)}_{\ell,\{\}}\bigr) \cup \bigl((0,0,2^\ell) + \mathcal{J}^{(3)}_{\ell,\{\}}\bigr) \\ & \cup \bigl((2^\ell,2^\ell,0) + \mathcal{J}^{(3)}_{\ell,\{1,2\}}\bigr) \cup \bigl((2^\ell,0,2^\ell) + \mathcal{J}^{(3)}_{\ell,\{1,3\}}\bigr) \cup \bigl((0,2^\ell,2^\ell) + \mathcal{J}^{(3)}_{\ell,\{2,3\}}\bigr) \\ & \cup \bigl((2^\ell,2^\ell,2^\ell) + \mathcal{J}^{(3)}_{\ell,\{1,2,3\}}\bigr)\,, \end{aligned}$$

where

$$\mathcal{J}^{(3)}_{\ell,\{1,2\}} = \bigl\{S_1 \times S_2 \times \{0, 2^\ell - 1\} \colon S_1 \times S_2 \in \mathcal{J}^{(2)}_{\ell,\{1,2\}}\bigr\}$$

with analogous expressions for $\mathcal{J}^{(3)}_{\ell,\{1,3\}}$ and $\mathcal{J}^{(3)}_{\ell,\{2,3\}}$. The set $\mathcal{J}^{(3)}_{3,\{1,2,3\}}$ is illustrated in Figure 5.2.

Proposition 5.6. *For each $d \geq 2$, the set $\mathcal{J}^{(d)}_{\ell,\{1,\dots,d\}}$ is a partition of $\{0,\dots,2^\ell-1\}^d$ with $\mathcal{O}(\ell^{d-2}2^\ell)$ elements, and for each $S \in \mathcal{J}^{(d)}_{\ell,\{1,\dots,d\}}$ there exists $\bar d \in \{1,\dots,d\}$ such that for all $j \in S$, we have $\max j = j_{\bar d}$.*

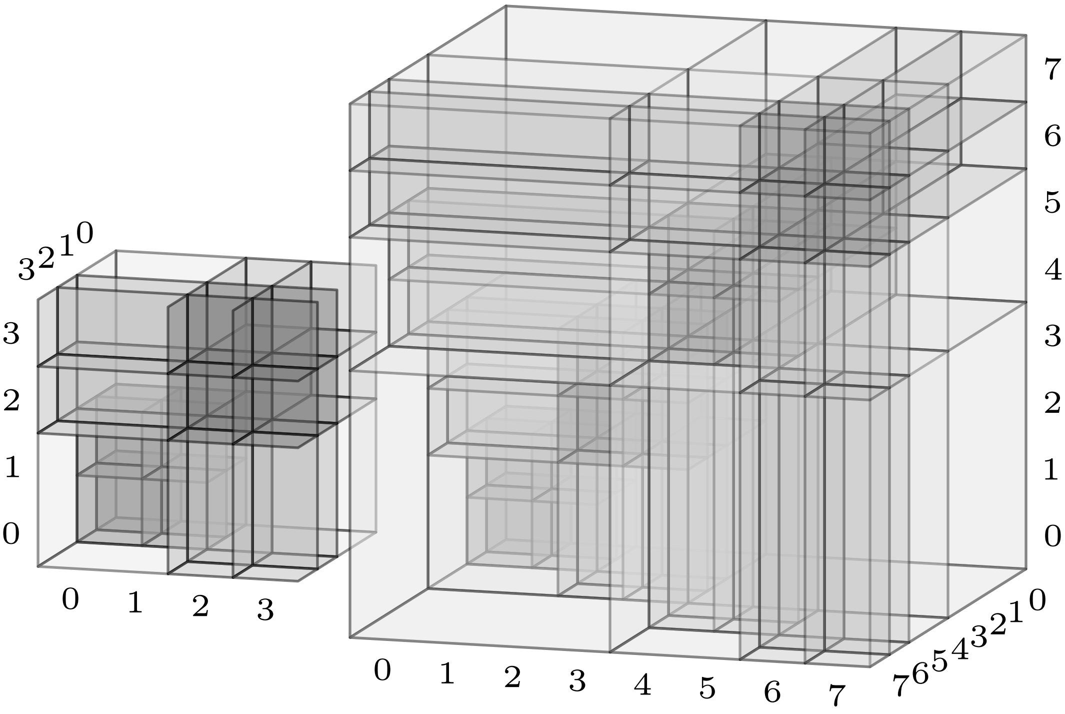

Figure 5.2. Structure of the partitions $\mathcal{J}^{(3)}_{\ell,\{1,2,3\}}$ for $\ell = 2, 3$.

The proof is given in Appendix A.3. Note that the statement of Proposition 5.6 concerning the cardinality of $\mathcal{J}^{(d)}_{\ell,\{1,\dots,d\}}$ can be rephrased as follows: for given $J \in \mathbb{N}$, a partition of $\{0,\dots,J\}^d$ generated by (5.34) has $\mathcal{O}(J \log^{d-2} J)$ elements.

Remark 5.7. *For $d = 2, 3, 4$, we have*

$$\begin{aligned} \#\mathcal{J}^{(2)}_{\ell,\{1,2\}} &= 3 \cdot 2^\ell - 2\,, \\ \#\mathcal{J}^{(3)}_{\ell,\{1,2,3\}} &= \tfrac{9}{2}\,\ell\,2^\ell - 2^{\ell+1} + 3\,, \\ \#\mathcal{J}^{(4)}_{\ell,\{1,\dots,4\}} &= \tfrac{9}{2}\,\ell^2\,2^\ell + \ell\,2^{\ell-1} + 5 \cdot 2^\ell - 4 \end{aligned}$$

for $\ell \in \mathbb{N}_0$.

On the basis of the partitions $\mathcal{J}^{(d)}_{\ell,\{1,\dots,d\}}$ of $\{0,\dots,2^\ell - 1\}^d$, we define a partition of $\mathbb{Z}^d_{j_0}$ by

$$\tilde{\mathcal{J}}^{(d)} = \bigcup_{\ell \in \mathbb{N}} \bigl(j_0 + \mathcal{J}^{(d)}_{\ell,\{1,\dots,d\}}\bigr)\,, \tag{5.37}$$

where we use that $\mathcal{J}^{(d)}_{\ell,\{1,\dots,d\}} \subset \mathcal{J}^{(d)}_{\ell+1,\{1,\dots,d\}}$, and additionally choose an enumeration of the countable set $\tilde{\mathcal{J}}^{(d)}$ to obtain the vector $(\mathcal{J}^{(d)}_n)_{n\in\mathbb{N}}$.

The above partitioning can in principle be used for any dimension parameter d, but for what follows we specialize the construction to the two cases that are relevant for the problems we will consider. We define sets of wavelet indices corresponding to $\tilde{\mathcal{J}}^{(3)}$ by

$$\bar\Lambda_{3,n} = \bigl\{\nu \in \nabla^3 \colon\ |\nu| \in \mathcal{J}^{(3)}_n\bigr\}\,, \tag{5.38a}$$

$$\bar\Lambda_{6,n} = \bigl\{\nu = (\nu_1,\nu_2,\nu_3) \in (\nabla^2)^3 \colon\ \bigl(\max|\nu_1|, \max|\nu_2|, \max|\nu_3|\bigr) \in \mathcal{J}^{(3)}_n\bigr\}\,. \tag{5.38b}$$

The sets $\bar\Lambda_{d,n}$, for $d = 3, 6$ and $n \in \mathbb{N}$, are pairwise disjoint and $\bigcup_n \bar\Lambda_{d,n} = \nabla^d$. Furthermore, each $\bar\Lambda_{d,n}$ can be written as a Cartesian product, and we denote by $\bar\Lambda^{(i)}_{d,n} \subset \nabla^{d/3}$, $i \in \{1,2,3\}$, the unique lower-dimensional index sets that satisfy $\bar\Lambda_{d,n} = \times_{i=1}^{3} \bar\Lambda_{d,n}^{(i)}$.

With the above preparations, we can define the class of tensor representations that we will rely on in what follows: for $d = 3, 6$ and $r = (r_n)_{n\in\mathbb{N}}$ with $r_n \in \mathbb{N}_0^3$, let

$$\mathcal{T}_d(r) := \bigl\{\mathbf{u} \in \ell_2(\nabla^d)\colon \#\operatorname{supp}\mathbf{u} < \infty \text{ and } \operatorname{rank}(\mathbf{u}|_{\bar\Lambda_{d,n}}) \le r_n \text{ for all } n \in \mathbb{N}\bigr\}\,. \tag{5.39}$$

Correspondingly, for $\mathbf{u} \in \ell_2(\nabla^d)$ we define the sequence of multilinear ranks

$$\operatorname{rank}(\mathbf{u}) := \bigl(\operatorname{rank}(\mathbf{u}|_{\bar\Lambda_{d,n}})\bigr)_{n\in\mathbb{N}}\,. \tag{5.40}$$

The following proposition, applied to $f(j) = 2^{-j}$, shows that $\mathbf{S}_d$ maps $\mathcal{T}_d(r)$ to $\mathcal{T}_d(r)$ for given r, that is, applying $\mathbf{S}_d$ to elements of $\mathcal{T}_d(r)$ does not increase their ranks as in (5.40).

Proposition 5.8. *Let $f\colon \mathbb{Z}_{j_0} \to \mathbb{R}$ and $r = (r_n)_{n\in\mathbb{N}}$ with $r_n \in \mathbb{N}_0^d$. If $\mathbf{u} \in \mathcal{T}_d(r)$, then*

$$\bigl(f(\max|\nu|)\,u_\nu\bigr)_{\nu\in\nabla^d} \in \mathcal{T}_d(r)\,,\quad d = 3, 6\,,$$

and for each n, there exist $\mathbf{S}_{d,n}^{(i)}$ such that $\mathbf{S}_d|_{\bar\Lambda_{d,n}} = \mathbf{S}_{d,n}^{(1)} \otimes \mathbf{S}_{d,n}^{(2)} \otimes \mathbf{S}_{d,n}^{(3)}$.

Proof. The statement follows from the observation made in Proposition 5.6 that by the construction of $\bar\Lambda_{d,n}$, for each $n \in \mathbb{N}$, there exist $i_3, i_6 \in \{1, 2, 3\}$ such that

$$\max|\nu| = |\nu_{i_3}| \quad\text{for}\quad \nu \in \bar\Lambda_{3,n}\,,\qquad \max|\tilde\nu| = \max|\tilde\nu_{i_6}| \quad\text{for}\quad \tilde\nu \in \bar\Lambda_{6,n}\,.$$

We assume without loss of generality that $i_3, i_6 = 1$ to simplify notation. Let $\mathbf{f} := \bigl(f(\max|\nu|)\bigr)_{\nu\in\nabla^d}$ and

$$\mathbf{f}^{(1)} := \begin{cases} \bigl(f(|\nu_1|)\bigr)_{\nu\in\nabla}\,, & d = 3\,,\\ \bigl(f(\max|\nu_1|)\bigr)_{\nu\in\nabla^2}\,, & d = 6\,.\end{cases}$$

In both cases, we thus obtain the representation

$$\mathbf{f}\,\mathbf{u}\,|_{\bar\Lambda_{d,n}} = \sum_k a_{n,k} (\mathbf{f}^{(1)}\,\mathbf{U}_{n,k_1}^{(1)}) \otimes \mathbf{U}_{n,k_2}^{(2)} \otimes \mathbf{U}_{n,k_3}^{(3)}\,,\quad d = 3, 6\,. \qquad \square$$

Note that the proof of Proposition 5.8 exposes a scheme for evaluating $\mathbf{S}_d\mathbf{u}$ for $\mathbf{u} \in \mathcal{T}_d(r)$ by rescaling one of the mode frames of each $\mathbf{u}|_{\bar\Lambda_{d,n}}$.

We have thus constructed a class of tensor representations of wavelet coefficients that, by imposing additional structure, enables us to efficiently perform rescaling operations required by iterative solvers for (5.9). The additional fixed subdivision by wavelet levels will in general lead to approximations which are slightly more expensive than those possible by a direct representation in the Tucker format (5.14) without further constraints. This approach can therefore be regarded as a compromise between approximation efficiency and feasibility of computational schemes. It should be noted, however, that the output $\mathbf{u} \in \mathcal{T}_d(r)$ of a computational scheme operating on separate tensor representations for each $\bar\Lambda_{d,n}$ can immediately be rewritten as a single tensor representation in the Tucker format (5.14) on all of ∇^d, with formal multilinear rank $\hat r := \sum_n r_n$. The actual multilinear rank required for approximating this single combined representation within the target accuracy can typically be expected to be smaller than $\hat r$, and such an approximate representation with smaller rank can be found by recursively combining the pieces $\mathbf{u}|_{\bar\Lambda_{d,n}}$ by hosvd with appropriate truncation tolerances.

Remark 5.9. *Let us now juxtapose the above constructed partitioned tensor representation to a direct tensor representation of wavelet coefficients for $\mathbf{u} \in \ell_2(\nabla^d)$,*

$$\mathbf{u} = \sum_k a_k\,\mathbf{U}_{k_1} \otimes \mathbf{U}_{k_2} \otimes \mathbf{U}_{k_3}\,. \tag{5.41}$$

Note that $\mathbf{S}_d$ *has the following separable expansion: Let* $\mathbf{P}_{\leq j}$ *denote the coordinate projection onto* $\bigcup_{i\leq j} \nabla_i$*, then*

$$\mathbf{S}_d = \sum_{j=j_0}^{\infty} 2^{-j-1} \bigotimes_{i=1}^{d} \mathbf{P}_{\leq j} \,. \tag{5.42}$$

In principle, this could be used directly to operate on vectors of wavelet coefficients represented as in (5.41)*. As we have seen in Subsection 5.2.2, the resulting bounds on the rank increase, in terms of the maximum arising wavelet level* j_{max}*, are substantially less favorable than for the subdivided tensor representation constructed above. However, although a higher power of* j_{max} *enters in the worst-case estimates for the direct application of* (5.42)*, there is no dependence on* d *in terms of* $\log j_{max}$ *as in the subdivided case.*

Remark 5.10. *The two cases of, on the one hand, a single tensor representation for all coefficients as in* (5.41)*, and on the other hand, a subdivided representation such that* $\mathbf{S}_d$ *leaves all ranks unchanged, may also be regarded as extreme cases of a more general class of subdivisions. One can group several* $\bar{\Lambda}_{d,n}$ *such that their union is again a Cartesian product, and use a single tensor representation on each such group. Then* $\mathbf{S}_d$ *does no longer have rank one, but on each group has some bounded rank depending only on the respective group.*

5.3 Basic Operations in Tensor Format

This section deals with the realization of basic building blocks for iterative solvers based on the format defined in (5.39). Here $\|\cdot\|$ and $\langle\cdot,\cdot\rangle$ always denote norm and scalar product, respectively, of ℓ_2 on the appropriate index set; for operators, $\|\cdot\|$ denotes the corresponding spectral norm. For wavelet index sets corresponding to the supports of mode frames, we introduce the notation

$$\Lambda_n(\mathbf{u}) := \bigtimes_{i=1}^{d} \Lambda_n^{(i)}(\mathbf{u}) \subset \nabla^d \,, \qquad \Lambda_n^{(i)}(\mathbf{u}) := \bigcup_k \operatorname{supp} \mathbf{U}_{n,k}^{(i)} \,, \tag{5.43}$$

so that, in particular, $\operatorname{supp} \mathbf{u}|_{\bar{\Lambda}_{d,n}} \subseteq \Lambda_n(\mathbf{u})$. Furthermore, let the matrices $\mathbf{a}_n^{(i)}$ and the vectors $\sigma_n^{(i)}$ of mode-i singular values be defined as in (5.17) for each $\mathbf{u}|_{\bar{\Lambda}_{d,n}}$.

5.3.1 Scaling, Addition, Inner Products, and Norms

For basic linear algebra operations, we only need to adapt the procedures commonly used for the Tucker tensor format – as treated in detail, e.g., in [72] – to our case with subdivision.

For $\mathbf{u} \in \mathcal{T}_d(r)$ and $\alpha \in \mathbb{R}$, we can obtain the tensor representation of $\alpha\mathbf{u}$ by simply rescaling the corresponding core tensors for $\mathbf{u}|_{\bar{\Lambda}_{d,n}}$.

Suppose further that $\tilde{\mathbf{u}} \in \mathcal{T}_d(\tilde{r})$. A tensor representation of $\mathbf{u} + \tilde{\mathbf{u}}$ is then given by a catenation of mode frames and core tensors, which formally leads to multilinear ranks $r + \tilde{r}$; a subsequent orthogonalization of the combined mode frames may yield lower ranks.

Provided that for each n, $\mathbf{u}|_{\bar{\Lambda}_{d,n}}$ is given with orthonormal mode frames corresponding to a core tensor $\mathbf{a}_n = (a_{n,k})_{k\in\mathcal{K}_3(r_n)}$, the norm of $\mathbf{u}$ can be obtained by

$$\|\mathbf{u}\|^2 = \sum_n \|\mathbf{u}|_{\bar{\Lambda}_{d,n}}\|^2 = \sum_n \sum_{k\in\mathcal{K}_3(r_n)} |a_{n,k}|^2 \,, \tag{5.44}$$

which can be evaluated in $\mathcal{O}(\sum_n \prod_i r_{n,i})$ operations.

Concerning the evaluation of inner products, since the $\bar{\Lambda}_{d,n}$ form a partition of ∇^d and by orthonormality of the wavelet basis, we have $\langle \mathbf{u}|_{\bar\Lambda_{d,n}}, \tilde{\mathbf{u}}|_{\bar\Lambda_{d,m}}\rangle = 0$ for $m \neq n$. We thus obtain

$$\langle \mathbf{u}, \tilde{\mathbf{u}}\rangle = \sum_n \langle \mathbf{u}|_{\bar\Lambda_{d,n}}, \tilde{\mathbf{u}}|_{\bar\Lambda_{d,n}}\rangle \,. \tag{5.45}$$

The number of operations required for the evaluation of $\langle \mathbf{u}|_{\bar\Lambda_{d,n}}, \tilde{\mathbf{u}}|_{\bar\Lambda_{d,n}}\rangle$ is of order

$$\mathcal{O}\bigl(|r_n|_\infty^2 |\tilde r_n|_\infty^2 + \sum_i r_{n,i}^2 \min\{\#\Lambda_n^{(i)}(\mathbf{u}), \#\Lambda_n^{(i)}(\tilde{\mathbf{u}})\}\bigr)\,,$$

and the total complexity is given by the sum over n.

5.3.2 Recompression and Coarsening

Applying the basic operations described in Subsection 5.3.1 and the approximate matrix-vector product described in Subsection 5.3.4 below to tensor representations will in general increase their ranks; in the case of the approximate application of operators it will also increase the support sizes of mode frames. We next describe routines that enable us to control the growth of these two quantities over the course of an iterative scheme.

In principle, one could attempt to find approximations to given tensor representations that have both lower ranks and mode frames of smaller support simultaneously. Performing the approximations with respect to these two degrees of freedom separately, however, enables us to make effective use of the orthogonality properties provided by hosvd in order to decouple dimensions in the error estimates.

For the error of approximation by lower-rank tensors, the following proposition provides a simple extension of the corresponding estimate (5.18) of Theorem 5.2.

Assumptions 5.11. Let $\mathbf{u} \in \mathcal{T}_d(r)$ with $d = 3, 6$ and $r \colon \mathbb{N} \to \mathbb{N}_0^3$ compactly supported. For each $n \in \mathbb{N}$, let $\mathbf{U}_n^{(i)}$, $i \in \{1,2,3\}$, and $\mathbf{a}_n$ be the mode frames and core tensor provided by hosvd$(\mathbf{u}|_{\bar\Lambda_{d,n}})$, and for $\mathbf{a}_n$ let $a_{n,kl}^i$ and $\sigma_{n,k}^{(i)}$ for $k,l \in \{1,\dots,r_i\}$ be defined according to (5.17), so that $a_{n,kl}^{(i)} = |\sigma_{n,k}^{(i)}|^2 \delta_{kl}$ with $\sigma_{n,k}^{(i)} \geq \sigma_{n,k+1}^{(i)}$.

Proposition 5.12. *Let* $\mathbf{u}$ *satisfy Assumptions 5.11. Then for* $\tilde r$ *with* $0 \leq \tilde r \leq r$ *componentwise and*

$$\tilde{\mathbf{u}} = \sum_n \sum_{k \in \mathcal{K}_3(\tilde r_n)} (\mathbf{U}_{n,k_1}^{(1)} \otimes \mathbf{U}_{n,k_2}^{(2)} \otimes \mathbf{U}_{n,k_3}^{(3)})\, a_{n,k}\,,$$

we have

$$\|\mathbf{u} - \tilde{\mathbf{u}}\|^2 \leq \sum_n \sum_{i=1}^3 \sum_{k=\tilde r_{n,i}+1}^{r_{n,i}} |\sigma_{n,k}^{(i)}|^2 \tag{5.46}$$

and

$$\|\mathbf{u} - \tilde{\mathbf{u}}\| \leq \sqrt{3} \inf_{\mathbf{w} \in \mathcal{T}_d(\tilde r)} \|\mathbf{u} - \mathbf{w}\|\,. \tag{5.47}$$

Proof. The estimate (5.46) follows from $\|\mathbf{u} - \tilde{\mathbf{u}}\|^2 = \sum_n \bigl\|(\mathbf{u} - \tilde{\mathbf{u}})|_{\bar\Lambda_{d,n}}\bigr\|^2$ and Theorem 5.2. By (5.18),

$$\sum_n \sum_{i=1}^3 \sum_{k=\tilde r_{n,i}+1}^{r_{n,i}} |\sigma_{n,k}^{(i)}|^2 \leq 3 \sum_n \inf_{\operatorname{rank}(\mathbf{w}_n) \leq \tilde r_n} \bigl\|\mathbf{u}|_{\bar\Lambda_{d,n}} - \mathbf{w}_n\bigr\|^2 = 3 \inf_{\mathbf{w} \in \mathcal{T}_d(\tilde r)} \|\mathbf{u} - \mathbf{w}\|^2\,. \qquad \square$$

On this basis, we obtain a simple routine that computes an approximation with prescribed error $\eta > 0$ satisfying the quasi-optimality property (5.47).

Algorithm 5.2 $\tilde{\mathbf{u}} = \mathsf{recompress}(\mathbf{u};\eta)$

```
input   $\mathbf{u} = \sum_n \sum_{k\in\mathcal{K}_3(r_n)} a_{n,k} \bigotimes_i \mathbf{U}^{(i)}_n$ satisfying Assumptions 5.11
output  $\tilde{\mathbf{u}} = \sum_n \sum_{k\in\mathcal{K}_3(\tilde r_n)} a_{n,k} \bigotimes_i \mathbf{U}^{(i)}_n$ with $\tilde r \le r$ such that $\|\mathbf{u}-\tilde{\mathbf{u}}\| \le \eta$ and (5.47) hold
$\tilde r \leftarrow r$
$(m,j) \leftarrow \arg\min_{\{(n,i)\colon r_n>0\}} \sigma^{(i)}_{n,r_{n,i}}$
$\hat\eta \leftarrow \sigma^{(j)}_{m,r_{m,j}}$
while $\hat\eta \le \eta$
    $\tilde r_{m,j} \leftarrow \tilde r_{m,j} - 1$
    $(m,j) \leftarrow \arg\min_{\{(n,i)\colon \tilde r_n>0\}} \sigma^{(i)}_{n,\tilde r_{n,i}}$
    $\hat\eta \leftarrow \big(\hat\eta^2 + |\sigma^{(j)}_{m,\tilde r_{m,j}}|^2\big)^{1/2}$
end while
```

Because of the implicit truncation of the core tensors $\mathbf{a}_n$, the output of the procedure recompress in Algorithm 5.2 will in general not satisfy Assumptions 5.11, since the corresponding $\mathbf{a}^{(i)}_n$ need not be diagonal any more.

Remark 5.13. *The routine* recompress *can be performed in at most* $\mathcal{O}(\sum_{n,i} r^2_{n,i})$ *operations; in fact, this is a rather coarse estimate, but it is in any case dominated by the cost for ensuring Assumptions 5.11 according to Remark 5.17.*

The next proposition provides an error estimate for coarsening the mode frames, i.e., for approximation by mode frames of smaller support.

Proposition 5.14. *Let* $\mathbf{u}$ *satisfy Assumptions 5.11. For* $n \in \mathbb{N}$, $i \in \{1,2,3\}$, *and* $\nu \in \nabla^{\hat d}$ *with* $\hat d = d/3$ *let*

$$\varepsilon^{(i)}_{n,\nu} := \sum_k \big|(\mathbf{U}^{(i)}_{n,k})_\nu\big|^2 \big|\sigma^{(i)}_{n,k}\big|^2 . \tag{5.48}$$

Let $N \in \mathbb{N}$ *and choose* $\mathcal{I}_N \subset \{(n,i,\nu)\colon \varepsilon^{(i)}_{n,\nu} \neq 0\}$ *minimizing* $\sum_{(n,i,\nu)\in\mathcal{I}_N} \varepsilon^{(i)}_{n,\nu}$ *subject to* $\#\mathcal{I}_N = N$. *For* $n \in \mathbb{N}$, $i \in \{1,2,3\}$ *define*

$$\tilde\Lambda^{(i)}_n := \Lambda^{(i)}_n(\mathbf{u}) \setminus \{\nu\colon (n,i,\nu) \in \mathcal{I}_N\} .$$

Then for $\tilde\Lambda = \bigcup_n \big(\times_{i=1}^3 \tilde\Lambda^{(i)}_n\big)$ *and* $\tilde{\mathbf{u}} := \mathbf{u}|_{\tilde\Lambda}$, *we have*

$$\|\mathbf{u} - \tilde{\mathbf{u}}\|^2 \le \sum_{(n,i,\nu)\in\mathcal{I}_N} \varepsilon^{(i)}_{n,\nu} , \tag{5.49}$$

and for any $\hat\Lambda = \bigcup_n \hat\Lambda_n$ *with* $\hat\Lambda_n = \times_{i=1}^3 \hat\Lambda^{(i)}_n \subset \bar\Lambda_{d,n}$ *satisfying* $\sum_{n,i} \#\big(\Lambda^{(i)}_n(\mathbf{u}) \setminus \hat\Lambda^{(i)}_n\big) \ge N$, *we have*

$$\|\mathbf{u} - \tilde{\mathbf{u}}\| \le \sqrt{3}\|\mathbf{u} - \mathbf{u}|_{\hat\Lambda}\| .$$

Proof. For $n \in \mathbb{N}$, let $\mathbf{u}_n := \mathbf{u}|_{\bar\Lambda_{d,n}}$ and $\tilde{\mathbf{u}}_n := \tilde{\mathbf{u}}|_{\bar\Lambda_{d,n}}$. Note that $\nu \in \Lambda^{(i)}_n(\mathbf{u}) \setminus \tilde\Lambda^{(i)}_n$ if and only if $(n,i,\nu) \in \mathcal{I}_N$ and hence

$$\begin{aligned}\|\tilde{\mathbf{u}}_n - \mathbf{u}_n\|^2 &\le \|\mathbf{u}_n|_{\tilde\Lambda^{(1)}_n \times \nabla^{2\hat d}} - \mathbf{u}_n\|^2 + \|\mathbf{u}_n|_{\nabla^{\hat d}\times\tilde\Lambda^{(2)}_n\times\nabla^{\hat d}} - \mathbf{u}_n\|^2 + \|\mathbf{u}_n|_{\nabla^{2\hat d}\times\tilde\Lambda^{(3)}_n} - \mathbf{u}_n\|^2 \\ &= \sum_{i=1}^3 \sum_{\nu\in\Lambda^{(i)}_n(\mathbf{u})\setminus\tilde\Lambda^{(i)}_n} \varepsilon^{(i)}_{n,\nu} ,\end{aligned}$$

where we have also used the orthonormality assumption on the mode frames. As the sets $\bar\Lambda_{d,n}$ are disjoint,

$$\|\mathbf{u} - \tilde{\mathbf{u}}\|^2 = \Big\|\sum_n (\mathbf{u}_n - \tilde{\mathbf{u}}_n)\Big\|^2 = \sum_n \|\mathbf{u}_n - \tilde{\mathbf{u}}_n\|^2 ,$$

and we obtain (5.49).

Let now $\hat{\Lambda}_n$ be as in the hypothesis, then by the choice of $\mathcal{I}_N$,

$$\begin{aligned} \|\mathbf{u} - \tilde{\mathbf{u}}\|^2 &\le \sum_{(n,i,\nu)\in\mathcal{I}_N} \varepsilon^{(i)}_{n,\nu} \le \sum_n \sum_{i=1}^3 \sum_{\nu\in\nabla^{\hat{d}}\setminus\bigcup_n \hat{\Lambda}^{(i)}_n} \varepsilon^{(i)}_{n,\nu} \\ &= \sum_n \Big(\|\mathbf{u}_n|_{\hat{\Lambda}^{(1)}_n \times \nabla^{2\hat{d}}} - \mathbf{u}_n\|^2 + \|\mathbf{u}_n|_{\nabla^{\hat{d}}\times\hat{\Lambda}^{(2)}_n\times\nabla^{\hat{d}}} - \mathbf{u}_n\|^2 + \|\mathbf{u}_n|_{\nabla^{2\hat{d}}\times\hat{\Lambda}^{(3)}_n} - \mathbf{u}_n\|^2 \Big) \\ &\le 3\|\mathbf{u} - \mathbf{u}|_{\hat{\Lambda}}\|^2 . \end{aligned}$$

□

A procedure based on Proposition 5.14 is given in Algorithm 5.3.

Algorithm 5.3 $\tilde{\mathbf{u}} = \mathsf{coarsen}(\mathbf{u};\eta)$

```
input   $\mathbf{u} = \sum_n \sum_{k\in\mathcal{K}_3(r_n)} a_{n,k} \bigotimes_i \mathbf{U}^{(i)}_n$ satisfying Assumptions 5.11
output  $\tilde{\mathbf{u}} = \sum_n \sum_{k\in\mathcal{K}_3(r_n)} a_{n,k} \bigotimes_i \tilde{\mathbf{U}}^{(i)}_n$ with $\tilde{\mathbf{U}}^{(i)}_n = \mathbf{U}^{(i)}_n|_{\tilde{\Lambda}^{(i)}_n}$ for $\tilde{\Lambda}^{(i)}_n \subseteq \Lambda^{(i)}_n(\mathbf{u})$ as in Proposition
        5.14, and $\|\mathbf{u} - \tilde{\mathbf{u}}\| \le \eta$
evaluate $\varepsilon^{(i)}_{n,\nu}$ for $n \in \mathbb{N}$, $i \in \{1,2,3\}$ with $\Lambda^{(i)}_n(\mathbf{u}) \ne \emptyset$ and $\nu \in \Lambda^{(i)}_n(\mathbf{u})$        ▷ as in (5.48)
sort $(\varepsilon^{(i)}_{n,\nu})_{n,i,\nu}$ to obtain the nondecreasing rearrangement $(\varepsilon^*_q)_{q\ge1}$        ▷ assuming bijection
                                                                                      $(n,i,\nu) \leftrightarrow q \in \mathbb{N}$
$N^* \leftarrow \max\{N\colon \sum_{q=1}^N \varepsilon^*_q \le \eta^2\}$
$\mathcal{I} \leftarrow \{(n(q), i(q), \nu(q))\colon 1 \le q \le N^*\}$
for all $i, n$
    $\tilde{\Lambda}^{(i)}_n \leftarrow \Lambda^{(i)}_n(\mathbf{u}) \setminus \{\nu\colon (n,i,\nu) \in \mathcal{I},\ \nu \in \bar{\Lambda}^{(i)}_{d,n}\}$
end for
```

Remark 5.15. *Evaluating all $\varepsilon^{(i)}_{n,\nu}$ takes $\mathcal{O}(\sum_{n,i} r_{n,i} \#\Lambda^{(i)}_n(\mathbf{u}))$ operations, and including the subsequent sorting step,* coarsen *requires work of order*

$$\mathcal{O}\Big(\sum_{n,i} (r_{n,i} + \log \#\Lambda^{(i)}_n(\mathbf{u}))\#\Lambda^{(i)}_n(\mathbf{u})\Big) .$$

The additional logarithmic dependency for sorting can be avoided by the adaptation of approximate sorting procedures as proposed for standard adaptive wavelet schemes in [7, 110], as been mentioned in Section 3.6.3.

Remark 5.16. *Dropping in Proposition 5.14 the assumption of diagonal $\mathbf{a}^{(i)}_n$ as provided by* hosvd*, one can still work directly with*

$$\varepsilon^{(i)}_{n,\nu} := \sum_{k,l} (\mathbf{U}^{(i)}_{n,k})_\nu (\mathbf{U}^{(i)}_{n,l})_\nu \, a^{(i)}_{n,kl} . \tag{5.50}$$

Precomputing the $\mathbf{a}^{(i)}_n$ then takes $\mathcal{O}(\sum_n |r_n|_\infty \prod_i r_{n,i})$ operations, and evaluating all $\varepsilon^{(i)}_{n,\nu}$ requires $\mathcal{O}(\sum_{n,i} r^2_{n,i} \#\Lambda^{(i)}_n(\mathbf{u}))$ operations. This modification therefore still yields the same overall asymptotic complexity as when first performing $\mathsf{hosvd}(\mathbf{u}|_{\bar{\Lambda}_{d,n}})$ *for each n.*

Note that if $\eta > 0$, neither recompress *nor* coarsen *preserve Assumptions 5.11; one can, however, first ensure Assumptions 5.11 by* hosvd*, then perform* recompress*, and finally perform* coarsen *using (5.50). This may offer a quantitative advantage over applying* hosvd *again to the result of* recompress*.*

5.3.3 Tensor Formats for Higher Dimensions

For a generalization of the framework developed above to tensor orders higher than three, the Tucker format (5.14) is not suitable: For a tensor of multilinear rank $(r, \dots, r)$ of order d, the core tensor $\mathbf{a}$ has r^d nonzero entries, and the complexity of performing hosvd directly for such a tensor is dominated by a term of order r^{d+1}. Due to this exponential dependence on d, the direct use of the Tucker representation therefore becomes too costly for large d.

The exponential scaling with respect to d can be overcome, however, by passing to different tensor formats that introduce additional structure, such as the above mentioned Hierarchical or $\mathcal{H}$–Tucker format. This format can be combined quite naturally with the considerations of this chapter, since it can be interpreted as a Tucker representation with certain additional structural constraints on the core tensor.

In the case $d = 4$, for instance, one possible form of $\mathcal{H}$–Tucker representation is

$$\mathbf{u} = \sum_{i_1=1}^{s_1} \sum_{i_2=1}^{s_2} \sum_{k \in \mathcal{K}_4(r)} B^{(\{1,2,3,4\})}_{i_1,i_2} B^{(\{1,2\})}_{i_1,k_1,k_2} B^{(\{3,4\})}_{i_2,k_3,k_4} \mathbf{U}^{(1)}_{k_1} \otimes \mathbf{U}^{(2)}_{k_2} \otimes \mathbf{U}^{(3)}_{k_3} \otimes \mathbf{U}^{(4)}_{k_4} \,.$$

This can be interpreted as a special case of a Tucker representation with

$$a_k = \sum_{i_1,i_2} B^{(\{1,2,3,4\})}_{i_1,i_2} B^{(\{1,2\})}_{i_1,k_1,k_2} B^{(\{3,4\})}_{i_2,k_3,k_4} \,, \tag{5.51}$$

with the additional orthogonality requirements

$$\sum_{k_1,k_2} B^{(\{1,2\})}_{i_1,k_1,k_2} B^{(\{1,2\})}_{j_1,k_1,k_2} = \delta_{j_1,i_1} \,, \quad \sum_{k_3,k_4} B^{(\{3,4\})}_{i_2,k_3,k_4} B^{(\{3,4\})}_{j_2,k_3,k_4} = \delta_{j_2,i_2} \,.$$

In order to obtain a gain in complexity over the Tucker format, the individual entries of $\mathbf{a}$ must never be used directly, but only implicitly via this representation.

An analogue of hosvd for the $\mathcal{H}$–Tucker format, which we shall henceforth abbreviate as $\mathcal{H}$–hosvd, has been introduced in [64]. The complexity of this procedure is determined by a modified notion of rank that depends on additional structural information on the tensor. For instance, in the above example, setting $R := \max\{\max_i r_i, \max_i s_i\}$, the number of operations required for $\mathcal{H}$–hosvd is of order

$$\mathcal{O}(dR^4 + dR^2 \max_{i,k} \#\Lambda^{(i)}_k) \,. \tag{5.52}$$

The crucial point is that for the recursive extension of the hierarchical decomposition (5.51) to higher orders d, the exponents in the corresponding estimate (5.52) remain the same, and d thus enters only as a linear factor.

Note that the quantities $\sigma^{(i)}_n$ corresponding to a core tensor represented as in (5.51) can be obtained in a straightforward manner as a byproduct of $\mathcal{H}$–hosvd. As a consequence, the procedures $\mathsf{recompress}$ and $\mathsf{coarsen}$ developed in the previous subsection immediately carry over to tensors represented in the $\mathcal{H}$–Tucker format, and in particular also to the slightly simpler special case of the Tensor Train format [121].

5.3.4 Adaptive Approximation of Operators

The aim of this subsection is the construction of a routine for approximately applying operators with prescribed accuracy, taking advantage both of sparsity in wavelet bases, and of low-rank structure and separability of the functions and operators of interest.

As in the case of the procedures $\mathsf{recompress}$ and $\mathsf{coarsen}$, the routine developed here for the Tucker format can be directly generalized to more advanced tensor formats for higher dimensions, such as the $\mathcal{H}$–Tucker format. The crucial point is that the procedure does not use information on individual entries of the core tensor, but only the mode-i singular values for $i = 1, \dots, d$. As noted above, these are obtained as by-products of hosvd or $\mathcal{H}$–hosvd, respectively.

We consider an operator $\mathbf{A}$ on $\ell_2(\nabla^d)$ for $d = 3, 6$ of the form

$$\mathbf{A} = \mathbf{S}_d(\mathbf{A}^{(1)} \otimes \mathbf{A}^{(2)} \otimes \mathbf{A}^{(3)})\mathbf{S}_d\,, \tag{5.53}$$

where $\mathbf{S}_d$ is given by (5.31). For what follows, let again $\hat{d} = d/3$.

For each $i \in \{1, 2, 3\}$, let a family of approximations $\mathbf{A}^{(i)}_{[p]}$, $p \in \mathbb{N}_0 \cup \{\infty\}$ be given, where we define $A^{(i)}_{[0]} := 0$ and formally set $\mathbf{A}^{(i)}_{[\infty]} := \mathbf{A}^{(i)}$. For these approximations, we assume the following to hold: there exist $C > 0$ and $\varepsilon_n \to 0$ such that for any choice $\{\Lambda^{(i)}_p\}_{p\in\mathbb{N}}$ of disjoint subsets of $\nabla^{\hat{d}}$, where we denote by $\mathbf{P}^{(i)}_p$ the ℓ_2–orthogonal projection onto $\Lambda^{(i)}_p$, we have

$$\begin{aligned}
&\Big\|\mathbf{S}_d\Big((\mathbf{A}^{(1)} - \mathbf{A}^{(1)}_{[p_1]}) \otimes \sum_{p_2\in\mathbb{N}} \mathbf{A}^{(2)}_{[p_2]}\mathbf{P}^{(2)}_{p_2} \otimes \sum_{p_3\in\mathbb{N}} \mathbf{A}^{(3)}_{[p_3]}\mathbf{P}^{(3)}_{p_3}\Big)\mathbf{S}_d\Big\| \le C\varepsilon_{p_1}\,,\\
&\Big\|\mathbf{S}_d\Big(\sum_{p_1\in\mathbb{N}} \mathbf{A}^{(1)}_{[p_1]}\mathbf{P}^{(1)}_{p_1} \otimes (\mathbf{A}^{(2)} - \mathbf{A}^{(2)}_{[p_2]}) \otimes \sum_{p_3\in\mathbb{N}} \mathbf{A}^{(3)}_{[p_3]}\mathbf{P}^{(3)}_{p_3}\Big)\mathbf{S}_d\Big\| \le C\varepsilon_{p_2}\,,\\
&\Big\|\mathbf{S}_d\Big(\sum_{p_1\in\mathbb{N}} \mathbf{A}^{(1)}_{[p_1]}\mathbf{P}^{(1)}_{p_1} \otimes \sum_{p_2\in\mathbb{N}} \mathbf{A}^{(2)}_{[p_2]}\mathbf{P}^{(2)}_{p_2} \otimes (\mathbf{A}^{(3)} - \mathbf{A}^{(3)}_{[p_3]})\Big)\mathbf{S}_d\Big\| \le C\varepsilon_{p_3}\,.
\end{aligned} \tag{5.54}$$

Note that approximations of precisely this type are provided by the wavelet compression schemes studied in Section 6.4, see Remarks 6.21, 6.28, 6.35.

Although for better clarity we formulate what follows only for separable operators of the form (5.53), the extension to operators of the form

$$\sum_j \mathbf{S}_d(\mathbf{A}^{(1)}_j \otimes \mathbf{A}^{(2)}_j \otimes \mathbf{A}^{(3)}_j)\mathbf{S}_d$$

required for our purposes is immediate.

Remark 5.17. *Performing* hosvd$(\mathbf{u}|_{\bar{\Lambda}_{d,n}})$ *for each* $n \in \mathbb{N}$, *for* $\mathbf{u} \in \mathcal{T}_d(r)$ *given in terms of mode frames and core tensors that do not necessarily have the orthogonality properties entailed by Assumptions 5.11, requires* $\mathcal{O}(\sum_n |r_n|_\infty \prod_i r_{n,i} + \sum_{n,i} \#\Lambda^{(i)}_n(\mathbf{u})\, r^2_{n,i})$ *operations by Remark 5.4.*

In the following lemma, we give an error estimate that serves as the basis for a numerical scheme for the approximate application of operators. Note that the approximations are adapted both to the higher-order singular values of the core tensor, and to the individual vectors in the mode frames.

Lemma 5.18. *Let* $\mathbf{u} = \sum_{n,k}(\bigotimes_i \mathbf{U}^{(i)}_{n,k_i})\, a_{n,k}$ *satisfy Assumptions 5.11. Let* $\mathbf{A} = \mathbf{S}_d(\mathbf{A}^{(1)} \otimes \mathbf{A}^{(2)} \otimes \mathbf{A}^{(3)})\mathbf{S}_d$, *and let* $\mathcal{D}_0 \subset \{1, 2, 3\}$ *such that* $\mathbf{A}^{(i)} = \mathrm{I}$ *for* $i \in \mathcal{D}_0$ *and* $\mathbf{A}^{(i)} \neq \mathrm{I}$ *for* $i \in \mathcal{D}_1 := \{1, 2, 3\}\backslash\mathcal{D}_0$.

For $n \in \mathbb{N}$, $k \in \mathcal{K}_3(r_n)$, *and* $i \in \{1, 2, 3\}$, *let* $\varepsilon^{(i)}_{n,k} > 0$, *and either*

(i) *let* $\mathcal{D}_0 = \emptyset$ *and for each* $n \in \mathbb{N}$, $k \in \mathcal{K}_3(r_n)$, *and* $i \in \{1, 2, 3\}$, *let* $\tilde{\mathbf{A}}^{(i)}_{n,k_i}$ *be approximations to* $\mathbf{A}^{(i)}$ *such that for* $\mathbf{B}^{(i)} \in \{\mathbf{A}^{(i)}, \tilde{\mathbf{A}}^{(i)}_{n,k_i}\}$,

$$\begin{aligned}
&\|\mathbf{S}_d((\mathbf{A}^{(1)} - \tilde{\mathbf{A}}^{(1)}_{n,k_1}) \otimes \mathbf{B}^{(2)} \otimes \mathbf{B}^{(3)})\mathbf{S}_d(\textstyle\bigotimes_i \mathbf{U}^{(i)}_{n,k_i})\| \le \varepsilon^{(1)}_{n,k_1}\,,\\
&\|\mathbf{S}_d(\mathbf{B}^{(1)} \otimes (\mathbf{A}^{(2)} - \tilde{\mathbf{A}}^{(2)}_{n,k_2}) \otimes \mathbf{B}^{(3)})\mathbf{S}_d(\textstyle\bigotimes_i \mathbf{U}^{(i)}_{n,k_i})\| \le \varepsilon^{(2)}_{n,k_2}\,,\\
&\|\mathbf{S}_d(\mathbf{B}^{(1)} \otimes \mathbf{B}^{(2)} \otimes (\mathbf{A}^{(3)} - \tilde{\mathbf{A}}^{(3)}_{n,k_3}))\mathbf{S}_d(\textstyle\bigotimes_i \mathbf{U}^{(i)}_{n,k_i})\| \le \varepsilon^{(3)}_{n,k_3}\,,
\end{aligned} \tag{5.55}$$

or

(ii) *let* $\mathcal{D}_0 \neq \emptyset$ *and for each* $n \in \mathbb{N}$, $k \in \mathcal{K}_3(r_n)$, *and* $i \in \{1,2,3\}$, *let* $\tilde{\mathbf{A}}^{(i)}_{n,k_i}$ *be approximations to* $\mathbf{A}^{(i)}$, *with* $\tilde{\mathbf{A}}^{(i)}_{n,k_i} = \mathrm{I}$ *if* $i \in \mathcal{D}_0$, *such that the following holds: let* $\mathbf{B}^{(i)} \in \{\mathbf{A}^{(i)}, \tilde{\mathbf{A}}^{(i)}_{n,k_i}\}$, *let* $L \in \mathbb{N}$ *and for* $\ell = 1,\ldots,L$, *let* $\mathbf{V}^{(i)}_\ell := \mathbf{U}^{(i)}_{n,k_i}$ *for* $i \in \mathcal{D}_1$, *then for any* $c_\ell \in \mathbb{R}$ *and any choice of* $\mathbf{V}^{(i)}_\ell$ *for* $i \in \mathcal{D}_0$ *and* $\ell = 1,\ldots,L$,

$$\begin{aligned}
&\Big\|\mathbf{S}_d\big((\mathbf{A}^{(1)} - \tilde{\mathbf{A}}^{(1)}_{n,k_1}) \otimes \mathbf{B}^{(2)} \otimes \mathbf{B}^{(3)}\big)\mathbf{S}_d\Big(\sum_{\ell=1}^{L} c_\ell \bigotimes_{i=1}^{3} \mathbf{V}^{(i)}_\ell\Big)\Big\| \leq \varepsilon^{(1)}_{n,k_1}\Big\|\sum_{\ell=1}^{L} c_\ell \bigotimes_{i\in\mathcal{D}_0} \mathbf{V}^{(i)}_\ell\Big\|\,,\\
&\Big\|\mathbf{S}_d\big(\mathbf{B}^{(1)} \otimes (\mathbf{A}^{(2)} - \tilde{\mathbf{A}}^{(2)}_{n,k_2}) \otimes \mathbf{B}^{(3)}\big)\mathbf{S}_d\Big(\sum_{\ell=1}^{L} c_\ell \bigotimes_{i=1}^{3} \mathbf{V}^{(i)}_\ell\Big)\Big\| \leq \varepsilon^{(2)}_{n,k_2}\Big\|\sum_{\ell=1}^{L} c_\ell \bigotimes_{i\in\mathcal{D}_0} \mathbf{V}^{(i)}_\ell\Big\|\,, \qquad (5.56)\\
&\Big\|\mathbf{S}_d\big(\mathbf{B}^{(1)} \otimes \mathbf{B}^{(2)} \otimes (\mathbf{A}^{(3)} - \tilde{\mathbf{A}}^{(3)}_{n,k_3})\big)\mathbf{S}_d\Big(\sum_{\ell=1}^{L} c_\ell \bigotimes_{i=1}^{3} \mathbf{V}^{(i)}_\ell\Big)\Big\| \leq \varepsilon^{(3)}_{n,k_3}\Big\|\sum_{\ell=1}^{L} c_\ell \bigotimes_{i\in\mathcal{D}_0} \mathbf{V}^{(i)}_\ell\Big\|\,.
\end{aligned}$$

Then for

$$\mathbf{w} := \sum_{n,k} a_{n,k}\mathbf{S}_d\Big(\bigotimes_{i=1}^{3} \tilde{\mathbf{A}}^{(i)}_{n,k_i}\Big)\mathbf{S}_d\Big(\bigotimes_{i=1}^{3} \mathbf{U}^{(i)}_{n,k_i}\Big)\,,$$

we have

$$\|\mathbf{A}\mathbf{u} - \mathbf{w}\| \leq \sqrt{\#\mathcal{D}_1}\Big(\sum_n \prod_{i\in\mathcal{D}_1} r_{n,i}\Big)^{\frac{1}{2}}\Big(\sum_n \sum_{i\in\mathcal{D}_1} \sum_{k_i=1}^{r_{n,i}} |\varepsilon^{(i)}_{n,k_i}|^2 |\sigma^{(i)}_{n,k_i}|^2\Big)^{\frac{1}{2}}\,. \qquad (5.57)$$

Concerning the extension of the estimate to tensors of order higher than three, besides the mentioned use of different underlying tensor formats, a certain feature of the error estimate that we obtain requires careful consideration: in the estimate (5.57), there is an additional dependence on the corresponding ranks via the factor $(\sum_n \prod_{i\in\mathcal{D}_1} r_{n,i})^{1/2}$. By the definition of $\mathcal{D}_1$, for each n one thus has a dependence on the product of all mode ranks $r_{n,i}$ for which $\mathbf{A}^{(i)} \neq \mathrm{I}$.

The operators arising in higher-dimensional problems of interest – in our case, the Laplacian and one-, two- and three-electron potential terms – typically only operate on a fixed number of dimensions, and are the identity operator on the remaining dimensions. In the example of the Laplacian in d dimensions, for instance, we have

$$\Delta = \mathrm{D}^2_{x_1} \otimes \mathrm{I}_{x_2} \otimes \cdots \otimes \mathrm{I}_{x_d} + \ldots + \mathrm{I}_{x_1} \otimes \cdots \otimes \mathrm{I}_{x_{d-1}} \otimes \mathrm{D}^2_{x_d}\,. \qquad (5.58)$$

Precisely when the underlying wavelet basis is L_2–orthonormal, the matrices representing the identity operators on the right hand side are identity matrices. In this case, when applying estimate (5.57) separately to each term on the right hand side of (5.58), the respective sets $\mathcal{D}_1$ each contain only one element.

In summary, provided that the wavelet basis is orthonormal, it is not the dimension of the problem that enters in the products of ranks in the estimate (5.57), but only the number of dimensions on which the tensor product operator under consideration is not the identity.

Proof. Note that $\mathbf{S}_d|_{\bar\Lambda_{d,n}} = \mathbf{S}^{(1)}_{d,n} \otimes \mathbf{S}^{(2)}_{d,n} \otimes \mathbf{S}^{(3)}_{d,n}$ according to Proposition 5.8. For $\tilde n \in \mathbb{N}$, let

$$\mathbf{W}^{(i)}_{n,k_i,\tilde n} := \mathbf{S}^{(i)}_{d,\tilde n}(\tilde{\mathbf{A}}^{(i)}_{n,k_i}\mathbf{S}^{(i)}_{d,n}\mathbf{U}^{(i)}_{n,k_i})|_{\bar\Lambda_{d,\tilde n}}\,,$$

then $\mathbf{w} = \sum_{\tilde n}\sum_{n,k} a_{n,k}\big(\bigotimes_i \mathbf{W}^{(i)}_{n,k_i,\tilde n}\big)$ and

$$\|\mathbf{A}\mathbf{u} - \mathbf{w}\|^2 = \sum_{\tilde n}\Big\|\sum_{n,k} a_{n,k}\big(\textstyle\bigotimes_i \mathbf{S}^{(i)}_{d,\tilde n}\mathbf{A}^{(i)}\mathbf{S}^{(i)}_{d,n}\mathbf{U}^{(i)}_{n,k_i} - \bigotimes_i \mathbf{W}^{(i)}_{n,k_i,\tilde n}\big)\Big\|^2\,. \qquad (5.59)$$

We first treat case (i), i.e., $\mathcal{D}_0 = \emptyset$. With the notation

$$\begin{aligned}
\varepsilon^{(1)}_{n,k,\tilde{n}} &:= \big\|\mathbf{S}_{d,\tilde{n}}\big[\big((\mathbf{A}^{(1)} - \tilde{\mathbf{A}}^{(1)}_{n,k_1}) \otimes \mathbf{A}^{(2)} \otimes \mathbf{A}^{(3)}\big)\mathbf{S}_d\big(\textstyle\bigotimes_i \mathbf{U}^{(i)}_{n,k_i}\big)\big]\big|_{\bar{\Lambda}_{d,\tilde{n}}}\big\| \,, \\
\varepsilon^{(2)}_{n,k,\tilde{n}} &:= \big\|\mathbf{S}_{d,\tilde{n}}\big[\big(\tilde{\mathbf{A}}^{(1)}_{n,k_1} \otimes (\mathbf{A}^{(2)} - \tilde{\mathbf{A}}^{(2)}_{n,k_2}) \otimes \mathbf{A}^{(3)}\big)\mathbf{S}_d\big(\textstyle\bigotimes_i \mathbf{U}^{(i)}_{n,k_i}\big)\big]\big|_{\bar{\Lambda}_{d,\tilde{n}}}\big\| \,, \\
\varepsilon^{(3)}_{n,k,\tilde{n}} &:= \big\|\mathbf{S}_{d,\tilde{n}}\big[\big(\tilde{\mathbf{A}}^{(1)}_{n,k_1} \otimes \tilde{\mathbf{A}}^{(2)}_{n,k_2} \otimes (\mathbf{A}^{(3)} - \tilde{\mathbf{A}}^{(3)}_{n,k_3})\big)\mathbf{S}_d\big(\textstyle\bigotimes_i \mathbf{U}^{(i)}_{n,k_i}\big)\big]\big|_{\bar{\Lambda}_{d,\tilde{n}}}\big\| \,,
\end{aligned}$$

a telescoping sum argument yields

$$\Big\|\sum_{n,k} a_{n,k}\big(\bigotimes_i \mathbf{S}^{(i)}_{d,\tilde{n}}(\mathbf{A}^{(i)}\mathbf{S}^{(i)}_{d,n}\mathbf{U}^{(i)}_{n,k_i})|_{\bar{\Lambda}_{d,n}} - \textstyle\bigotimes_i \mathbf{W}^{(i)}_{n,k_i,\tilde{n}}\big)\Big\| \le \displaystyle\sum_{n,k}|a_{n,k}|\sum_{i=1}^{3}\varepsilon^{(i)}_{n,k,\tilde{n}} \,,$$

which by the Cauchy-Schwarz inequality can be estimated further by

$$\sqrt{3}\Big(\sum_n \prod_{i=1}^{3} r_{n,i}\Big)^{\frac{1}{2}}\Big(\sum_{n,k}\sum_{i=1}^{3}|\varepsilon^{(i)}_{n,k,\tilde{n}}|^2|a_{n,k}|^2\Big)^{\frac{1}{2}} .$$

Inserting this into (5.59), noting that $\sum_{\tilde{n}}|\varepsilon^{(i)}_{n,k,\tilde{n}}|^2 \le |\varepsilon^{(i)}_{n,k_i}|^2$ by (5.55), and recalling that by our assumptions on the $\mathbf{a}_n$, we have

$$\sum_{k_2,k_3}|a_{n,k}|^2 = |\sigma^{(1)}_{n,k_1}|^2 \,, \quad \ldots \,, \quad \sum_{k_1,k_2}|a_{n,k}|^2 = |\sigma^{(3)}_{n,k_3}|^2 \,, \tag{5.60}$$

we obtain the assertion in the case $\mathcal{D}_0 = \emptyset$.

For part (ii), we now consider $\mathcal{D}_0 = \{3\}$, $\mathcal{D}_1 = \{1,2\}$ and $\mathcal{D}_0 = \{2,3\}$, $\mathcal{D}_1 = \{1\}$; all other cases with $\mathcal{D}_0 \ne \emptyset$ can be treated analogously.

Let $\mathcal{D}_0 = \{3\}$. Recall that in this case, $\mathbf{A}^{(3)} = \tilde{\mathbf{A}}^{(3)}_{n,k_3} = \mathrm{I}$ for all n and k_3. We set

$$\begin{aligned}
\hat{\varepsilon}^{(1)}_{n,k_1,k_2,\tilde{n}} &:= \big\|\mathbf{S}_{d,\tilde{n}}\big[\big((\mathbf{A}^{(1)} - \tilde{\mathbf{A}}^{(1)}_{n,k_1}) \otimes \mathbf{A}^{(2)} \otimes \mathrm{I}\big)\mathbf{S}_d\big(\mathbf{U}^{(1)}_{n,k_1} \otimes \mathbf{U}^{(2)}_{n,k_2} \otimes \textstyle\sum_{k_3} a_{n,k}\mathbf{U}^{(3)}_{n,k_3}\big)\big]\big|_{\bar{\Lambda}_{d,\tilde{n}}}\big\| \,, \\
\hat{\varepsilon}^{(2)}_{n,k_1,k_2,\tilde{n}} &:= \big\|\mathbf{S}_{d,\tilde{n}}\big[\big(\tilde{\mathbf{A}}^{(1)}_{n,k_1} \otimes (\mathbf{A}^{(2)} - \tilde{\mathbf{A}}^{(2)}_{n,k_2}) \otimes \mathrm{I}\big)\mathbf{S}_d\big(\mathbf{U}^{(1)}_{n,k_1} \otimes \mathbf{U}^{(2)}_{n,k_2} \otimes \textstyle\sum_{k_3} a_{n,k}\mathbf{U}^{(3)}_{n,k_3}\big)\big]\big|_{\bar{\Lambda}_{d,\tilde{n}}}\big\| \,.
\end{aligned}$$

Proceeding as above, we obtain

$$\|\mathbf{A}\mathbf{u} - \mathbf{w}\|^2 \le 2\Big(\sum_n \prod_{i=1}^{2} r_{n,i}\Big)\Big(\sum_{\tilde{n}}\sum_n \sum_{k_1,k_2}\sum_{i=1}^{2}|\hat{\varepsilon}^{(i)}_{n,k_1,k_2,\tilde{n}}|^2\Big) .$$

From (5.56) with $L = 1$, $\mathbf{V}^{(3)}_1 = \sum_{k_3} a_{n,k}\mathbf{U}^{(3)}_{n,k_3}$ we conclude

$$\sum_{\tilde{n}}|\hat{\varepsilon}^{(i)}_{n,k_1,k_2,\tilde{n}}|^2 \le |\varepsilon^{(i)}_{n,k_i}|^2\Big\|\sum_{k_3} a_{n,k}\mathbf{U}^{(3)}_{n,k_3}\Big\|^2$$

for each n, k_1, k_2, and i. Since

$$\Big\|\sum_{k_3} a_{n,k}\mathbf{U}^{(3)}_{n,k_3}\Big\|^2 = \sum_{k_3}|a_{n,k}|^2 \,,$$

the assertion follows as before.

In the case $\mathcal{D}_0 = \{2,3\}$, analogously to the previous cases we obtain

$$\|\mathbf{A}\mathbf{u}-\mathbf{w}\|^2 \le \Big(\sum_n r_{n,1}\Big)\Big(\sum_{n,k_1}\Big\|\mathbf{S}_d\big((\mathbf{A}^{(1)}-\tilde{\mathbf{A}}^{(1)}_{n,k_1})\otimes \mathrm{I}\otimes\mathrm{I}\big)\mathbf{S}_d\Big(\mathbf{U}^{(1)}_{n,k_1}\otimes\Big[\sum_{k_2,k_3} a_{n,k}\mathbf{U}^{(2)}_{n,k_2}\otimes\mathbf{U}^{(3)}_{n,k_3}\Big]\Big)\Big\|^2\Big),$$

and by (5.56), the right hand side can be estimated further by

$$\Big(\sum_n r_{n,1}\Big)\Big(\sum_{n,k_1}|\varepsilon^{(1)}_{n,k_1}|^2\Big\|\sum_{k_2,k_3} a_{n,k}\mathbf{U}^{(2)}_{n,k_2}\otimes\mathbf{U}^{(3)}_{n,k_3}\Big\|^2\Big) = \Big(\sum_n r_{n,1}\Big)\Big(\sum_{n,k_1}|\varepsilon^{(1)}_{n,k_1}|^2\sum_{k_2,k_3}|a_{n,k}|^2\Big).$$

Using again (5.60), we arrive at the assertion also in this case. □

A scheme based on Lemma 5.18 for approximating the action of $\mathbf{A}$ up to an error $\eta > 0$ is given in Algorithm 5.4. Here $\alpha \in \ell_1(\mathbb{N})$ is a fixed positive sequence with $\sum_n \alpha_n = 1$.

Algorithm 5.4 $\mathbf{w} = \mathsf{apply}_{\mathbf{A}}(\mathbf{u};\eta)$

```
input   $\mathbf{u} = \sum_n \sum_{k\in\mathcal{K}_3(r_n)} a_{n,k}(\bigotimes_i \mathbf{U}^{(i)}_{n,k})$ satisfying Assumptions 5.11
output  $\mathbf{w} \in \mathcal{T}_d(s)$ for some $s = (s_n)_{n\in\mathbb{N}}$, $s_n \in \mathbb{N}_0^3$, with $\|\mathbf{A}\mathbf{u}-\mathbf{w}\| \le \eta$ and $\#\operatorname{supp}\mathbf{w} < \infty$
    $c_0 := (\#\mathcal{D}_1)^{\frac12}\big(\sum_n \prod_{i\in\mathcal{D}_1} r_{n,i}\big)^{\frac12}$.
1: for all $n$, $i$, and $k = 1,\dots,r_{n,i}$,
2:     $\varepsilon^{(i)}_{n,k_i} := \frac12(\#\mathcal{D}_1)^{-\frac12}(\alpha_n\alpha_{k_i})^{\frac12}(c_0\,\sigma^{(i)}_{n,k_i})^{-1}\eta$,      ▷ $\alpha_q > 0$, $\sum_q \alpha_q = 1$
3:     Construct $\tilde{\mathbf{A}}^{(i)}_{n,k_i}$ such that conditions (5.56) hold.
4: end for
5: for all $n$,
6:     $\hat{\mathbf{w}}_n \leftarrow \sum_k a_{n,k}\bigotimes_i\big(\mathbf{A}^{(i)}_{n,k_i}\mathbf{S}^{(i)}_{d,n}\mathbf{U}^{(i)}_{n,k_i}\big)$,
7:     $\mathbf{w} \leftarrow \mathbf{w} + \mathbf{S}_d\hat{\mathbf{w}}_n$,
8:     $\mathbf{w} \leftarrow \mathsf{recompress}(\mathbf{w};\frac12\alpha_n\eta)$.
9: end for
```

The basic rationale, as suggested by the error estimate, is to use a more accurate approximation of $\mathbf{A}^{(i)}$ for large, a less accurate approximation for small mode-i singular values. In addition, the approximations to $\mathbf{A}^{(i)}$ are adapted to each individual vector in the mode frames, where again coarser approximations are sufficient for smaller entries.

The addition in line 7 of Algorithm 5.4 can be done by a simple concatenation of tensor representations, or, for improved numerical stability, by concatenation followed by a reorthogonalization of mode frames of intermediate results. We combine this addition with a rank reduction of intermediate results by the routine based on hosvd from the previous subsection in line 8, where the tolerances are chosen so as to preserve the desired error bound for the final result.

For the construction of approximate operators as used in line 3 of Algorithm 5.4, one can, with only slight modifications, follow the strategy for adaptive application of operators based on s^*–compressiblity as discussed in Section 3.6 – that is, appropriately subdividing the corresponding $\mathbf{U}^{(i)}_{n,k_i}$ and applying approximations as in (5.54) to each of the pieces to meet the target accuracies required in (5.55) and (5.56).

More specifically, assuming (5.54) we proceed as follows. For $i \in \mathcal{D}_0$, for which $\mathbf{A}^{(i)} = \mathrm{I}$, we set $\tilde{\mathbf{A}}^{(i)}_{n,k_i} = \mathrm{I}$ for all n and k_i. For $i \in \mathcal{D}_1$, for which $\mathbf{A}^{(i)} \neq \mathrm{I}$, again with $\alpha_p > 0$ such that $\sum_p \alpha_p = 1$, and for given $\varepsilon^{(i)}_{n,k_i}$ and $\mathbf{U}^{(i)}_{n,k_i}$, we choose disjoint subsets $\tilde{\Lambda}^{(i)}_{n,k_i,p}$, $p \in \mathbb{N}_0$, such that with ε_p as in (5.54) we have

$$\sum_{p\in\mathbb{N}_0} C\varepsilon_p\big\|\mathbf{U}^{(i)}_{n,k_i}|_{\tilde{\Lambda}^{(i)}_{n,k_i,p}}\big\| \le \varepsilon^{(i)}_{n,k_i}\,. \tag{5.61}$$

Denoting by $\tilde{\mathbf{P}}^{(i)}_{n,k_i,p}$ the ℓ_2–orthogonal projection onto $\tilde{\Lambda}^{(i)}_{n,k_i,p}$, we define

$$\tilde{\mathbf{A}}^{(i)}_{n,k_i} := \sum_{p\in\mathbb{N}_0} \mathbf{A}^{(i)}_{[p]}\tilde{\mathbf{P}}^{(i)}_{n,k_i,p} .$$

The constructed operators then satisfy assumptions (5.55) if $\mathcal{D}_0 = \emptyset$, and (5.56) if $\mathcal{D}_0 \neq \emptyset$.

Operator compression results that yield the assumptions (5.54) on the $\mathbf{A}^{(i)}_{[p]}$ with suitable ε_p will be considered in Section 6.4. Specifically, for the operators of interest in our case, this is clear for the Laplacian by Proposition 6.1, and is a direct consequence of Remarks 6.21, 6.28, and 6.35 for the separable approximations of potential terms.

Under the given assumptions, a choice of $\tilde{\Lambda}^{(i)}_{n,k_i,p}$ as in (5.61) is always possible, since $\|\mathbf{U}^{(i)}_{n,k_i}\| = 1$ and $\varepsilon_p \to 0$. A procedure for making the choice that leads to the best overall complexity, however, mainly depends on knowledge about the decay of $\mathbf{u}|_{\bar{\Lambda}_{d,n}}$ for each n, which may differ from the decay properties of $\mathbf{u}$ itself. Since this point therefore depends on further properties of the exact solution, we do not consider this issue in further detail here.

Remark 5.19. *In the given form, the support of the output of Algorithm 5.4 in general has larger support than the input. However, Algorithm 5.4 can be used in exactly the same way to operate on a fixed set of basis elements, that is, with the constraint that the support of the output be contained in the support of the input. This can be used, e.g., for solving Galerkin problems for a fixed wavelet discretization.*

5.4 Adaptive Methods

With the algorithmic components given in the previous section, the adaptive wavelet schemes outlined in Section 3.6 can be adapted in a straightforward manner to operate on low-rank representations of wavelet coefficients.

We obtain a convergence analysis with all involved constants depending only on the operator and the wavelet basis under consideration. This is in contrast to tensor iterative methods based on simpler discretizations: for a fixed discretization, it is of course always possible to choose iteration parameters sufficiently small to ensure convergence, but the precise dependence of such a choice on the underlying discretization generally remains opaque. In our context, we find that – as in standard adaptive wavelet schemes – it suffices to choose the error tolerances on the order of the current residual to ensure convergence.

5.4.1 Iterative Solution of Linear Operator Equations

We first give an iterative solver for operator equations that uses a low-rank tensor representation of wavelet coefficients. With the routines developed in this chapter as a prerequisite, the basic scheme of the standard adaptive wavelet solver in Algorithm 3.1 carries over to our setting with only two modifications: The first is the additional use of recompress described in Algorithm 5.2 in the inner iteration, which is required for practical feasibility; the second is the substitution of the coarsening step in the outer iteration by a combination of the tensor coarsening described in Algorithm 5.3 and a recompression. Note that here we additionally assume the availability of a routine rhs that produces approximations of the right hand side $\mathbf{f}$ in the tensor format.

Under the same boundedness and ellipticity assumptions on $\mathbf{A}$ as in Section 3.6.1, we obtain the following convergence result.

Proposition 5.20. *Let the step size $\alpha > 0$ in Algorithm 5.5 satisfy $\|\mathrm{I} - \alpha\mathbf{A}\| \leq \rho < 1$. Then the intermediate steps $\mathbf{u}_i$ of Algorithm 5.5 satisfy $\|\mathbf{u}_i - \mathbf{u}\| \leq \theta^i\delta$, and in particular, The output $\mathbf{u}_\varepsilon$ of Algorithm 5.5 satisfies $\|\mathbf{u}_\varepsilon - \mathbf{u}\| \leq \varepsilon$.*

Proof. Taking into account the adjustment of iteration parameters for the additional recompression step in each inner iteration, the statement follows exactly as in Proposition 3.20. □

Algorithm 5.5 $\mathbf{u}_\varepsilon = \mathsf{tensor\_solve}(\mathbf{A}, \mathbf{f}; \varepsilon)$

```
input   $\alpha > 0$ and $\rho \in (0,1)$ such that $\|\mathrm{I} - \alpha\mathbf{A}\| \leq \rho$, $\theta, \kappa \in (0,1)$, and $\beta > 0$.
output  $\mathbf{u}_\varepsilon$ satisfying $\|\mathbf{u}_\varepsilon - \mathbf{u}\| \leq \varepsilon$.
$\mathbf{u}_0 := 0$, $\delta := c_{\mathbf{A}}^{-1}\|\mathbf{f}\|$
$i := 0$, $K := \min\{k\colon \rho^k(1 + (\alpha + \beta)k) \leq \kappa\theta\}$
while $\theta^i\delta > \varepsilon$
    $\mathbf{w}_0 := \mathbf{u}_i$
    repeat
        $\eta_j := \rho^{j+1}\theta^i\delta$
        $\mathbf{r}_j := \mathsf{apply}(\mathbf{w}_j; \frac{1}{2}\eta_j) - \mathsf{rhs}(\frac{1}{2}\eta_j)$
        $\mathbf{w}_{j+1} := \mathsf{recompress}(\mathbf{w}_j - \alpha\mathbf{r}_j; \beta\eta_j)$
        $j \leftarrow j + 1$.
    until $(j \geq K \quad \vee \quad c_{\mathbf{A}}^{-1}\rho\|\mathbf{r}_{j-1}\| + (c_{\mathbf{A}}^{-1}\rho + \alpha + \beta)\eta_{j-1} \leq \kappa\theta^{i+1}\delta)$
    $\mathbf{u}_{i+1} := \mathsf{coarsen}\big(\mathsf{recompress}(\mathbf{w}_j; \frac{1}{2}(1-\kappa)\theta^{i+1}\delta); \frac{1}{2}(1-\kappa)\theta^{i+1}\delta\big)$
    $i \leftarrow i + 1$
end while
$\mathbf{u}_\varepsilon := \mathbf{u}_i$
```

5.4.2 Iterative Solution of Eigenvalue Problems

With exactly the same minor changes as in the case of operator equations considered above, the adaptive wavelet eigensolver of Algorithm 3.2 for symmetric, elliptic operators can be modified to a method operating on low-rank representations of wavelet coefficients as well. The resulting scheme is given in Algorithm 5.6.

Under the same assumptions on $\mathbf{A}$ and $\mathbf{M}$ as made in Section 3.6.2 for Algorithm 3.2, we obtain the following convergence result for the error in the eigenspace corresponding to the lowest eigenvalue.

Proposition 5.21. *Let the parameters α, ρ, E, C_1 in Algorithm 5.6 be chosen as in Lemma 3.23, and let the starting vector $\mathbf{v}_0 \in \ell_2$ with $\|\mathbf{v}_0\| = 1$ satisfy $\|e_\perp(\mathbf{v}_0)\| \leq \delta$, where δ satisfies*

$$0 < \delta < \min\bigl\{(1 + C_1^2)^{1/2} - C_1, (E^{-1} + (C_2\alpha)^2)^{1/2} - (C_2\alpha)\bigr\} \tag{5.62}$$

with $C_2 := \frac{1}{2}(1-\rho)^{-1}\|\mathbf{M}\|$. Then the iterates $\mathbf{v}_i$ in Algorithm 5.6 satisfy $\|e_\perp(\mathbf{v}_i)\| \leq \theta^i\delta$ with $\|\mathbf{v}_i\| = 1$, and in particular, we have $\|e_\perp(\mathbf{u}_\varepsilon)\| \leq \varepsilon$ with $\|\mathbf{u}_\varepsilon\| = 1$.

Proof. Taking into account the adjustment of iteration parameters for the additional recompression step in each inner iteration, the statement follows exactly as in Proposition 3.24. □

The practical realization of this algorithm, in particular for the model problems of Section 2.3, will be considered in Chapter 7. Before coming to this point, in the following chapter we study in detail the required approximation of the relevant operators.

Remark 5.22. *The statement of Remark 3.28 concerning nonsymmetric eigenvalue problems, as in the explicitly correlated formulation* (2.11), *applies here as well, that is, Algorithm 5.6 and Proposition 5.21 require symmetric* $\mathbf{A}$. *A construction of an adaptive scheme for nonsymmetric eigenvalue problems, which we leave for future work, can be based on inexact inverse iteration, using Algorithm 5.5 – which is directly applicable to nonsymmetric elliptic problems – as a solver for the arising operator equations.*

5.4.3 Discussion

The adaptive methods based on low-rank tensor formats that we have constructed are in their basic structure completely analogous to known adaptive wavelet methods. This raises the question

Algorithm 5.6 $\mathbf{u}_\varepsilon = \mathsf{tensor\_evpsolve}(\mathbf{A}, \mathbf{v}_0; \varepsilon)$

```
input  $\alpha$, $\rho$, $E$, $C_1$ as in Lemma 3.23, and $R$ as in (3.40); $\mathbf{v}_0$ with $\|\mathbf{v}_0\| = 1$ such that $\|e_\perp(\mathbf{v}_0)\| \le \delta$
    with $\delta$ as in (3.41); $\theta, \kappa \in (0,1)$.
output  $\mathbf{u}_\varepsilon$ with $\|\mathbf{u}_\varepsilon\| = 1$ and $\|e_\perp(\mathbf{u}_\varepsilon)\| \le \varepsilon$.
$i := 0$, $\varepsilon_0 := \delta$
while $\varepsilon_i > \varepsilon$
    $\mathbf{w}_0 \leftarrow \mathbf{v}_i$
    $\xi_i := \rho + \alpha\|\mathbf{M}\|(1 - E\varepsilon_i^2)^{-1}E\varepsilon_i$
    $\tilde{\eta}_i := \alpha^{-1}(1 + \varepsilon_i)^{-1}\varepsilon_i(1 - \xi_i)$
    $\varepsilon_{i+1} := \theta\varepsilon_i$
    $K_i := \min\bigl\{k\colon \bigl(\prod_{l=0}^{k-1}(1 - \xi_i^{l+1}\alpha\tilde{\eta}_i)\bigr)^{-1}\xi_i^k(\varepsilon_i + k\alpha\tilde{\eta}_i) \le \kappa\varepsilon_{i+1}\bigr\}$
    $j \leftarrow 0$
    repeat
        $\eta_j \leftarrow \xi_i^{j+1}\,\tilde{\eta}_i$
        $\mathbf{r}_j \leftarrow \mathsf{apply}(\mathbf{w}_j; \frac{1}{4}\eta_j) - \mathsf{rayleigh}(\mathbf{w}_j; \frac{1}{4}\|\mathbf{M}\|^{-1}\eta_j)\,\mathbf{M}\mathbf{w}_j$
        $\hat{\mathbf{w}}_{j+1} \leftarrow \mathsf{recompress}(\mathbf{w}_j - \alpha\mathbf{r}_j; \frac{1}{2}\alpha\eta_j)$
        $\mathbf{w}_{j+1} \leftarrow \|\hat{\mathbf{w}}_{j+1}\|^{-1}\,\hat{\mathbf{w}}_{j+1}$
        $j \leftarrow j + 1$
    until $(j \ge K_i \quad \vee \quad (1 - \alpha\eta_{j-1})^{-1}(\xi_i R(\mathbf{w}_{j-1})\|\mathbf{r}_{j-1}\| + (\alpha + \xi_i R(\mathbf{w}_{j-1}))\eta_{j-1}) \le \kappa\varepsilon_{i+1})$
    $\tau_{i+1} := (1 + \varepsilon_{i+1}^2)^{-1}\bigl[\bigl(\kappa^2 + (1 - \kappa^2)(1 + \varepsilon_{i+1}^2)\bigr)^{1/2} - \kappa\bigr]$
    $\hat{\mathbf{v}}_{i+1} := \mathsf{coarsen}\bigl(\mathsf{recompress}(\mathbf{w}_j; \frac{1}{2}\tau_{i+1}\varepsilon_{i+1});\ \frac{1}{2}\tau_{i+1}\,\varepsilon_{i+1}\bigr)$
    $\mathbf{v}_{i+1} := \|\hat{\mathbf{v}}_{i+1}\|^{-1}\hat{\mathbf{v}}_{i+1}$
    $i \leftarrow i + 1$
end while
$\mathbf{u}_\varepsilon := \mathbf{v}_i$
```

whether the new methods can make in a similar sense optimal use of wavelet compressibility properties of operator and solution. What one can hope to achieve here is to come close to the best N-term rate for approximation of the mode frames. In this context, a crucial role is played by a new aspect, the evolution of tensor ranks over the course of the iteration. These complexity considerations are left for future work.

Since a main motivation for these low-rank schemes is the treatment of higher-dimensional problems, a further important question concerns their dimension dependencies, which we shall now summarize.

In the approach followed here, the tensor order may in general enter via the number of active elements in the levelwise subdivision we have used for the tensor representation. For a worst case estimate, we consider the approximation of a wavelet coefficient sequence up to an error ε by tensors of order d in the subdivided format. The maximum required wavelet level in the corresponding approximation is then proportional to $|\log \varepsilon|$; according to Proposition 5.6, the number of elements in the subdivision can thus be estimated by $\mathcal{O}(|\log \varepsilon|(\log|\log \varepsilon|)^{d-2})$. More general subdivisions, as outlined in Remark 5.10, may therefore be of interest in higher dimensions. Note, however, that the above estimate for the number of active subdivision elements may be very pessimistic, in particular in the case of coefficient sequences with a pronounced sparse grid structure.

A second dependence on the dimension appears in the estimate of Lemma 5.18, which forms the basis of our routine for the adaptive application of operators. For each separable term in the operator, the number of lower-dimensional component operators that do not equal the identity enters exponentially in the error estimate. In typical cases, such as the Laplacian or one- and two-electron potentials, the corresponding exponents are independent of the total problem dimension, and this therefore does not represent a severe restriction. It is unclear at this point whether this dependence can actually be removed from the estimate.

The only other place where the tensor order d enters explicitly is the underlying tensor format. Since the complexity estimates for the Tucker format, which is sufficient for the model problems considered here, depend exponentially on d, it is not suitable for a generalization to larger d. As noted in Subsection 5.3.3, however, all required operations can be realized in the same manner for the $\mathcal{H}$-Tucker format, which is in principle suitable for very high-dimensional problems, and Algorithms 5.5 and 5.6 are therefore applicable in combination with this format as well.

6 Approximation of Operators

The numerical cost of obtaining approximations to wave functions by iterative schemes depends not only on the approximability of such functions as discussed in Chapter 4, but also on the cost of approximating the action of the corresponding Hamiltonian operators. In this chapter, we study approximations to both the self-adjoint electronic Schrödinger Hamiltonian and to the nonsymmetric two-electron operator arising in the explicitly correlated formulation (2.16).

We are dealing with three different aspects of approximating these operators. In Section 6.3, we consider the convergence properties of approximations by sums of separable functions for the potential terms

$$\frac{1}{|x|}\,, \quad \frac{1}{|x-y|}\,, \quad \frac{x-y}{|x-y|}\cdot(\mathrm{D}_x-\mathrm{D}_y)\,, \quad x,y\in\mathbb{R}^3\,,$$

based on the exponential sum approximations of Section 4.3.1, and subsequently study wavelet compression of the resulting approximate operators in Section 6.4. A third approximation becomes necessary because in general, the required integrals cannot be evaluated exactly: in Sections 6.5 and 6.6, we consider integration schemes for the corresponding matrix entries that are applicable to a large class of wavelet bases.

Before coming to these points, we give an overview of suitable choices of wavelet bases in the following section, and discuss compression of the Laplacian in such bases in Section 6.2.

6.1 Choice of Wavelet Basis

The adaptive schemes reviewed in Section 3.6 and their counterparts based on low-rank tensor representations considered in Chapter 5 can be expected to be efficient in our context only under quite restrictive conditions on the underlying wavelet bases. This concerns in particular the choice of univariate wavelets $\{\psi_\nu\}_{\nu\in\nabla}$ that serve as the basis of the higher-dimensional tensor product constructions.

A fundamental requirement is the transformation of the original problem to a well-posed infinite matrix problem on an ℓ_2–space. We therefore need to work with wavelets that are sufficiently regular to become, with an appropriate rescaling, a Riesz basis for the corresponding energy space. In our case, this is always H^1; that is, the univariate wavelet needs to be H^1–stable. For the resulting problem to be reasonably well-conditioned, however, the condition number of the corresponding Riesz basis of H^1 needs to be small. In the higher-dimensional case, this leads to a further fundamental restriction on the wavelets. Recall from Remark 3.17 that the condition number will always increase exponentially with the space dimension, unless the wavelet basis is L_2–*orthonormal*, in which case the condition number stays uniformly bounded with increasing dimension. In higher dimensions, orthonormality thus becomes indispensable.

The two restrictions of L_2–orthonormality and H^1–stability by themselves are not too severe. What is required in addition to ensure efficiency of adaptive schemes, however, is near-sparsity of the basis representations both of the solution and of the operator.

The solutions of the problems considered in this work are smooth on the complement of a certain set of localized singularities. In order to take advantage of this property, the wavelet basis functions need to be sufficiently well localized, which leads us to consider *compactly supported* wavelets. In principle, one could also consider globally supported wavelets with sufficiently rapid decay towards infinity. We are, however, not aware of orthonormal wavelets of this type that are more favorable for our purposes than the known compactly supported constructions. We therefore restrict our considerations to wavelets of compact support.

The decay of solution coefficients corresponding to wavelet basis functions on whose supports the approximand is smooth is then in general limited by the *approximation order* of the wavelets. In the case of, e.g., hydrogenic ground states, as we have seen in Section 4.2, the convergence rate of best N-term approximation by a wavelet basis is limited only by the approximation order of that basis. For problems with electron interaction cusps, we have seen that one instead obtains an intrinsic limitation on the convergence rates that can be achieved by tensor product wavelets. Even in this case, however, wavelets of higher approximation orders can yield approximations that are quantitatively more efficient. Recall that in the orthonormal case, the approximation order equals the number of vanishing moments of the wavelet.

The combination of the requirements encountered so far is quite restrictive. The most important options have already been mentioned in Section 3.1. One possible choice are Daubechies wavelets [37]. A further variant of interest are the wavelets constructed, following the same principle, by Ojanen [119]. For given support size the latter have less vanishing moments, but higher Sobolev regularity than the classical Daubechies wavelets. Due to the fractal nature of such Daubechies-type wavelets, the construction of quadrature schemes for the computation of matrix entries is not straightforward. Specialized methods for evaluating required integrals will be considered in Sections 6.5 and 6.6.

From the point of view of quadrature, spline wavelets are an ideal choice. As noted in Section 3.1, the construction of wavelets that are orthonormal, have compact support and are additionally piecewise polynomial is not possible. These requirements can, however, be realized simultaneously by multiwavelets, where a multiresolution analysis is generated by several different scaling functions and wavelets. Families of compactly supported, orthonormal, and piecewise polynomial multiwavelets have been constructed by Donovan, Gernonimo, and Hardin in [45, 46]. These multiwavelets are available with C^0, C^1, and C^2 smoothness and with arbitrarily high approximation orders. A piecewise linear and continuous variant has been used in adaptive wavelet schemes for higher-dimensional problems in [44] and [90].

Besides the less problematic evaluation of integrals, when represented in a basis of spline wavelets, certain operators, including the Laplacian, have better s^*–compressibility properties. We shall consider this point in more detail in Section 6.2.

Although polynomial multiwavelets therefore have some important advantages over Daubechies wavelets, there is also a major disadvantage: with increasing approximation orders and smoothness requirements, the number of different multiwavelet basis functions in the one-dimensional construction increases, and this number in turn enters exponentially with respect to space dimension in the number of basis functions per dyadic grid point that need to be considered in the higher-dimensional case. For a direct wavelet discretization, this presents a serious practical obstruction. In the setting of nonlinearly parameterized wavelet expansions of Chapter 5, however, this point is less problematic, since only the (multi)wavelet expansions of lower-dimensional factors are required. In this chapter, all results are formulated for the notationally simpler case of wavelets, but directly carry over to multiwavelet bases.

Apart from the choice of univariate wavelet basis functions, there is also a choice between two types of tensor product wavelet constructions. Recall that for a direct (linearly parametrized) wavelet representation, one-electron wavefunctions could either be represented in a basis indexed by $\nabla^{(3)}$, which corresponds to isotropic basis functions, or by a fully anisotropic tensor product basis ∇^3. Similarly, for two-electron wavefunctions one could use partially anisotropic bases indexed by $(\nabla^{(3)})^2$, or the fully anisotropic variants ∇^6.

For the low-rank representations of wavelet coefficients considered in Section 4.3 and Chapter 5, however, the wavelet index sets need to have an appropriate tensor product structure, and therefore only the fully anisotropic variants ∇^3 and ∇^6 are suitable. In fact, the latter are also advantageous in direct wavelet representations. When the potential terms are replaced by separable approximations as considered in Section 6.4, the arising factor matrices have suitable compressibility properties only in the case of fully anisotropic wavelet bases. Compression schemes for these factor matrices are given in Section 6.4.

6.2 Approximation of the Laplacian

In the approximate application of operators required by adaptive wavelet schemes, the notion of s^*–compressibility of operators plays a central role. As we have seen in Section 5.3.4, one can proceed similarly in the context of low-rank representations. The complexity of the corresponding Algorithm 5.4 is, however, influenced by an additional aspect: the bounds on the ranks of intermediate results become more favorable with less interaction between the elements $\bar{\Lambda}_{d,n}$ (cf. (5.38)) of the level subdivision. Thus it is not only the number of nonzero elements in the columns of sparse approximations that influences the complexity in this modified setting, but also the *levelwise* decay of entries.

In this section, we summarize standard results concerning wavelet compression of the Laplacian. For the fully anisotropic tensor product wavelets, this can be obtained as a direct consequence of the corresponding compression estimate in the one-dimensional case.

For the derivation of this one-dimensional estimate, let $\psi \in \mathrm{H}^\tau(\mathbb{R})$ for some $\tau > 1$ be orthonormal with p vanishing moments. Note that in view of Remark 3.4, we have $p \geq \lfloor \tau \rfloor + 1$. By integration by parts, ψ' has $p+1$ vanishing moments. Let I be a closed interval such that $\operatorname{supp}\psi \subset I$. For $\nu, \mu \in \nabla$ with $|\nu| \geq |\mu|$ and $\mathrm{s}(\nu) \neq 0$ we thus obtain as in [8, 29] the estimate

$$\begin{aligned}\left|\int \psi'_\mu \psi'_\nu \,\mathrm{d}x\right| &\leq \|\psi'_\nu\|_{\mathrm{L}_2} \inf_{g \in \Pi_p} \|\psi'_\mu - g\|_{\mathrm{L}_2(2^{-|\nu|}(I+\mathrm{k}(\nu)))} \lesssim 2^{|\nu|} 2^{-(\tau-1)|\nu|} |\psi'_\mu|_{\mathrm{H}^{\tau-1}(2^{-|\nu|}(I+\mathrm{k}(\nu)))} \\ &\lesssim 2^{-(\tau-1)(|\nu|-|\mu|)} 2^{|\mu|+|\nu|} |\psi|_{\mathrm{H}^\tau(2^{|\mu|-|\nu|}(I+\mathrm{k}(\nu))-\mathrm{k}(\mu))}\,,\end{aligned}$$

with the symmetric estimate for $|\nu| < |\mu|$, which altogether yields

$$2^{-|\mu|-|\nu|}\left|\int \psi'_\mu \psi'_\nu \,\mathrm{d}x\right| \lesssim 2^{-(\tau-1)||\nu|-|\mu||}\,. \tag{6.1}$$

This can be used in conjunction with the following result from [30]. Since we are exclusively interested in local operators in this work, we reproduce it here with some adaptations to this particular case. Here, χ_1 is defined as in (3.19).

Proposition 6.1 (cf. [30, Proposition 3.4]). *Let* $\mathbf{A} = (a_{\nu\mu})_{\nu,\mu\in\nabla}$ *with* $|a_{\nu\mu}| \leq c_A 2^{-||\mu|-|\nu||\sigma} \chi_1(\mu,\nu)$ *for a* $\sigma > 1/2$, *and let* $s^* := \sigma - 1/2$. *Then for given* $s \leq s^*$ *there exists for every* $\ell \in \mathbb{N}$ *a matrix* $\mathbf{A}_\ell$ *with at most* 2^ℓ *entries in each row and column such that*

$$\|\mathbf{A} - \mathbf{A}_\ell\| \leq C 2^{-s\ell}\,. \tag{6.2}$$

Specifically, such $\mathbf{A}_\ell$ *can be obtained from* $\mathbf{A}$ *by fixing* $\alpha \in \ell_1$ *and setting to zero all entries* $a_{\nu\mu}$ *for which* $||\nu| - |\mu|| > \ell$ *or* $|a_{\nu\mu}| \leq \alpha_{||\nu|-|\mu||} 2^{-||\nu|-|\mu||/2}\, 2^{-s\ell}$.

Proof. Let $\ell \in \mathbb{N}$ and $\alpha \in \ell_1$, and let $\tilde{a}_{\nu\mu} = a_{\nu\mu}$ if $||\nu| - |\mu|| \geq \ell$, and $\tilde{a}_{\nu\mu} = 0$ otherwise. For $\nu \in \nabla$, let $\omega_\nu = 2^{-|\nu|/2}$. We have

$$\begin{aligned}\omega_\nu^{-1} \sum_\mu \omega_\mu |a_{\mu\nu} - \tilde{a}_{\mu\nu}| &= \omega_\nu^{-1} \sum_{\{\mu\colon ||\nu|-|\mu||>\ell\}} \omega_\mu |a_{\mu\nu}| \\ &\lesssim \sum_{j<|\nu|-\ell} 2^{(|\nu|-j)/2}\, 2^{-(|\nu|-j)\sigma} + \sum_{j>|\nu|+\ell} 2^{(|\nu|-j)/2}\, 2^{j-|\nu|}\, 2^{-(j-|\nu|)\sigma} \\ &\lesssim \sum_{l>\ell} 2^{-(\sigma-1/2)l} \lesssim 2^{-s\ell}\,.\end{aligned}$$

The number of nonzero entries per row and column of $(\tilde a_{\nu\mu})$ can be estimated by $\sum_{l=0}^{\ell} 2^l \lesssim 2^\ell$.

In a second compression step, let $\hat a_{\nu\mu} = \tilde a_{\nu\mu}$ if $|\tilde a_{\nu\mu}| > \alpha_{||\nu|-|\mu||} 2^{-||\nu|-|\mu||/2}\, 2^{-s\ell}$, and $\hat a_{\nu\mu} = 0$ otherwise, then

$$\omega_\nu^{-1} \sum_\mu \omega_\mu |\hat a_{\mu\nu} - \tilde a_{\mu\nu}| \lesssim \sum_{|\nu|-\ell \le j \le |\nu|} \alpha_{|\nu|-j} 2^{-s\ell} + \sum_{|\nu| < j \le |\nu|+\ell} \alpha_{j-|\nu|} 2^{-s\ell} \le \|\alpha\|_{\ell_1} 2^{-s\ell} ,$$

and we obtain the assertion with Lemma 6.8 for $\mathbf{A}_\ell := (\hat a_{\nu\mu})$. □

Applying (6.1) and Proposition 6.1, one obtains s^*-compressibility of the one-dimensional Laplacian[1] with $s^* \le \tau - \frac{3}{2}$ for wavelets in $\mathrm{H}^\tau(\mathbb{R})$. Here the second part of the prescription for obtaining a suitable $\mathbf{A}_\ell$ in Proposition 6.1 is not necessary for the asymptotic rate, but can be important in practice for a further reduction of the number of required entries.

Remark 6.2. *The estimate* (6.1) *holds under the assumption that the wavelets have sufficient global regularity. Substantially better compressibility properties for a certain class of operators, including the Laplacian, are obtained in [135] for piecewise polynomial wavelets. In our particular case of interest, the underlying observation is that for a spline wavelet basis* $\{\psi_\nu\}_{\nu\in\nabla}$*, unless the support of* ψ_μ *contains a node of the spline function* ψ_ν *or vice versa, the vanishing moment property yields*

$$\int \psi'_\mu \psi'_\nu \,\mathrm{d}x = 0\,.$$

The number of nonzero coefficients is thus uniformly bounded for each combination of levels $|\nu|$, $|\mu|$*. Consequently, the representation of the one-dimensional Laplacian in a spline wavelet basis is* s^**–compressible for* any $s^* > 0$.

An additional restriction to spline functions as in Remark 6.2 excludes Daubechies-type wavelets; if orthonormality is required one can, as pointed out in [44], instead use piecewise polynomial multiwavelets. In our case, however, the limitation of compressibility due to the smoothness of the wavelets is not a decisive point, since in the following subsections we will obtain even more severe restrictions on the compressibility of discretized two-electron potential terms, which will eventually limit the compressibility of the full Hamiltonians.

Remark 6.3. *As mentioned in the beginning of this section, for applying wavelet compression in the low-rank schemes of Chapter 5 as in Algorithm 5.4, it is advantageous to keep the interactions between level subdivision elements* $\bar\Lambda_{d,n}$ *to a minimum. In the case of the Laplacian, this means that the exponent* $\sigma := \tau - 1$ *in the estimate* (6.1) *– and thus the Sobolev regularity index* τ *of the wavelets – should be as large as possible. In this regard, spline wavelets of low global regularity are less favorable; for splines in* C^0*, for instance, one only obtains* $\sigma < \frac{1}{2}$.

From the above result for $\{\psi_\nu\}_{\nu\in\nabla}$, the compressibility of the higher-dimensional Laplacian in a corresponding (fully anisotropic) tensor product basis $\{\Psi_\nu\}_{\nu\in\nabla^d}$ with the same s^* follows for orthonormal wavelets from [44, Theorem 3.5]. We recapitulate the argument in the following proposition.

Proposition 6.4. *Let the infinite matrices with entries* $m_{\nu\mu}$, $\tilde m_{\nu\mu}$, $\nu, \mu \in \nabla$*, be symmetric and such that*

$$\mathbf{E}^{(1)} := \bigl(2^{-|\nu|-|\mu|}(m_{\nu\mu} - \tilde m_{\nu\mu})\bigr)_{\nu,\mu\in\nabla}$$

---

[1] A result similar to (6.1) can be derived for higher-dimensional isotropic tensor product wavelet bases $\{\Psi_\nu\}_{\nu\in\nabla^{(d)}}$, where one instead obtains $s^* \le \frac{\tau-1}{d} - \frac{1}{2}$, see e.g. [33, 135]; since in our context it is necessary, as discussed in Section 6.1, to work with fully anisotropic tensor product bases $\{\Psi_\nu\}_{\nu\in\nabla^d}$, we will not need this latter result.

satisfies $\|\mathbf{E}^{(1)}\|_{\ell_2(\nabla)\to\ell_2(\nabla)} \leq \varepsilon$. *Then for any* $d \in \mathbb{N}$ *and*

$$\mathbf{E}^{(d)} := \Bigl(\Bigl(\sum_{i=1}^{d} 2^{2|\nu_i|}\Bigr)^{-\frac{1}{2}} \Bigl(\sum_{i=1}^{d} 2^{2|\mu_i|}\Bigr)^{-\frac{1}{2}} \sum_{i=1}^{d} (m_{\nu_i\mu_i} - \tilde{m}_{\nu_i\mu_i}) \prod_{j\neq i} \delta_{\nu_j\mu_j} \Bigr)_{\nu,\mu\in\nabla^d} ,$$

we also have $\|\mathbf{E}^{(d)}\| \leq \varepsilon$.

Proof. We follow the lines of [44, Theorem 3.5]. For each finitely supported vector $\mathbf{v}$ on ∇, by assumption,

$$-\varepsilon \sum_{\nu\in\nabla} 2^{2|\nu|}|v_\nu|^2 \leq \sum_{\nu,\mu\in\nabla} (m_{\nu\mu} - \tilde{m}_{\nu\mu}) v_\nu v_\mu \leq \varepsilon \sum_{\nu\in\nabla} 2^{2|\nu|}|v_\nu|^2 .$$

Applying this d times, for any finitely supported vector $\mathbf{w}$ on ∇^d we obtain

$$-\varepsilon \sum_{i=1}^{d} \sum_{\nu\in\nabla^d} 2^{2|\nu_i|}|w_\nu|^2 \leq \sum_{\nu,\mu\in\nabla^d} \Bigl(\sum_{i=1}^{d} (m_{\nu_i\mu_i} - \tilde{m}_{\nu_i\mu_i}) \prod_{j\neq i} \delta_{\nu_j\mu_j}\Bigr) w_\nu w_\mu \leq \varepsilon \sum_{i=1}^{d} \sum_{\nu\in\nabla^d} 2^{2|\nu_i|}|w_\nu|^2 ,$$

and thus the assertion. □

To arrive at compressibility of the Laplacian in an L_2–orthonormal[2] tensor product wavelet basis, we use Proposition 6.4 with $m_{\nu\mu} = \int \psi'_\nu \psi'_\mu \,\mathrm{d}x$, and $\tilde{m}_{\nu\mu}$ the corresponding entries of a compressed approximation as provided, e.g., by Proposition 6.1. The representation matrix of the associated compressed approximation of the higher-dimensional Laplacian is thus given by

$$\Bigl(\Bigl(\sum_{i=1}^{d} 2^{2|\nu_i|}\Bigr)^{-\frac{1}{2}} \Bigl(\sum_{i=1}^{d} 2^{2|\mu_i|}\Bigr)^{-\frac{1}{2}} \sum_{i=1}^{d} \tilde{m}_{\nu_i\mu_i} \prod_{j\neq i} \delta_{\nu_j\mu_j} \Bigr)_{\nu,\mu\in\nabla^d} .$$

As the Laplacian is given explicitly as a sum of tensor product operators, the results of this section can be applied directly in the framework of Chapter 5. In the following section, we consider approximations by sums of tensor product operators for the potential terms, which themselves do not have this structure.

6.3 Separable Approximation of Potentials

The approximations of potentials by sums of separable functions described in this section are useful for tensor product wavelet schemes in general, but are especially crucial for exploiting approximate low-rank structures of wave functions by the methods developed in Chapter 5.

Separable expansions for potential terms generated by exponential sum approximations have been used for a variety of related purposes, for instance, in [109, 25, 48] as part of an integration scheme for higher-dimensional integrals of potentials with wavelets, in [12, 79, 60] for the approximation of Green's functions, or as part of low-rank tensor methods for Hartree-Fock problems in [94].

The necessity of approximations of the type considered here for schemes based on low-rank structures has already been discussed in Section 5.1; however, they are also important for the practical feasibility of direct wavelet discretizations: The application of the full discretization matrices arising from the the potential terms, which in our case are of the form

$$\int_{\mathbb{R}^3} \frac{1}{|x|} \Psi_\mu \Psi_\nu \,\mathrm{d}x , \quad \int_{\mathbb{R}^6} \frac{1}{|x-y|} \Psi_\mu \Psi_\nu \,\mathrm{d}(x,y) , \quad \int_{\mathbb{R}^6} \frac{x-y}{|x-y|} \cdot (\mathrm{D}_x - \mathrm{D}_y) \Psi_\mu \, \Psi_\nu \,\mathrm{d}(x,y) , \qquad (6.3)$$

---

[2] Note that without orthonormality assumption, a similar result for the higher-dimensional Laplacian can be obtained from the more involved construction given in [115, Section 3.8].

is too expensive to be feasible numerically. A main reason is that the number of nonzero entries per column in these matrices basically scales with the third or sixth power, respectively, of the support size of the scaling functions, which is generally large for higher-order wavelets. Furthermore, the algorithms mentioned in Section 3.5 for efficiently applying matrices arising in sparse grid-type discretizations are based on separability properties of operators. Separable approximations enable the use of these schemes, which by successively operating along dimensions also yield a linear or quadratic scaling, respectively, with respect to the basis function support size.

With this aim of efficiently applying operators in a direct wavelet discretization, the approach we pursue here has also been taken in [154], and the estimates of this section can be regarded as an extension of the error estimates for the energy error given there. We additionally derive bounds for the eigenfunction error, obtain estimates for the nonsymmetric explicitly correlated two-electron term, and in particular obtain qualitatively improved estimates for the energy error by taking the H^2-regularity of wave functions into account. We also consider the interplay of separable approximations with wavelet discretization, where it turns out that for higher wavelet levels, coarser approximations of the potentials suffice. Our results in this section have previously been published in [3].

Note first that Theorem 4.15 yields an error estimate for the approximation of the Coulomb potential on $B_R(0) \setminus B_r(0) \subset \mathbb{R}^3$,

$$\sup_{\{x\in\mathbb{R}^3 :\, r\leq|x|\leq R\}} \left| \frac{1}{|x|} - p_{N,r,R}(x) \right| \leq r^{-1}\delta(N, r^{-2}R^2)\,, \quad p_{N,r,R}(x) := \sum_{k=1}^{N} \frac{\omega_k}{r} \exp\Bigl(-\frac{\alpha_k}{r^2}|x|^2\Bigr)\,, \tag{6.4}$$

with $\delta(N,S) = 8\sqrt{2}\exp(-(\pi^2 N)/(\ln 8S))$ as in (4.10). This provides a concrete construction for an approximation of the form (5.5). The following results rely solely on uniform approximation for $r \leq |x| \leq R$, and therefore a different type of separable approximation providing an error estimate of this type could be used just as well, for instance the approximation based on sinc quadrature as provided by Theorem 4.17; however, in practice the best approximation as in Theorem 4.15 turns out to be substantially more efficient.

In the following subsections, we always denote by φ the univariate scaling function from which the tensor product wavelet bases $\{\Psi_\nu\}_{\nu\in\nabla^3}$ and $\{\Psi_\nu\}_{\nu\in\nabla^6}$ are constructed. Recall also the notation $\mathbb{Z}_{j_0}$ introduced in (3.5). We shall make repeated use of the following sets of infinite matrices on $\mathbb{Z}^D_{j_0}$ for $D \in \mathbb{N}$,

$$\begin{aligned} W_D := \bigl\{\tau \in \mathbb{R}^{\mathbb{Z}^D_{j_0}\times\mathbb{Z}^D_{j_0}} :\ &\tau_{i,j} = \tau_{j,i} \text{ and } \tau_{i,j} > 0 \text{ for all } i,j \in \mathbb{Z}^D_{j_0}, \\ &\text{and } \sup_{i\in\mathbb{Z}^D_{j_0}} \sum_{j\in\mathbb{Z}^D_{j_0}} \tau_{i,j} < \infty \bigr\}\,. \end{aligned} \tag{6.5}$$

Arbitrary elements of these sets will serve as weighting factors in several estimates. To give a specific example, one has

$$\Bigl((1 + i_1^2 + \ldots + i_D^2)^{-\beta}(1 + j_1^2 + \ldots + j_D^2)^{-\beta}\Bigr)_{i,j\in\mathbb{Z}^D_{j_0}} \in W_D$$

for any $\beta > \frac{D}{2}$.

6.3.1 Approximation of One-Electron Potentials

We now estimate the error in operator norm caused by approximations of the type (6.4) when combined with a wavelet discretization.

Theorem 6.5. *Let* $0 < r < R$, $\varepsilon_0 > 0$, *and* $s \in \{1, 2\}$. *Let* $\varphi \in \mathrm{H}^\tau(\mathbb{R})$ *for a* $\tau > s$. *For each* $N \in \mathbb{N}$, *let* $p_N := p_{N,r,R}$. *Furthermore, let* $\Lambda \subset \nabla^3$ *such that* $\operatorname{supp}\Psi_\nu \subset B_R(0)$ *for all* $\nu \in \Lambda$; *let*

$\tau \in W_3$ and for $\alpha, \beta \in \mathbb{Z}^3_{j_0}$, let $N_{\alpha,\beta}$ be chosen such that

$$r^{-1}\delta(N_{\alpha,\beta}, r^{-2}R^2) \leq \Big(\sum_{k,l=1}^{3} 2^{2s(\alpha_k+\beta_l)}\Big)^{\frac{1}{2}} \tau_{\alpha,\beta}\, \varepsilon_0 \,. \tag{6.6}$$

Let $A_\Lambda, \tilde{A}_\Lambda \colon \mathrm{H}^s(\mathbb{R}^3) \to \mathrm{H}^{-s}(\mathbb{R}^3)$ be the operators defined by the matrices $(a_{\nu\mu})_{\nu,\mu\in\Lambda}$, $(\tilde{a}_{\nu\mu})_{\nu,\mu\in\Lambda}$ with

$$a_{\nu\mu} = \int_{\mathbb{R}^3} \frac{1}{|x|} \Psi_\mu\, \Psi_\nu \,\mathrm{d}x\,, \quad \tilde{a}_{\nu\mu} = \int_{\mathbb{R}^3} p_{N_{|\mu|,|\nu|}}\, \Psi_\mu\, \Psi_\nu \,\mathrm{d}x\,,$$

extended to $\mu, \nu \in \nabla^3 \setminus \Lambda$ by zero. Then there exist $C_s, C_{\psi,j_0,s,\tau} > 0$ independent of r, R, ε_0 and Λ such that for $s \in \{1,2\}$, we have

$$\big\| A_\Lambda - \tilde{A}_\Lambda \,\big|\, \mathrm{H}^s(\mathbb{R}^3) \to \mathrm{H}^{-s}(\mathbb{R}^3) \big\| \leq C_s\, r^s + C_{\psi,j_0,s,\tau}\, \varepsilon_0 \,. \tag{6.7}$$

The practical implication of the condition (6.6) is that the separable approximation need not be uniformly accurate, but can be coarser for combinations of wavelets on higher levels. The fact that one obtains faster decay of the approximation error as $r \to 0$ when measuring the error as an operator from H^2 to H^{-2} will be used in Subsection 6.3.3 to obtain improved estimates for eigenvalue approximations. The impact of the choice of r, mainly via the sizes of the exponents in the approximations $p_{N,r,R}$ as in (6.4), will become clearer in Sections 6.4 and 6.6.

The proof of Theorem 6.5 is based on several auxiliary results, some of which will also be used in the following subsection. To obtain the estimate (6.7), the error will be split into two components corresponding to the domains $B_r(0)$ and $B_R(0)\setminus B_r(0)$. The first part is dealt with by the following proposition; for the case $s = 1$, this was shown in [154].

Proposition 6.6. *Let either $s = 1$ or $s > \frac{3}{2}$. There exists a $C > 0$ such that for $r > 0$,*

$$\sup\Big\{ \int_{B_r(0)} \frac{1}{|x|} f(x)\, g(x) \,\mathrm{d}x : \ f, g \in \mathrm{H}^s(\mathbb{R}^3),\ \|f\|_s = \|g\|_s = 1 \Big\} \leq C r^{\eta_s}\,,$$

where $\eta_1 = 1$, and $\eta_s = 2$ for $s > \frac{3}{2}$.

Proof. For $s = 1$, we use the argument from [154]: using $r|x|^{-1} > 1$ on $B_r(0)$, for any $f, g \in \mathrm{H}^1(\mathbb{R}^3)$, we obtain

$$\Big| \int_{B_r(0)} \frac{1}{|x|} f(x)\, g(x) \,\mathrm{d}x \Big| \leq r \int_{B_r(0)} \frac{1}{|x|^2} |f(x)\, g(x)| \,\mathrm{d}x \leq r \| |x|^{-1} f \|_{\mathrm{L}_2(\mathbb{R}^3)} \| |x|^{-1} g \|_{\mathrm{L}_2(\mathbb{R}^3)}$$

and by Lemma 2.1, the latter can be estimated by

$$\leq C r \|f\|_1 \|g\|_1 \,.$$

In the case $s > \frac{3}{2}$, for any $f, g \in \mathrm{H}^s(\mathbb{R}^3)$, the claim follows by Hölder's inequality and continuity of the imbedding $\mathrm{H}^s(\mathbb{R}^3) \hookrightarrow \mathrm{L}_\infty(\mathbb{R}^3)$ according to the assumption on s (cf. [1, Theorem 7.34]). □

The following lemma will be used in estimating the error component corresponding to $B_R(0) \setminus B_r(0)$; for the formulation, recall the definition of χ_d in (3.19). The proof is an adaptation of standard arguments, cf. [29, Section 4.6]

Lemma 6.7. *Let $d, D \in \mathbb{N}$ and $s > 0$, and let $\varphi \in \mathrm{H}^\tau(\mathbb{R})$ for a $\tau > s$. Let $M \colon \mathrm{H}^s(\mathbb{R}^{dD}) \to \mathrm{H}^{-s}(\mathbb{R}^{dD})$ be a local operator, and $m_{\nu\mu} = \langle M\Psi_\mu, \Psi_\nu \rangle$ for $\mu, \nu \in (\nabla^{(d)})^D$. If for $\tau = (\tau_{i,j})_{i,j\in\mathbb{Z}^D_{j_0}} \in$*

W_D and $\varepsilon_0 > 0$,

$$|m_{\nu\mu}| \lesssim \varepsilon_0 \Big(\sum_{i=1}^{D} 2^{2s|\nu_i|} \sum_{j=1}^{D} 2^{2s|\mu_j|}\Big)^{\frac{1}{2}} 2^{-\frac{d}{2}\sum_i ||\mu_i|-|\nu_i||} \tau_{|\nu|,|\mu|} \prod_{k=1}^{D} \chi_d(\mu_k,\nu_k)\,,$$

then the estimate $\|M \,|\, \mathrm{H}^s(\mathbb{R}^{dD}) \to \mathrm{H}^{-s}(\mathbb{R}^{dD})\| \lesssim \varepsilon_0$ holds, with constant depending only on d, D, s, τ, and the wavelet basis.

Recall that for $M\colon \mathrm{H}^s(\mathbb{R}^{dD}) \to \mathrm{H}^{-s}(\mathbb{R}^{dD})$, under the assumptions of Lemma 6.7, by Remark 3.16 we have

$$\|M \,|\, \mathrm{H}^s \to \mathrm{H}^{-s}\| \sim \left\| \bigg(\Big(\sum_{i=1}^{D} 2^{2s|\mu_i|}\Big)^{-\frac{1}{2}} \Big(\sum_{i=1}^{D} 2^{2s|\nu_i|}\Big)^{-\frac{1}{2}} \langle M\Psi_\mu, \Psi_\nu\rangle \bigg)_{\mu,\nu} \right\|_{\ell^2((\nabla^{(d)})^D) \to \ell^2((\nabla^{(d)})^D)} . \tag{6.8}$$

With (6.8), the proof of Lemma 6.7 can be reduced to the following lemma, which will also play a prominent role in the remainder of this chapter.

Lemma 6.8 (Schur's Lemma, e.g. [111])**.** *Let $M = (m_{ij})_{i,j\in\mathbb{N}}$ be an infinite matrix and let $\omega_i > 0, i \in \mathbb{N}$. Suppose that*

$$\sum_j |m_{ij}|\,\omega_j \le c\,\omega_i\,, \quad \sum_i |m_{ij}|\,\omega_i \le \tilde{c}\,\omega_j\,,$$

then $M\colon \ell^2 \to \ell^2$ is bounded with $\|M\| \le \sqrt{c\,\tilde{c}}$.

Proof. Let $x \in \ell^2$, then

$$\begin{aligned}\sum_i \Big|\sum_j m_{ij}x_j\Big|^2 &\le \sum_i \Big(\sum_j |m_{ij}|\omega_j\Big)\Big(\sum_j |m_{ij}|\omega_j^{-1}|x_j|^2\Big) \\ &\le c\sum_i \omega_i \sum_j |m_{ij}|\omega_j^{-1}|x_j|^2 = c\sum_j \omega_j^{-1}|x_j|^2 \sum_i |m_{ij}|\omega_i\,,\end{aligned}$$

and the right hand side can be estimated by $c\tilde{c}\|x\|^2$, which yields the assertion. ☐

Proof of Lemma 6.7. Let $s_j := \big(\sum_i 2^{2sj_i}\big)^{-1/2}$ for $j \in \mathbb{Z}^D$. For suitable positive weight sequences $\{\omega_\nu\}$,

$$\omega_\nu^{-1} \sum_{\mu\in(\nabla^{(d)})^D} \omega_\mu |m_{\nu\mu}| s_{|\mu|} s_{|\nu|} \lesssim \varepsilon_0\, \omega_\nu^{-1} \sum_{\mu\in(\nabla^{(d)})^D} \omega_\mu 2^{-\frac{d}{2}\sum_i ||\mu_i|-|\nu_i||} \tau_{|\nu|,|\mu|} \prod_{k=1}^{D} \chi_d(\mu_k,\nu_k)\,. \tag{6.9}$$

With the choice $\omega_\nu = 2^{-\frac{d}{2}\sum_i |\nu_i|}$, the right hand side of (6.9) can be rewritten as

$$\varepsilon_0\, 2^{\frac{d}{2}\sum_i |\nu_i|} \sum_{j\in\mathbb{Z}^D_{j_0}} \tau_{|\nu|,j} \prod_{k=1}^{D} 2^{-\frac{d}{2}j_k} \sum_{|\mu_k|=j_k} 2^{-\frac{d}{2}|j_k-|\nu_k||}\chi_d(\mu_k,\nu_k)\,.$$

Using the estimate $\sum_{|\mu_k|=j_k} 2^{-\frac{d}{2}|j_k-|\nu_k||}\chi_d(\mu_k,\nu_k) \lesssim 2^{-\frac{d}{2}(|\nu_k|-j_k)}$, we obtain

$$\omega_\nu^{-1} \sum_{\mu\in(\nabla^{(d)})^D} \omega_\mu |m_{\nu\mu}| s_{|\mu|} s_{|\nu|} \lesssim \varepsilon_0 \sum_{j\in\mathbb{Z}^D_{j_0}} \tau_{|\nu|,j} \le C_\tau\, \varepsilon_0\,,$$

which with (6.8) implies the assertion. ☐

Proof of Theorem 6.5. Let $X := \mathrm{H}^s(\mathbb{R}^3)$ and denote by X_Λ the closure of $\operatorname{span}\{\Psi_\nu\}_{\nu\in\Lambda}$ in X. For $u \in X_\Lambda$, in what follows u_ν denotes the corresponding coefficients of the wavelet expansion of u.

The operator norm $\|A_\Lambda - \tilde{A}_\Lambda \,|\, \mathrm{H}^s(\mathbb{R}^3) \to \mathrm{H}^{-s}(\mathbb{R}^3)\|$ can be estimated by

$$\sup_{\substack{u,v\in X_\Lambda\\ \|u\|_X=\|v\|_X=1}} \langle (A_\Lambda - \tilde{A}_\Lambda)u, v\rangle \leq \sup_{\substack{u,v\in X\\ \|u\|_X=\|v\|_X=1}} \int_{B_r(0)} \frac{1}{|x|}\, u\, v\, dx$$

$$+ \sup_{\substack{u,v\in X_\Lambda\\ \|u\|_X=\|v\|_X=1}} r^{-1}\delta(N_{|\mu|,|\nu|}, r^{-2}R^2) \Big(\int_{\mathbb{R}^3\setminus B_r(0)} |\Psi_\nu \Psi_\mu| \,\mathrm{d}x \Big) u_\mu\, v_\nu \,.$$

For the first term on the right hand side, we can apply Proposition 6.6. Note that since φ and ψ are uniformly bounded by our regularity assumptions,

$$\int_{\mathbb{R}^3} |\Psi_\mu \Psi_\nu| \,\mathrm{d}x \lesssim 2^{-\frac{1}{2}\sum_i ||\mu_i|-|\nu_i||} \prod_{i=1}^{3} \chi_1(\mu_i,\nu_i)\,,$$

and with (6.6), we obtain for the second term

$$r^{-1}\delta(N_{|\mu|,|\nu|}, r^{-2}R^2) \int_{\mathbb{R}^3\setminus B_r(0)} |\Psi_\nu \Psi_\mu| \,\mathrm{d}x$$

$$\leq \varepsilon_0 \Big(\sum_{i,j=1}^{3} 2^{2s(|\mu_i|+|\nu_j|)} \Big)^{\frac{1}{2}} \tau_{|\mu|,|\nu|}\, 2^{-\frac{1}{2}\sum_i ||\mu_i|-|\nu_i||} \prod_{i=1}^{3} \chi_1(\mu_i,\nu_i)\,.$$

Hence Lemma 6.7 gives the assertion. □

A similar statement also holds for the isotropic three-dimensional wavelets corresponding to $\nabla^{(3)}$, where we can apply Lemma 6.7 with a different combination of parameters.

The estimate (6.7) can be transferred to the three-dimensional Coulomb potential acting on higher-dimensional functions, since, e.g., $\mathrm{H}^s(\mathbb{R}^{3+n}) \subset \mathrm{H}^s(\mathbb{R}^3) \otimes \mathrm{L}_2(\mathbb{R}^n)$ for any n by Lemma 3.15.

6.3.2 Approximation of Two-Electron Operators

We now use the same strategy as in the previous subsection for both the two-electron Coulomb potential, and the two-electron term in the explicitly correlated formulation. For the following, let $S_\rho := \{x, y \in \mathbb{R}^3 \colon\ |x-y| < \rho\}$ for $\rho > 0$.

Theorem 6.9. *Let $0 < r < R$, $\varepsilon_0 > 0$, and $s \in \{1,2\}$. Let $\varphi \in \mathrm{H}^\tau(\mathbb{R})$ for a $\tau > s$. For each $N \in \mathbb{N}$, let $p_N := p_{N,r,R}$. Furthermore, let $\Lambda \subset \nabla^6$ such that $\operatorname{supp}\Psi_\nu \subset S_R$ for all $\nu \in \Lambda$; let $\tau \in W_6$ and for $\alpha, \beta \in \mathbb{Z}^6_{j_0}$, let $N_{\alpha,\beta}$ be chosen such that*

$$r^{-1}\delta(N_{\alpha,\beta}, r^{-2}R^2) \leq \Big(\sum_{k,l=1}^{6} 2^{2s(\alpha_k+\beta_l)} \Big)^{\frac{1}{2}} \tau_{\alpha,\beta}\, \varepsilon_0\,. \tag{6.10}$$

Let $A_\Lambda, \tilde{A}_\Lambda \colon \mathrm{H}^s(\mathbb{R}^6) \to \mathrm{H}^{-s}(\mathbb{R}^6)$ be the operators defined by the matrices $(a_{\nu\mu})_{\nu,\mu\in\Lambda}$, $(\tilde{a}_{\nu\mu})_{\nu,\mu\in\Lambda}$ with

$$a_{\nu\mu} = \int_{\mathbb{R}^6} \frac{1}{|x-y|} \Psi_\mu \Psi_\nu \,\mathrm{d}(x,y)\,, \quad \tilde{a}_{\nu\mu} = \int_{\mathbb{R}^6} p_{N_{|\mu|,|\nu|}}(x-y)\, \Psi_\mu \Psi_\nu \,\mathrm{d}(x,y)\,,$$

extended to $\mu, \nu \in \nabla^6 \setminus \Lambda$ by zero. Then there exist $C_s, C_{\psi,j_0,s,\tau} > 0$ independent of r, R, ε_0 and Λ such that for $s \in \{1,2\}$, we have

$$\|A_\Lambda - \tilde{A}_\Lambda \,|\, \mathrm{H}^s(\mathbb{R}^6) \to \mathrm{H}^{-s}(\mathbb{R}^6)\| \leq C_s\, r^s + C_{\psi,j_0,s,\tau}\, \varepsilon_0\,. \tag{6.11}$$

Similarly to the previous subsection, the following proposition is used to estimate the error on the domain S_ρ.

Proposition 6.10. *Let either $s = 1$ or $s > \frac{3}{2}$. Then there exists $C > 0$ such that for $r > 0$,*

$$\sup\biggl\{ \int_{|x-y|<r} \frac{1}{|x-y|} f\, g \,\mathrm{d}(x,y) :\ f,g \in \mathrm{H}^s(\mathbb{R}^6),\ \|f\|_s = \|g\|_s = 1 \biggr\} \leq C r^{\eta_s} ,$$

where $\eta_1 = 1$, and $\eta_s = 2$ for $s > \frac{3}{2}$.

Proof. Applying a coordinate rotation, we find that it suffices to estimate the supremum over

$$\sup\biggl\{ \int_{B_r(0)\times\mathbb{R}^3} \frac{1}{|x|} f\, g \,\mathrm{d}(x,y) \colon\ f,g \in \mathrm{H}^s(\mathbb{R}^6)\,,\ \|f\|_s = \|g\|_s = 1 \biggr\} . \tag{6.12}$$

Lemma 3.15 yields $\mathrm{H}^s(\mathbb{R}^6) \subset \mathrm{H}^s(\mathbb{R}^3) \otimes \mathrm{L}_2(\mathbb{R}^3)$, and since the bilinear form in (6.12) has the corresponding tensor product structure as well, with Theorem 3.12 the statement follows from the three-dimensional result in Proposition 6.6. ☐

Proof of Theorem 6.9. We follow the lines of the proof of Theorem 6.5, combining Proposition 6.10 with Lemma 6.7. ☐

For the modified potential $|x-y|^{-1}(x-y)\cdot(\mathrm{D}_x - \mathrm{D}_y)$, we additionally obtain from (4.10) the exponential sum approximation

$$\sup_{\{x\in\mathbb{R}^3\colon\, r\leq|x|\leq R\}} \biggl| \frac{x}{|x|} - x \sum_{k=1}^{N} \frac{\omega_k}{r} \exp\Bigl(-\frac{\alpha_k}{r^2}|x|^2\Bigr) \biggr|_{\ell^2} \leq r^{-1} R\, \delta(N, r^{-2}R^2) . \tag{6.13}$$

Theorem 6.11. *Let $0 < r < R$, $\varepsilon_0 > 0$, and $s \in \{1,2\}$. Let $\varphi \in \mathrm{H}^\tau(\mathbb{R})$ for a $\tau > s$. For each $N \in \mathbb{N}$, let $p_N := p_{N,r,R}$. Furthermore, $\Lambda \subset \nabla^6$ such that* $\operatorname{supp}\Psi_\nu \subset S_R$ *for all $\nu \in \Lambda$; let $\tau \in W_6$ and for $\alpha,\beta \in \mathbb{Z}^6_{j_0}$, let $N_{\alpha,\beta}$ be chosen such that*

$$r^{-1} R\, \delta(N_{\alpha,\beta}, r^{-2}R^2) \leq \Bigl(\sum_{k=1}^{6} 2^{2\alpha_k}\Bigr)^{-\frac{1}{2}} \Bigl(\sum_{k,l=1}^{6} 2^{2s(\alpha_k+\beta_l)}\Bigr)^{\frac{1}{2}} \tau_{\alpha,\beta}\, \varepsilon_0 . \tag{6.14}$$

Let $A_\Lambda, \tilde{A}_\Lambda \colon \mathrm{H}^s(\mathbb{R}^6) \to \mathrm{H}^{-s}(\mathbb{R}^6)$ be the operators defined by the matrices $(a_{\nu\mu})_{\nu,\mu\in\Lambda}$, $(\tilde{a}_{\nu\mu})_{\nu,\mu\in\Lambda}$ with

$$\begin{aligned} a_{\nu\mu} &= \int_{\mathbb{R}^6} \frac{x-y}{|x-y|} \cdot \bigl(\mathrm{D}_x - \mathrm{D}_y\bigr)\Psi_\mu\ \Psi_\nu \,\mathrm{d}(x,y)\,, \\ \tilde{a}_{\nu\mu} &= \int_{\mathbb{R}^6} \bigl[(x-y)\, p_{N_{|\mu|,|\nu|}}(x-y)\bigr] \cdot \bigl(\mathrm{D}_x - \mathrm{D}_y\bigr)\Psi_\mu\ \Psi_\nu \,\mathrm{d}(x,y)\,, \end{aligned}$$

extended to $\mu,\nu \in \nabla^6 \setminus \Lambda$ by zero. Then there exist $C_s, C_{\psi,j_0,s,\tau} > 0$ independent of r, R, ε_0 and Λ such that for $s \in \{1,2\}$, we have

$$\bigl\| A_\Lambda - \tilde{A}_\Lambda \,\big|\, \mathrm{H}^s(\mathbb{R}^6) \to \mathrm{H}^{-s}(\mathbb{R}^6) \bigr\| \leq C_s\, r^{\eta_s} + C_{\psi,j_0,s,\tau}\, \varepsilon_0 . \tag{6.15}$$

where $\eta_1 = 1$, and $\eta_2 = \frac{5}{2}$.

Note the slight difference in powers of r between (6.11) and (6.15), which is related to the following proposition.

Proposition 6.12. *Let either* $s = 1$ *or* $s = 2$*, then there exists* $C > 0$ *such that for* $r > 0$,

$$\sup\biggl\{ \int_{|x-y|<r} \frac{x-y}{|x-y|} \cdot (\mathrm{D}_x - \mathrm{D}_y) f \, g \, \mathrm{d}(x,y) : \; f,g \in \mathrm{H}^s(\mathbb{R}^6), \; \|f\|_s = \|g\|_s = 1 \biggr\} \leq C r^{\eta_s} ,$$

where $\eta_1 = 1$*,* $\eta_2 = \frac{5}{2}$*.*

Proof. We use a rotation of coordinates and $\mathrm{H}^s(\mathbb{R}^6) \subset \mathrm{H}^s(\mathbb{R}^3) \otimes \mathrm{L}_2(\mathbb{R}^3)$ as in Proposition 6.10. In the case $s = 1$, it thus suffices to estimate, for $f, g \in \mathrm{H}^1(\mathbb{R}^3)$,

$$\int_{B_r(0)} \frac{x}{|x|} \cdot \mathrm{D}_x f \, g \, \mathrm{d}x \leq \bigl\| |x|^{-1} |x| \bigr\|_{\mathrm{L}_3(B_r(0))} \|f\|_{\mathrm{H}^1(\mathbb{R}^3)} \|g\|_{\mathrm{L}_6(\mathbb{R}^3)} \lesssim \biggl(\int_0^r s^2 \, ds \biggr)^{1/3} \|f\|_{\mathrm{H}^1(\mathbb{R}^3)} \|g\|_{\mathrm{H}^1(\mathbb{R}^3)} ,$$

where we have used the imbedding $\mathrm{H}^1(\mathbb{R}^3) \hookrightarrow \mathrm{L}_6(\mathbb{R}^3)$. In the case $s = 2$, for $f, g \in \mathrm{H}^2(\mathbb{R}^3)$,

$$\begin{aligned} \int_{B_r(0)} \frac{x}{|x|} \cdot \mathrm{D}_x f \, g \, \mathrm{d}x &\lesssim \bigl\| |x|^{-1} |x| \bigr\|_{\mathrm{L}_{6/5}(B_r(0))} \bigl\| |\mathrm{D}_x f| \bigr\|_{\mathrm{L}_6(\mathbb{R}^3)} \|g\|_{\mathrm{H}^2(\mathbb{R}^3)} \\ &\lesssim \biggl(\int_0^r s^2 \, ds \biggr)^{5/6} \|f\|_{\mathrm{H}^2(\mathbb{R}^3)} \|g\|_{\mathrm{H}^2(\mathbb{R}^3)} , \end{aligned}$$

where we have used the imbedding $\mathrm{H}^2(\mathbb{R}^3) \hookrightarrow \mathrm{L}_\infty(\mathbb{R}^3)$, Hölder's inequality, and the imbedding $\mathrm{H}^1(\mathbb{R}^3) \hookrightarrow \mathrm{L}_6(\mathbb{R}^3)$. ☐

Proof of Theorem 6.11. Following the lines of the proof of Theorem 6.5, combining Proposition 6.12 with Lemma 6.7. ☐

Remark 6.13. *Theorems 6.5, 6.9, and 6.11 are formulated for the particular type of error estimate provided by Theorem 4.15, which is of most practical relevance. The same proofs, however, yield an analogous result for exponential sum approximations on infinite intervals* $[r, \infty)$*, as provided by Theorem 4.17.*

Remark 6.14. *In principle, the above constructions can be adapted to bounded correlation factors with suitable structure. For instance, let* κ *be a univariate function that is sufficiently smooth and even, such that* $\kappa > 0$*,* $\kappa(0) = 1$*, and* $\kappa(r) \lesssim r^{-1}$ *for* $r \to \infty$*. Replacing the correlation factor* $\exp(-\frac{1}{2}|x-y|)$ *by* $\exp(-\frac{1}{2}K(x-y)|x-y|)$*, where* $K(x) = \prod_{i=1}^3 \kappa(x_i)$ *for* $x \in \mathbb{R}^3$*, the resulting modified Hamiltonian for helium takes the form*

$$\begin{aligned} &-\frac{1}{2}\Delta - \frac{2}{|x|} - \frac{2}{|y|} + \frac{1-K}{|x-y|} - (\mathrm{D}K) \cdot \frac{x-y}{|x-y|} - \frac{1}{2}|x-y| \Delta K \\ &- \frac{1}{2}\Bigl(K \frac{x-y}{|x-y|} + (\mathrm{D}K)|x-y| \Bigr) \cdot (\mathrm{D}_x - \mathrm{D}_y) - \frac{1}{4}\bigl(|K|^2 + |\mathrm{D}K|^2 |x-y|^2 \bigr) - \frac{1}{2} K (\mathrm{D}K) \cdot (x-y) . \end{aligned}$$

Here we have used the abbreviations $K = K(x-y)$*,* $\mathrm{D}K = (\mathrm{D}K)(x-y)$*,* $\Delta K = (\Delta K)(x-y)$*. As* K *is assumed to be separable – one may, for instance, choose* $\kappa(r) = e^{-\gamma r^2}$ *for some* $\gamma > 0$ *– what is required to treat this case in addition to what we have considered here is a suitable separable approximation for* $|x-y|$*.*

Since the focus of this work is on the two-electron case, we do not treat the three-electron terms arising in the explicitly correlated formulation for more than two electrons; although one could in principle proceed along similar lines, the question of how to best construct such approximations is connected to a number of further difficulties that appear in the case of several electrons.

6.3.3 Complexity and Eigenpair Error Estimates

Concerning the asymptotics of the number of summands in the exponential sums required for a certain error in operator norm, note that for a total error $\varepsilon > 0$ in the estimates (6.7), (6.11) and

(6.15), which are all of the form

$$\|A_\Lambda - \tilde{A}_\Lambda\| \lesssim r^\eta + \varepsilon_0\,,$$

we need to choose $r \sim \varepsilon^{\eta^{-1}}$, and subsequently N such that $\delta(N, \varepsilon^{-2\eta^{-1}} R^2) \lesssim \varepsilon^{1+\eta^{-1}}$. By Theorem 4.15, this leads to

$$N = \mathcal{O}\big(\ln(\varepsilon^{-2\eta^{-1}} R^2) \ln \varepsilon^{-2}\big) = \mathcal{O}\big(|\ln \varepsilon|^2 + \ln R\, |\ln \varepsilon|\big)\,.$$

In view of the exponential decay of solutions of the electronic Schrödinger equation, one typically also has $\ln R \sim |\ln \varepsilon|$.

We now give some general estimates concerning the effects of perturbations in the potentials on the solutions of the Galerkin discretizations of the eigenvalue problems, and subsequently apply these to the separable approximations we have constructed; to avoid technicalities, we restrict ourselves to the case of main interest in our context, the approximation of the ground state, which we assume to correspond to a simple eigenvalue. Note that in the case of the modified problem involving the nonsymmetric potential term arising in (4.3), although the exact eigenvalues of interest are unchanged by the discussion in Section 2.2, it cannot necessarily be guaranteed that the eigenvalues remain real for the perturbed potentials. Thus we need to work on spaces of complex-valued functions at this point.

Let $d \in \mathbb{N}$, let $V \subset \mathrm{H}^1(\mathbb{R}^d, \mathbb{C})$ be a closed subspace, and let the real linear operators $A, A_n \colon V \to V'$ be bounded and invertible. Let $\lambda_0 \in \mathbb{C}$ be an isolated simple eigenvalue with eigenfunction u_0 of A and let $\|A - A_n\| \leq \varepsilon_n \to 0$. Recall that $\langle \cdot, \cdot \rangle$ denotes the duality product induced by the inner product on $\mathrm{L}_2(\mathbb{R}^d, \mathbb{C})$, and $\|\cdot\|$ denotes the norm on $\mathrm{H}^1(\mathbb{R}^d, \mathbb{C})$.

We define the operators $T, T_n \colon V \to V$ by

$$\langle ATu, v\rangle = \langle u, v\rangle_{\mathrm{L}_2}\,, \quad \langle A_n T_n u, v\rangle = \langle u, v\rangle_{\mathrm{L}_2} \qquad \text{for all } u, v \in V.$$

Note that in terms of the mapping $R \colon V \subset \mathrm{L}_2 \to (\mathrm{L}_2)' \subset V'$, $u \mapsto Ru = \langle u, \cdot\rangle_{\mathrm{L}_2}$, we have $T = A^{-1}R$ and $T_n = A_n^{-1} R$. With these definitions, $\mu_0 := \lambda_0^{-1}$ is isolated simple eigenvalue of T, and we can choose a $\delta > 0$ such that $\{|z - \mu_0| \leq \delta\} \cap (\sigma(T) \setminus \{\mu_0\}) = \emptyset$; for this δ, let $\Gamma := \{z \in \mathbb{C} \colon |z - \mu_0| = \delta\}$.

Theorem 6.15. *For sufficiently large n, there exist isolated simple eigenvalues $\mu_{0,n}$ of T_n with corresponding eigenfunctions $u_{0,n}$, as well as $C_1, C_2 > 0$, such that*

$$|\mu_0 - \mu_{0,n}| \leq C_1 \varepsilon_n\,, \quad \|u_0 - u_{0,n}\| \leq C_2 \varepsilon_n\,.$$

Proof. Let $M_\Gamma = \max_{z\in\Gamma} \|(T - z)^{-1}\|$. Without restriction of generality, we can assume $\varepsilon_n M_\Gamma \leq \frac{1}{2}$, which implies $\|(T_n - z)^{-1}\| \leq 2\|(T - z)^{-1}\| \leq 2M_\Gamma$ for all $z \in \Gamma$ and all n, see e.g. [89, IV, Theorem 1.16]. Thus in particular $\Gamma \subset \rho(T_n)$ for all n. We can therefore define the spectral projections

$$P = -\frac{1}{2\pi i} \int_\Gamma (T - \zeta)^{-1}\, d\zeta\,, \quad P_n = -\frac{1}{2\pi i} \int_\Gamma (T_n - \zeta)^{-1}\, d\zeta$$

and obtain for $u \in \mathrm{H}^1(\mathbb{R}^d, \mathbb{C})$, following the lines of [22, Proposition 5.3],

$$\|(P - P_n)u\| = \frac{1}{2\pi} \left\| \int_\Gamma (T_n - \zeta)^{-1} (T_n - T)(T - \zeta)^{-1} u \,\mathrm{d}\zeta \right\| \leq 2\delta M_\Gamma^2\, \varepsilon_n \|u\|\,,$$

and hence $\|P - P_n\| \to 0$.

From $\|P - P_n\| < 1$ it follows that $\dim \operatorname{range} P = \dim \operatorname{range} \tilde{P}_n = 1$, see [22, p. 87]. Consequently, by [89, p. 182], for large enough n, T_n has an isolated simple eigenvalue $\mu_{0,n}$ inside Γ with corresponding eigenfunction $u_{0,n}$, normalized as u_0, such that for an n-independent $C_2 > 0$, $\|u_0 - u_{0,n}\| \leq C_2 \varepsilon_n$. The identity

$$T(u_0 - u_{0,n}) + (T - T_n) u_{0,n} = \mu_0 (u_0 - u_{0,n}) + (\mu_0 - \mu_{0,n}) u_{0,n}$$

now yields $|\mu_0 - \mu_{0,n}| \leq C_1\varepsilon_n$ for a $C_1 > 0$. $\square$

Remark 6.16. *Theorem 6.15 applies also to the adjoints* T^*, T_n^*, *i.e., if* u_0^* *is the adjoint eigenfunction for* $\mu_0 = \lambda_0^{-1}$, *we obtain* $u_{0,n}^*$ *with* $\|u_0^* - u_{0,n}^*\| \leq C_2\varepsilon_n$ *as well.*

Note furthermore that if $\varepsilon_n \leq (2C_1|\lambda_0|)^{-1}$, *the estimate* $|\mu_0 - \mu_{0,n}| \leq C_1\varepsilon_n$ *implies* $|\lambda_{0,n}| \leq 2|\lambda_0|$ *and hence* $|\lambda_0 - \lambda_{0,n}| \leq 2C_1|\lambda_0|^2\varepsilon_n$.

We now apply Theorem 6.15 to the approximations from Theorems 6.5, 6.9, and 6.11, where a potential operator A_Λ is approximated by a family of separable substitutes $\tilde{A}_\Lambda$ with error in operator norm dependent on the two parameters r, ε_0, with the latter tied to the rank of the separable expansions by (6.6), (6.10), or (6.14), respectively. Thus the Hamiltonians formed with the respective A_Λ need to be invertible, which can be ensured by adding appropriate shifts, and the eigenvalues of interest need to be isolated and simple. Then Theorem 6.15 yields

$$|\lambda_0 - \tilde{\lambda}_0| \lesssim r + \varepsilon_0\,, \quad \|u_0 - \tilde{u}_0\|_{\mathrm{H}^1} \lesssim r + \varepsilon_0\,, \quad \|u_0^* - \tilde{u}_0^*\|_{\mathrm{H}^1} \lesssim r + \varepsilon_0\,,$$

where u_0, u_0^* can be direct and adjoint eigenfunctions of discretizations of the electronic Schrödinger Hamiltonian, where $u_0 = u_0^*$, or of the explicitly correlated formulation (4.3) according to the considered A_Λ, and $\tilde{u}_0$, $\tilde{u}_0^*$ those obtained with approximate potentials. An estimate of the same order in r, ε_0 for $|\lambda_0 - \tilde{\lambda}_0|$ based on Rayleigh quotient estimates that applies to the self-adjoint electronic Schrödinger Hamiltonian has also been given in [154].

We can additionally obtain an estimate for $|\lambda_0 - \tilde{\lambda}_0|$ that is quadratic instead of linear in r, provided that the approximate wave functions under consideration are H^2-regular. The connection of the corresponding operator norm estimates of Theorems 6.5, 6.9, and 6.11 to the eigenvalue error is provided by the following result.

Proposition 6.17. *Let* $A, \tilde{A} \colon \mathrm{H}^1(\mathbb{R}^d, \mathbb{C}) \to \mathrm{H}^{-1}(\mathbb{R}^d, \mathbb{C})$ *be bounded with*

$$\big\|A - \tilde{A} \mid \mathrm{H}^2(\mathbb{R}^d, \mathbb{C}) \to \mathrm{H}^{-2}(\mathbb{R}^d, \mathbb{C})\big\| \leq \varepsilon\,.$$

Moreover, let $u, \tilde{u}_0, u_0^*, \tilde{u}_0^* \in \mathrm{H}^2(\mathbb{R}^d, \mathbb{C})$ *and* $\lambda_0, \tilde{\lambda}_0 \in \mathbb{C}$ *with* $Au_0 = \lambda_0 u_0$, $\tilde{A}\tilde{u}_0 = \tilde{\lambda}_0\tilde{u}_0$, $A^*u_0^* = \overline{\lambda_0}u_0^*$, $\tilde{A}^*\tilde{u}_0^* = \overline{\tilde{\lambda}_0}\tilde{u}_0^*$, *with the normalizations* $\langle u_0, u_0^*\rangle = \langle \tilde{u}_0, \tilde{u}_0^*\rangle = 1$. *Then*

$$|\lambda_0 - \tilde{\lambda}_0| \lesssim \|u_0 - \tilde{u}_0\|\,\|u_0^* - \tilde{u}_0^*\| + \varepsilon\,\|\tilde{u}_0\|_{\mathrm{H}^2(\mathbb{R}^d,\mathbb{C})}\,\|\tilde{u}_0^*\|_{\mathrm{H}^2(\mathbb{R}^d,\mathbb{C})}\,. \tag{6.16}$$

Proof. We have

$$\begin{aligned}\langle A(u_0 - \tilde{u}_0), u_0^* - \tilde{u}_0^*\rangle &= \langle Au_0, u_0^*\rangle + \langle A\tilde{u}_0, \tilde{u}_0^*\rangle - \langle Au_0, \tilde{u}_0^*\rangle - \langle A\tilde{u}_0, u_0^*\rangle \\ &= \lambda_0 + \tilde{\lambda}_0 + \langle (A - \tilde{A})\tilde{u}_0, \tilde{u}_0^*\rangle - \lambda_0(\langle u_0, \tilde{u}_0^*\rangle + \langle \tilde{u}_0, u_0^*\rangle) \\ &= -\lambda_0 + \tilde{\lambda}_0 + \langle (A - \tilde{A})\tilde{u}_0, \tilde{u}_0^*\rangle + \lambda_0\langle u_0 - \tilde{u}_0, u_0^* - \tilde{u}_0^*\rangle\,,\end{aligned}$$

and therefore $|\lambda_0 - \tilde{\lambda}_0| \leq \|A - \lambda_0\mathrm{I}\|\,\|u_0 - \tilde{u}_0\|\,\|u_0^* - \tilde{u}_0^*\| + \varepsilon\,\|\tilde{u}_0\|_{\mathrm{H}^2(\mathbb{R}^d,\mathbb{C})}\,\|\tilde{u}_0^*\|_{\mathrm{H}^2(\mathbb{R}^d,\mathbb{C})}$. $\square$

Remark 6.18. *For self-adjoint operators, it suffices to consider real-valued function spaces and real eigenvalues. With the additional assumption that* λ_0, $\tilde{\lambda}_0$ *are the lowest eigenvalues, and if* $u_0, \tilde{u}_0 \in \mathrm{H}^2$, *the characterization by the Rayleigh quotient yields* $|\lambda_0 - \tilde{\lambda}_0| \leq \varepsilon \max\{\|u_0\|^2_{\mathrm{H}^2(\mathbb{R}^d)}, \|\tilde{u}_0\|^2_{\mathrm{H}^2(\mathbb{R}^d)}\}$ *in place of* (6.16).

In order to additionally employ Proposition 6.17, we assume the underlying univariate wavelet basis to be H^τ-regular with $\tau > 2$, which by H^2-regularity of the exact solutions implies in particular that $u_0, u_0^* \in \mathrm{H}^2$. If it can additionally be ensured that also for the solutions with approximate potentials, $\|\tilde{u}_0\|_{\mathrm{H}^2}, \|\tilde{u}_0^*\|_{\mathrm{H}^2} \leq C$ with some $C > 0$ uniformly for all considered $\tilde{A}_\Lambda$, then (6.16) and Theorems 6.5, 6.9, and 6.11 yield

$$|\lambda_0 - \tilde{\lambda}_0| \lesssim (r + \varepsilon_0)^2 + r^2 + \varepsilon_0\,.$$

In the symmetric case, if λ_0, $\tilde\lambda_0$ are the lowest eigenvalues, by Remark 6.18 we have $|\lambda_0 - \tilde\lambda_0| \lesssim r^2 + \varepsilon_0$.

In other words, provided that one has H^2-regularity of the approximate solutions, and if one chooses $\varepsilon_0 \sim r^2$, the error in energy induced by the separable approximations is not just of order $\mathcal{O}(r)$ as provided by Theorem 6.15, but of order $\mathcal{O}(r^2)$. On the one hand, in view of the estimates (6.4), (6.13), this yields a quantitative improvement in the ranks of the separable approximations required for a certain error in energy. On the other hand, a larger choice of r leads to lower exponents in the corresponding exponential sum approximations, which will turn out to be very beneficial in the context of the schemes for operator compression and matrix element computation considered in the following two sections.

Example 6.19. As an example, we consider a Galerkin discretization for the hydrogen model problem. In this case, we use least asymmetric Daubechies wavelets of approximation order 6. The basis comprises functions on levels $j = 0, \dots, 7$ with a total of 241,844 unknowns. In a computation with the exact potential term, on the basis of the wavelet coefficient estimates in [50] we can expect an H^1–error of order $\approx 10^{-4}$ in the ground state eigenfunction, and thus an error of order $\approx 10^{-8}$ in the eigenvalue. This discretization is combined with a highly accurate exponential sum approximation with 51 summands from [70]. As can be seen from Figure 6.1, up to the discretization error one obtains the expected dependence of the eigenvalue error on r of order $\mathcal{O}(r^{-2})$.

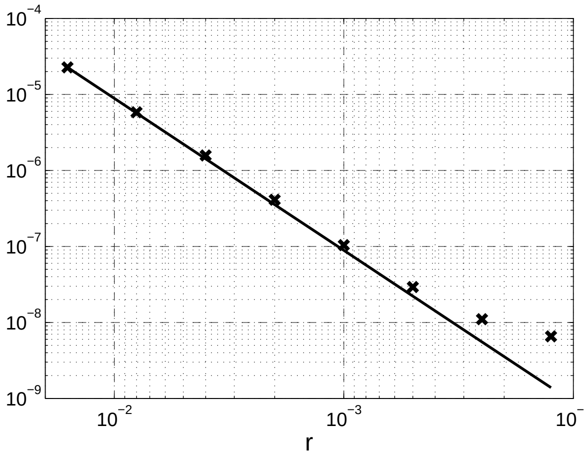

Figure 6.1. Dependence of the eigenvalue error in the discretization of Example 6.19 on the potential approximation parameter r.

6.4 Wavelet Compression of Approximate Potentials

We now turn to the compression of the potential approximations constructed in Section 6.3. As has been noted in Section 6.1, the following considerations apply only to the fully anisotropic wavelet bases $\{\Psi_\nu\}_{\nu\in\nabla^3}$ and $\{\Psi_\nu\}_{\nu\in\nabla^6}$.

We construct compression schemes for factor matrices arising in the wavelet approximation of separable expansions of the form

$$\frac{1}{|x|} \approx \sum_{k=1}^{N} r^{-1}\omega_k e^{-r^{-2}\alpha_k|x|^2}\,, \qquad \frac{1}{|x-y|} \approx \sum_{k=1}^{N} r^{-1}\omega_k e^{-r^{-2}\alpha_k|x-y|^2}\,, \tag{6.17}$$

where $x, y \in \mathbb{R}^3$, as well as

$$\frac{x-y}{|x-y|} \cdot (\mathrm{D}_x - \mathrm{D}_y) \approx \sum_{k=1}^{N} r^{-1} \omega_k (x-y)\, e^{-r^{-2}\alpha_k |x-y|^2} \cdot (\mathrm{D}_x - \mathrm{D}_y)\,. \tag{6.18}$$

The expressions on the right hand sides of (6.17) and (6.18) are considered in each case as multiplication operators $\mathrm{H}^1 \to \mathrm{H}^{-1}$, and the compression of factor matrices is done in such a way that error estimates in operator norm for the complete expansions are facilitated.

Suitable parameters $\{\alpha_k\}$, $\{\omega_k\}$ in (6.17), (6.18) are provided by both Theorem 4.15 and Theorem 4.17. The former yields more efficient approximations and is therefore generally preferable in practice. However, in order to obtain error estimates for compression of the complete separable expansions we need further information on $\{\alpha_k\}$, $\{\omega_k\}$ that is only available for the explicit construction in Theorem 4.17, which we therefore use for what follows. In particular, by Corollary 4.20, we have

$$r^{-1}\omega_k \leq \frac{\pi^2}{|\ln \delta|} \sqrt{r^{-2}\alpha_k}\,, \tag{6.19}$$

where $\delta > 0$ is the error in the exponential sum approximation on $[1, \infty)$ as in Theorem 4.17. We shall use (6.19) in the following way: let, for instance, $A(\alpha)\colon \mathrm{H}^1(\mathbb{R}^3) \to \mathrm{H}^{-1}(\mathbb{R}^3)$ be defined as multiplication by $\exp(-\alpha|x|^2)$, and let $\tilde{A}_\varepsilon(\alpha)$ be a family of compressed operators with $\|A(\alpha) - \tilde{A}_\varepsilon(\alpha)\|_{\mathrm{H}^1 \to \mathrm{H}^{-1}} \leq \varepsilon$, then

$$\Bigl\| \sum_{k=1}^{N} r^{-1}\omega_k \bigl(A(r^{-2}\alpha_k) - \tilde{A}_{\varepsilon_k}(r^{-2}\alpha_k)\bigr) \Bigr\|_{\mathrm{H}^1 \to \mathrm{H}^{-1}} \leq \frac{\pi^2}{|\ln \delta|} \sum_{k=1}^{N} \sqrt{r^{-2}\alpha_k} \bigl\| A(r^{-2}\alpha_k) - \tilde{A}_{\varepsilon_k}(r^{-2}\alpha_k) \bigr\|_{\mathrm{H}^1 \to \mathrm{H}^{-1}}\,.$$

In the following subsection, we therefore derive compression estimates for $\sqrt{\alpha}\bigl\|A(\alpha) - \tilde{A}_\varepsilon(\alpha)\bigr\|$ in dependence on $\alpha > 0$, which can be applied to the one-electron Coulomb potential, and analogous estimates for the two-electron potential terms.

For what follows, we fix a $j_0 \in \mathbb{Z}$ and denote by ∇ the index set corresponding to a one-dimensional compactly supported wavelet basis $\{\psi_\nu\}_{\nu \in \nabla}$ with scaling functions on level j_0. At several points, we shall use an estimate for the support size of the basis functions,

$$L := \max\{|\operatorname{supp} \varphi|, |\operatorname{supp} \psi|\}\,. \tag{6.20}$$

To $\alpha > 0$, we assign

$$j_\alpha := \max\{j_0,\, \tfrac{1}{2}\log_2(2\alpha)\}\,,$$

which plays the role of a 'characteristic wavelet level' corresponding to α; furthermore, we will be dealing repeatedly with expressions involving

$$h_\alpha(i) := \max i - \max\{j_\alpha, \min i\}\,, \quad i \in \mathbb{Z}^2\,. \tag{6.21}$$

Recall also the definition of the sets of weighting factors W_D from (6.5).

6.4.1 One-Electron Coulomb Potentials

We begin with the compressibility of factor matrices of approximations of the one-electron Coulomb potential. Without restriction of generality, we consider the case of the potential with singularity at the origin.

Theorem 6.20. *Let $\alpha > 0$ and $\psi \in \mathrm{W}^p_\infty(\mathbb{R})$ for a $p \in \mathbb{N}$, then the matrix $(a_{\nu\mu})_{\nu,\mu \in \nabla}$ with entries*

$$a_{\nu\mu} = \int e^{-\alpha x^2}\, \psi_\mu(x)\, \psi_\nu(x)\, \mathrm{d}x \tag{6.22}$$

satisfies

$$\|(|a_{\nu\mu}|)_{\nu,\mu\in\nabla}\|_{\ell_2(\nabla)\to\ell_2(\nabla)} \lesssim \max\{1, j_\alpha - j_0\}\,, \tag{6.23}$$

and for each $\ell > 0$ there exists a symmetric infinite matrix $(\tilde a^{(\ell)}_{\nu\mu})$ for which

$$\big\|\big(\sqrt{\alpha}\, 2^{-|\mu|-|\nu|}|a_{\nu\mu} - \tilde a^{(\ell)}_{\nu\mu}|\big)_{\nu,\mu\in\nabla}\big\|_{\ell_2(\nabla)\to\ell_2(\nabla)} \lesssim 2^{-\ell} \tag{6.24}$$

with maximum number of entries per row and column bounded by

$$C\big((1+\sqrt{\ell + (\ln\alpha)_+})2^{(p+1/2)^{-1}\ell} + (\ln\alpha)_+\big)\,, \tag{6.25}$$

where $C > 0$ is independent of ℓ and α. In particular, $\tilde a^{(\ell)}_{\nu\mu} = 0$ for $\nu,\mu\in\nabla$ if

$$\tfrac{1}{2}(|\nu|+|\mu|) + p\big(h_\alpha(|\nu|,|\mu|)\big)_+ > \ell\,. \tag{6.26}$$

Remark 6.21. *The error for the tensor product operator $\sqrt{\alpha}\exp(-\alpha|\cdot|^2)\colon \mathrm{H}^1(\mathbb{R}^3)\to\mathrm{H}^{-1}(\mathbb{R}^3)$, which corresponds to a single term in the separable approximation of the Coulomb potential, is given by*

$$\Big\|\sqrt{\alpha}\Big(2^{-\max|\mu|-\max|\nu|}\Big(\prod_{i=1}^{3} a_{\nu_i\mu_i} - \prod_{i=1}^{3}\tilde a^{(\ell_i)}_{\nu_i\mu_i}\Big)\Big)_{\nu,\mu\in\nabla^3}\Big\|_{\ell_2(\nabla^3)\to\ell_2(\nabla^3)} \tag{6.27}$$

for any given accuracy parameters ℓ_i, $i = 1,2,3$. By a telescoping sum argument, this can be estimated by

$$3\max\big\{\|(a_{\nu\mu})\|, \max_{i=1,2,3}\|(\tilde a^{(\ell_i)}_{\nu\mu})\|\big\}^2 \max_{i=1,2,3}\big\|\big(\sqrt{\alpha}\,2^{-|\mu|-|\nu|}(a_{\nu\mu} - \tilde a^{(\ell_i)}_{\nu\mu})\big)\big\|\,,$$

where $\|\cdot\| = \|\cdot\|_{\ell_2(\nabla)\to\ell_2(\nabla)}$. To make use of the latter, besides (6.24) *an estimate of $\|(\tilde a_{\nu\mu})\|$ is required. We will obtain $(\tilde a_{\nu\mu})$ by setting certain entries of $(a_{\nu\mu})$ to zero. In this situation, we generally cannot obtain a useful estimate of $\|(\tilde a_{\nu\mu})\|$ in terms of $\|(a_{\nu\mu})\|$ unless the entries in $(a_{\nu\mu})$ are nonnegative. Instead, we therefore use the estimate* (6.23)*, from which an estimate for $\|(\tilde a_{\nu\mu})\|$ follows by $\|(|\tilde a_{\nu\mu}|)\| \le \|(|a_{\nu\mu}|)\|$. Compression error estimates of the type* (6.27) *are relevant in particular for the methods considered in Chapter 5.*

Remark 6.22 (s^*-compressibility of exponential sum approximations)**.** *Provided that $(\ln\alpha)_+ \lesssim \ell$, which will always be the case in our context, Theorem 6.20 shows that exponential sum approximations for the one-electron Coulomb potential are s^*-compressible, with values $s^* > 0$ limited only by order and smoothness of the underlying wavelet basis. A result to the same effect for direct compression of the Coulomb potential in isotropic wavelet bases $\{\Psi_\nu\}_{\nu\in\nabla^{(3)}}$ has been obtained in [52].*

For estimates of wavelet coefficients in the proof of Theorem 6.20, we shall need the following auxiliary result.

Lemma 6.23. *Let $\alpha > 0$, then there exists a $C > 0$ such that for any $x\in\mathbb{R}$ and $n\in\mathbb{N}$,*

$$|\mathrm{D}^n_x e^{-\alpha x^2}| \le C(2\alpha)^{n/2}\sqrt{n!}\,e^{-\alpha x^2/2}\,. \tag{6.28}$$

Proof of Lemma 6.23. Recall the definition of the Hermite polynomials $H_n(x) := (-1)^n e^{x^2}(\mathrm{D}^n_x e^{-x^2})$. By Cramérs inequality [80, eq. (28)],

$$|H_n(x)| \le C\sqrt{2^n n!}\,e^{x^2/2}\,, \tag{6.29}$$

with $C > 0$ independent of x, n. Furthermore, for $n\in\mathbb{N}$ we have

$$\mathrm{D}^n_x e^{-\alpha x^2} = (-\sqrt{\alpha})^n e^{-\alpha x^2} H_n(\sqrt{\alpha}x)\,,$$

which combined with (6.29) yields the assertion. □

Proof of Theorem 6.20. We derive estimates for the entries of $(a_{\nu\mu})$ and define a suitable compression rule such that the operator norm estimates (6.23) and (6.24) follow with Lemma 6.8. It then remains to estimate the number of entries in the compressed matrix. For what follows, for $\nu, \mu \in \nabla$, let S_ν and $S_{\nu\mu}$ denote the smallest closed intervals such that $\operatorname{supp}\psi_\nu \subseteq S_\nu$ and $\operatorname{supp}\psi_\nu\psi_\mu \subseteq S_{\nu\mu}$.

Step 1 (Estimates for matrix entries): By Remark 3.4, ψ has at least $p+1$ vanishing moments. For $\nu, \mu \in \nabla$ with $|\nu| \geq |\mu|$, using the vanishing moments of the wavelets and Hölder's inequality, we have

$$|a_{\nu\mu}| \leq \|\psi_\nu\|_{\mathrm{L}_\infty} 2^{-p|\nu|} \|\mathrm{D}_x^p(e^{-\alpha x^2}\psi_\mu)\|_{\mathrm{L}_1(S_{\nu\mu})}\,,$$

and using Lemma 6.23 to estimate derivatives of the Gaussian term, this can be estimated further by

$$\begin{aligned}
&\lesssim 2^{|\nu|/2}\, 2^{-p|\nu|} \sum_{i=0}^{p} \sqrt{i!}\,(2\alpha)^{i/2}\, 2^{(p-i+1/2)|\mu|} \|\mathrm{D}_x^{p-i}\psi\|_{\mathrm{L}_\infty} \int_{S_{\nu\mu}} e^{-\frac{\alpha}{2}x^2}\,\mathrm{d}x \\
&\lesssim 2^{-p(|\nu|-|\mu|)} 2^{\frac{1}{2}(|\nu|+|\mu|)} \sum_{i=0}^{p} (2\alpha)^{i/2}\, 2^{-i|\mu|} \|\psi\|_{\mathrm{W}_\infty^p} \int_{S_{\nu\mu}} e^{-\frac{\alpha}{2}x^2}\,\mathrm{d}x \\
&\lesssim 2^{-p(|\nu|-|\mu|)} 2^{\frac{1}{2}(|\nu|+|\mu|)} \max\bigl\{1, (2\alpha)^{p/2} 2^{-p|\mu|}\bigr\} \int_{S_{\nu\mu}} e^{-\frac{\alpha}{2}x^2}\,\mathrm{d}x\,,
\end{aligned} \tag{6.30}$$

where the involved constants depend on p. Note that

$$\int_{S_{\nu\mu}} e^{-\frac{\alpha}{2}x^2}\,\mathrm{d}x \lesssim \min\bigl\{\alpha^{-1/2}, 2^{-|\nu|} \sup_{x\in S_{\nu\mu}} e^{-\frac{\alpha}{2}x^2}\bigr\}\,, \tag{6.31}$$

and that with h_α defined as in (6.21), we have

$$2^{-p(|\nu|-|\mu|)} \max\bigl\{1, (2\alpha)^{p/2} 2^{-p|\mu|}\bigr\} = 2^{-p(|\nu|-\max\{j_\alpha,|\mu|\})} = 2^{-p\,h_\alpha(|\nu|,|\mu|)}\,.$$

In summary, we thus obtain

$$|a_{\nu\mu}| \leq C_{p,\psi} 2^{-p\,h_\alpha(|\nu|,|\mu|)} 2^{\frac{1}{2}(|\nu|+|\mu|)} \min\bigl\{2^{-j_\alpha}, 2^{-\max\{|\nu|,|\mu|\}} \sup_{x\in S_{\nu\mu}} e^{-\frac{\alpha}{2}x^2}\bigr\}\,. \tag{6.32}$$

By symmetry the same estimate holds for $\nu, \mu \in \nabla$ with $|\mu| \geq |\nu|$.

Noting furthermore that

$$\sum_{\mu\in\nabla_j} \int_{S_{\nu\mu}} e^{-\frac{\alpha}{2}x^2}\,\mathrm{d}x \lesssim \int_{S_\nu} e^{-\frac{\alpha}{2}x^2}\,\mathrm{d}x \lesssim \min\bigl\{2^{-j_\alpha}, 2^{-|\nu|} \sup_{x\in S_{\nu\mu}} e^{-\frac{\alpha}{2}x^2}\bigr\} \tag{6.33}$$

because of local support of the wavelets, we also obtain

$$\sum_{\mu\in\nabla_j} |a_{\nu\mu}| \lesssim C_{p,\psi} 2^{-p\,h_\alpha(|\nu|,j)} 2^{\frac{1}{2}(|\nu|+j)} \min\bigl\{2^{-j_\alpha}, 2^{-|\nu|} \sup_{x\in S_{\nu\mu}} e^{-\frac{\alpha}{2}x^2}\bigr\}\,. \tag{6.34}$$

Without using the vanishing moment property, Hölder's inequality directly yields

$$|a_{\nu\mu}| \leq C_{0,\psi} 2^{\frac{1}{2}(|\nu|+|\mu|)} \min\bigl\{2^{-j_\alpha}, 2^{-\max\{|\nu|,|\mu|\}} \sup_{x\in S_{\nu\mu}} e^{-\alpha x^2}\bigr\}\,,$$

and, again by (6.33), we conclude

$$\sum_{\mu\in\nabla_j} |a_{\nu\mu}| \lesssim C_{0,\psi} 2^{\frac{1}{2}(|\nu|+j)} \min\bigl\{2^{-j_\alpha}, 2^{-|\nu|} \sup_{x\in S_{\nu\mu}} e^{-\alpha x^2}\bigr\}\,. \tag{6.35}$$

For $\nu \in \nabla$ and $j \in \mathbb{Z}_{j_0}$ with $|\nu|, j \leq j_\alpha$, we have $h_\alpha(|\nu|, j) \leq 0$ and therefore in this case (6.35) provides a better estimate than (6.34).

Fix a $\theta \in W_1$ and for $i, j \in \mathbb{Z}_{j_0}$ and $S \subseteq \mathbb{R}$, let

$$f^{(i,j)}(S) := \begin{cases} \sup_{x\in S} e^{-\alpha x^2}\,, & i,j \leq j_\alpha\,, \\ \sup_{x\in S} e^{-\frac{\alpha}{2}x^2}\,, & \text{otherwise.} \end{cases}$$

For $t \in \mathbb{R}$, we define the set of pairs of wavelet indices $\hat\Lambda(t)$ by

$$\hat\Lambda(t) := \bigl\{(\nu,\mu) \in \nabla^2\colon\; f^{(|\nu|,|\mu|)}(S_{\nu\mu}) \leq \theta_{|\nu|,|\mu|} 2^{-t}\bigr\}\,. \tag{6.36}$$

With a suitable choice of t, the index set $\hat\Lambda(t)$ will correspond to those matrix entries that can be dropped because the Gaussian factor is sufficiently small. As a consequence of (6.34) and (6.35), we have

$$\sum_{\substack{\mu\in\nabla_j \\ (\nu,\mu)\in\hat\Lambda(t)}} |a_{\nu\mu}| \lesssim C_{p,\psi} 2^{-\frac{1}{2}(|\nu|-j)} 2^{-p(h_\alpha(|\nu|,j))_+} \theta_{|\nu|,j} 2^{-t}\,. \tag{6.37}$$

Step 2 (Proof of (6.23)): Let $\omega_j = 2^{-\frac{1}{2}j}$ and $\nu \in \nabla$. If $|\nu| > j_\alpha$, by (6.34)

$$\omega_{|\nu|}^{-1} \sum_{\mu\in\nabla} \omega_{|\mu|} |a_{\nu\mu}| \;\lesssim\; \sum_{j=j_0}^{\lfloor j_\alpha \rfloor} 2^{-p(|\nu|-j_\alpha)} + \sum_{j=\lfloor j_\alpha\rfloor+1}^{\infty} 2^{-p|j-|\nu||} \lesssim \max\{1, j_\alpha - j_0\}\,,$$

and if $|\nu| \leq j_\alpha$, by (6.35) and (6.34)

$$\omega_{|\nu|}^{-1} \sum_{\mu\in\nabla} \omega_{|\mu|} |a_{\nu\mu}| \;\lesssim\; 2^{|\nu|-j_\alpha} \sum_{j=j_0}^{\lfloor j_\alpha \rfloor} 1 \,+\, 2^{|\nu|-j_\alpha} \sum_{j=\lfloor j_\alpha\rfloor+1}^{\infty} 2^{-p(j-j_\alpha)} \lesssim \max\{1, j_\alpha - j_0\}\,,$$

which together by Lemma 6.8 implies (6.23).

Step 3 (Construction of compressed matrices and proof of (6.24)): For $\ell > 0$ and $\nu, \mu \in \nabla$, we define

$$c_1(|\nu|,|\mu|) := \frac{1}{2}\bigl(|\nu| + |\mu|\bigr) + p\bigl(h_\alpha(|\nu|,|\mu|)\bigr)_+ \tag{6.38}$$

and, with $\hat\Lambda(\cdot)$ defined as in (6.36), the set of indices

$$\hat\Lambda^{(\ell)}_{|\nu|,|\mu|} := \hat\Lambda\bigl(\ell - c_1(|\nu|,|\mu|) + (j_\alpha - \min\{|\nu|,|\mu|\})_+\bigr)\,. \tag{6.39}$$

We verify the error estimate (6.24) for the compressed infinite matrix $(\tilde a^{(\ell)}_{\nu\mu})$ defined by

$$\tilde a^{(\ell)}_{\nu\mu} := \begin{cases} 0\,, & c_1(|\nu|,|\mu|) > \ell \quad \text{or} \quad (\nu,\mu) \in \hat\Lambda^{(\ell)}_{|\nu|,|\mu|} \\ a_{\nu\mu}\,, & \text{otherwise.} \end{cases} \tag{6.40}$$

In what follows, we use the simplified notation $\hat\Lambda_{|\nu|,|\mu|}$ and $\tilde a_{\nu\mu}$ without reference to ℓ for (6.39) and

(6.40), respectively. We employ Lemma 6.8 with weights $\omega_j \equiv 1$. Note first that

$$2^{j_\alpha}\sum_{\mu\in\nabla} 2^{-|\nu|-|\mu|}|a_{\nu\mu}-\tilde a_{\nu\mu}| = 2^{j_\alpha}\Big(\sum_{\mu\colon c_1(|\nu|,|\mu|)>\ell} 2^{-|\nu|-|\mu|}|a_{\nu\mu}| + \sum_{\substack{\mu\colon c_1(|\nu|,|\mu|)\le\ell,\\ (\nu,\mu)\in\hat\Lambda_{|\nu|,|\mu|}}} 2^{-|\nu|-|\mu|}|a_{\nu\mu}|\Big)\,. \tag{6.41}$$

For the first summand on the right hand side of (6.41), we apply the estimate (6.34); if $|\nu|\le j_\alpha$,

$$\sum_{\mu\colon c_1(|\nu|,|\mu|)>\ell} 2^{j_\alpha}2^{-|\nu|-|\mu|}|a_{\nu\mu}| \lesssim \sum_{2\ell-|\nu|\le j\le j_\alpha} 2^{-\frac12(j+|\nu|)} \\ + \sum_{\substack{j>j_\alpha\\ (p+\frac12)j>\ell+pj_\alpha-\frac12|\nu|}} 2^{-p(j-j_\alpha)-\frac12(j+|\nu|)} \lesssim 2^{-\ell}\,,$$

and if $|\nu|>j_\alpha$,

$$\sum_{\mu\colon c_1(|\nu|,|\mu|)>\ell} 2^{j_\alpha}2^{-|\nu|-|\mu|}|a_{\nu\mu}| \lesssim \sum_{\substack{j\le j_\alpha\\ \frac12 j>\ell+pj_\alpha-(p+\frac12)|\nu|}} 2^{-p(|\nu|-j_\alpha)-\frac12(j+|\nu|)} \\ + \sum_{\substack{j>j_\alpha\\ p||\nu|-j|+\frac12(|\nu|+j)>\ell}} 2^{-p||\nu|-j|-\frac12(|\nu|+j)} \lesssim 2^{-\ell}\,.$$

For the second summand on the right hand side of (6.41), with (6.37) we obtain

$$\sum_{\substack{\mu\colon c_1(|\nu|,|\mu|)\le\ell,\\ (\nu,\mu)\in\hat\Lambda_{|\nu|,|\mu|}}} 2^{j_\alpha}2^{-|\nu|-|\mu|}|a_{\nu\mu}| \lesssim \sum_{\substack{j\in\mathbb{Z}_{j_0}\\ c_1(|\nu|,j)\le\ell}} 2^{j_\alpha}2^{-c_1(|\nu|,j)}2^{-|\nu|}\theta_{|\nu|,j}2^{-\ell+c_1(|\nu|,j)-j_\alpha+|\nu|} \le C_\theta 2^{-\ell}\,,$$

where $C_\theta := \sup_{i\ge j_0}\sum_{j\ge j_0}\theta_{i,j}$. By Lemma 6.8, we thus obtain (6.24).

Step 4 (Estimates for the number of matrix entries): It remains to estimate the maximum number of nonzero entries per row and column in $(\tilde a_{\nu\mu})$. The nonzero entries satisfy the conditions

$$c_1(|\nu|,|\mu|) = \tfrac12(|\nu|+|\mu|) + p(h_\alpha(|\nu|,|\mu|))_+ \le \ell\,, \tag{6.42a}$$

$$(\nu,\mu)\in\nabla^2\setminus\hat\Lambda\big(\ell-\tfrac12(|\nu|+|\mu|)-p(h_\alpha(|\nu|,|\mu|))_+ + (j_\alpha-\min\{|\nu|,|\mu|\})_+\big)\,. \tag{6.42b}$$

Concerning (6.42b), note that for $x\in S_\nu$, $\nu\in\nabla$, and $0<\varepsilon<1$, the condition $\exp(-\alpha|x|^2)<\varepsilon$ is implied by $\exp(-2^{2j_\alpha}(2^{-|\nu|}(\mathrm{k}(\nu)-L))^2)<\varepsilon$, with L defined in (6.20). The latter condition is ensured by

$$|\,\mathrm{k}(\nu)| > L + 2^{|\nu|-j_\alpha}\sqrt{-\ln\varepsilon}\,. \tag{6.43}$$

Up to a constant factor, the same follows for $\exp(-\frac{\alpha}{2}|x|^2)$. Hence, for $j_1,j_2\in\mathbb{Z}_{j_0}$,

$$\#\big\{(\nu,\mu)\in\nabla^2\setminus\hat\Lambda(t)\colon\ |\nu|=j_1,|\mu|=j_2\big\} \sim L+2^{\max\{j_1,j_2\}-j_\alpha}\sqrt{t}\,,\quad t>0\,.$$

For given $\nu\in\nabla$ and $j\in\mathbb{Z}_{j_0}$, if condition (6.42a) is satisfied for $|\nu|,j$ we thus have

$$n_\ell(\nu,j) := \#\{\mu\colon |\mu|=j \text{ and } \tilde a_{\nu\mu}\ne 0\} \lesssim \begin{cases} 1+\sqrt{\ell+(j_\alpha-j_0)_+}\,2^{j-j_\alpha}\,, & |\nu|\le j_\alpha\,,\\ \max\{1,2^{j-|\nu|}\}\,, & |\nu|>j_\alpha\,,\end{cases}$$

where we have used that $\nabla^2\setminus\hat\Lambda(t)$ grows monotonically in t; recall that if (6.42a) is violated for ν,j and ℓ, then $n_\ell(\nu,j)=0$.

For what follows, we introduce the abbreviations $d_\alpha := (j_\alpha - j_0)_+$ and $\tau_p = (p + \frac{1}{2})$. Considering first the case $|\nu| \leq j_\alpha$ and supposing that $\ell > (j_\alpha + |\nu|)/2$,

$$\begin{aligned}\sum_{j\in\mathbb{Z}_{j_0}} n_\ell(\nu, j) &\lesssim \sum_{j=j_0}^{\lfloor j_\alpha \rfloor} (1 + \sqrt{\ell + d_\alpha}\, 2^{j-j_\alpha}) + \sum_{j=\lfloor j_\alpha\rfloor+1}^{\lfloor \tau_p^{-1}(\ell + pj_\alpha - \frac{1}{2}|\nu|)\rfloor} (1 + \sqrt{\ell + d_\alpha}\, 2^{j-j_\alpha}) \\ &\leq \lfloor j_\alpha \rfloor - j_0 + 1 + 2\sqrt{\ell + d_\alpha} \\ &\qquad + \tau_p^{-1}(\ell + pj_\alpha - |\nu|/2) - \lfloor j_\alpha \rfloor + \sqrt{\ell + d_\alpha}\, 2^{\tau_p^{-1}(\ell + pj_\alpha - \frac{1}{2}|\nu|) - j_\alpha} \\ &\lesssim \ell + d_\alpha + \sqrt{\ell + d_\alpha}(1 + 2^{(2p-1)^{-1}j_0} 2^{\tau_p^{-1}\ell}) \,. \end{aligned} \tag{6.44}$$

In case that $|\nu| \leq j_\alpha$ and $\ell \leq (j_\alpha + |\nu|)/2$, by (6.42a),

$$\sum_{j\in\mathbb{Z}_{j_0}} n_\ell(\nu, j) \lesssim \sum_{j=j_0}^{\lfloor 2\ell - |\nu|\rfloor} (1 + \sqrt{\ell + d_\alpha}\, 2^{j-j_\alpha}) \leq d_\alpha + 2\sqrt{\ell + d_\alpha}\,. \tag{6.45}$$

Let now $|\nu| > j_\alpha$. If $\ell < |\nu|$, then $c_1(|\nu|, j) \leq \ell$, as in (6.42a), for $j \in \mathbb{Z}_{j_0}$ implies that $j < j_\alpha$, and consequently

$$\sum_{j\in\mathbb{Z}_{j_0}} n_\ell(\nu, j) \lesssim 2\ell - |\nu| - 2p(|\nu| - j_\alpha) < |\nu| + (j_\alpha - |\nu|) - (2p-1)(|\nu| - j_\alpha) < j_\alpha\,. \tag{6.46}$$

If $|\nu| > j_\alpha$ and $\ell \geq |\nu|$, inspecting the different cases possible in the condition $c_1(|\nu|, j) \leq \ell$, we find that either $j \leq j_\alpha$ and $j \leq 2\ell - 2\tau_p|\nu| + 2pj_\alpha \leq 2\ell - j_\alpha$, or $j_\alpha < j \leq |\nu|$ and $(\tau_p - 1)^{-1}\bigl(\tau_p|\nu| - \ell\bigr) \leq j \leq |\nu|$, or $j > |\nu|$ and $|\nu| + 1 \leq j \leq \tau_p^{-1}\bigl(\ell + (\tau_p - 1)|\nu|\bigr)$. Putting this together,

$$\begin{aligned}\sum_{j\in\mathbb{Z}_{j_0}} n_\ell(\nu, j) &\lesssim \bigl(\min\{j_\alpha, 2\ell - j_\alpha\} - j_0\bigr)_+ + |\nu| - (\tau_p - 1)^{-1}\bigl(\tau_p|\nu| - \ell\bigr) + \sum_{j=|\nu|+1}^{\lfloor \tau_p^{-1}(\ell + (\tau_p-1)|\nu|)\rfloor} 2^{j-|\nu|} \\ &\lesssim d_\alpha + (\tau_p - 1)^{-1}\ell + 2^{-\tau_p^{-1}\max\{j_\alpha, j_0\}} 2^{\tau_p^{-1}\ell}\,. \end{aligned} \tag{6.47}$$

Combining (6.44), (6.45), (6.46), and (6.47), we obtain the assertion. □

Remark 6.24. *For the sake of simplicity, in Theorem 6.20 we have only used an integral-order differentiability assumption on the wavelet – that is,* $\psi \in \mathrm{W}^p_\infty$ *for* $p \in \mathbb{N}$. *Using interpolation theory, however, the proof can be adapted to make use of fractional-order smoothness as well.*

In particular, if we assume that ψ *is in the Hölder-Zygmund space* $\mathcal{C}^s(\mathbb{R}) = \mathrm{B}^s_{\infty,\infty}(\mathbb{R})$ *(cf. [143]) with* $k > s$ *vanishing moments, the statements in* (6.25) *and* (6.26) *still hold with* p *replaced by* s.

Proof. For the results from interpolation theory we shall use here, we refer to [142]. Let $\nu, \mu \in \nabla$ with $|\nu| \geq |\mu|$. We have

$$\int e^{-\alpha x^2} \psi_\nu \psi_\mu \,\mathrm{d}x = \int e^{-(2^{-2|\mu|})x^2} \psi_{(|\nu|-|\mu|, \mathrm{k}(\nu), \mathrm{s}(\nu))} \psi_{(0, \mathrm{k}(\mu), \mathrm{s}(\mu))} \,\mathrm{d}x\,.$$

For the functional

$$\Phi v := \int e^{-(2^{-2|\mu|})x^2} \psi_{(|\nu|-|\mu|, \mathrm{k}(\nu), \mathrm{s}(\nu))} v \,\mathrm{d}x\,,$$

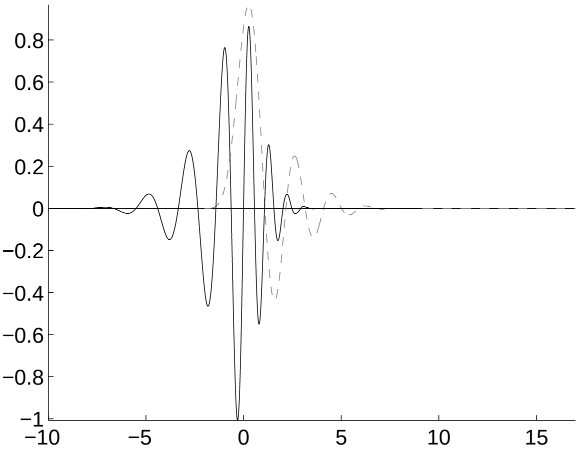

Figure 6.2. Wavelet ψ (solid line) and scaling function φ (dashed line) from [119] with support length 19 and 6 vanishing moments.

as in (6.30) we obtain, for v with support in S_μ,

$$|\Phi v| \leq 2^{\frac{1}{2}(|\nu|+|\mu|)} \int_{S_{\nu\mu}} e^{-\frac{\alpha}{2}x^2}\,\mathrm{d}x\,\|v\|_{\mathrm{C}^0(\mathbb{R})}\,,$$

$$|\Phi v| \leq 2^{-k(h_\alpha(|\nu|,|\mu|))_+} 2^{\frac{1}{2}(|\nu|+|\mu|)} \int_{S_{\nu\mu}} e^{-\frac{\alpha}{2}x^2}\,\mathrm{d}x\,\|v\|_{\mathrm{C}^k(\mathbb{R})}\,.$$

By [142, Theorem 2.7.2/1], $(\mathrm{C}^0(\mathbb{R}), \mathrm{C}^k(\mathbb{R}))_{\frac{s}{k},\infty} = \mathcal{C}^s(\mathbb{R})$, and therefore also

$$|\Phi v| \leq 2^{-s(h_\alpha(|\nu|,|\mu|))_+} 2^{\frac{1}{2}(|\nu|+|\mu|)} \int_{S_{\nu\mu}} e^{-\frac{\alpha}{2}x^2}\,\mathrm{d}x\,\|v\|_{\mathcal{C}^s(\mathbb{R})}.$$

Using this for $v = \psi_\mu$, we obtain the assertion of Theorem 6.20 with s in place of p. □

Example 6.25. To assess the quality of the matrix entry estimates (6.34) and (6.35) on which the compression scheme is based, we consider the actual values of

$$L_j := \sqrt{\alpha}\, 2^{-j} \sum_{\mu\in\nabla_j} \left| \int e^{-\alpha x^2}\, \psi_\mu\, \psi_{\nu_0}\,\mathrm{d}x \right|$$

with $\nu_0 = (0,0,0)$ and $\alpha = 1, 10^2, 10^4, 10^6$, corresponding to $j_\alpha = 0.5, 3.82, 7.14, 10.47$.

In view of the estimates in the proof of Theorem 6.20, for $j \geq 0$ we expect

$$L_j \leq C 2^{-\frac{1}{2}j}\, 2^{-p(j-j_\alpha)_+} \tag{6.48}$$

with some $C > 0$ and with p determined by regularity and vanishing moments of the wavelets. For the test, we use a wavelet constructed by Ojanen [119] with support length 19, shown in Figure 6.2. It has 6 vanishing moments and, according to the estimate given in [119], is contained in $\mathrm{H}^s(\mathbb{R})$ for $s \approx 4.32$. We can therefore expect the decay estimate to hold at least for some $p \in [s - \frac{1}{2}, s) \approx [3.82, 4.32)$.

As can be seen from Figure 6.3, the estimate (6.48) reproduces the qualitative behaviour, but the values for j_α and p that we have arrived at are slightly too pessimistic. The lines with markers show the actual values of L_j for each value of α. The dashed grey lines show the right hand side of (6.48) with $C = 3$, $p = 4.3$, and j_α as above, whereas the dashed black lines show these reference values with $C = 3$, $p = 5.4$, and $j_\alpha = -0.3, 2.5, 6.0, 9.3$. Whereas the former reference curves overestimate the true values for $j > j_\alpha$, the latter reproduce the observed decay fairly accurately for the whole range of j.

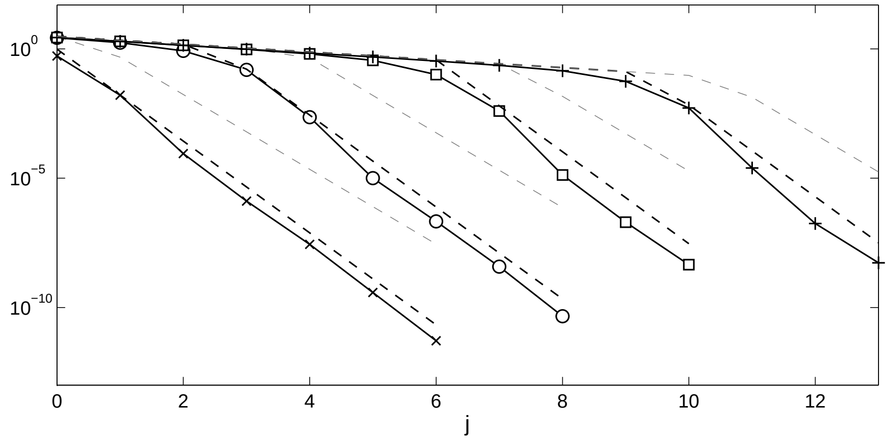

Figure 6.3. Levelwise decay of L_j as in Example 6.25, with the following markers for different values of α: $\times$ 10^0, $\circ$ 10^2, $\Box$ 10^4, $+$ 10^6.

Remark 6.26. *For large* α, *the* L_2*-inner product with* $\sqrt{\pi^{-1}\alpha}\, e^{-\alpha x^2}$ *is an approximate point evaluation at zero. The results for the target error* (6.24) *are therefore related to the compressibility properties of the operator* $\delta_0 \colon \mathrm{H}^1(\mathbb{R}) \to \mathrm{H}^{-1}(\mathbb{R})$ *induced by the bilinear form* $(u\,v)|_{x=0}$ *for* $u, v \in \mathrm{H}^1(\mathbb{R})$. *For the individual entries of the matrix representation on* ℓ_2, *we have the estimate*

$$\bigl|2^{-(|\nu|+|\mu|)}\langle \delta_0 \psi_\nu, \psi_\mu\rangle\bigr| = \bigl|2^{-(|\nu|+|\mu|)}(\psi_\nu \psi_\mu)|_{x=0}\bigr| \lesssim 2^{-\frac{1}{2}(|\mu|+|\nu|)} .$$

For a given accuracy parameter $\ell \in \mathbb{N}$, *a compressed approximation of this infinite matrix can be defined by setting to zero all entries with* $|\mu| + |\nu| > \ell$. *The error in spectral norm can be estimated using Lemma 6.8, with weight sequence* $\omega_j = 1$, *by*

$$\sum_{j > \max\{j_0, \ell - |\nu|\}} 2^{-\frac{1}{2}(j+|\nu|)} \lesssim 2^{-\frac{1}{2}\ell} .$$

The number of nonzero entries per row and column in the compressed matrix is of order $\mathcal{O}(\ell)$, *and hence* δ_0 *is* s^**-compressible for any* $s^* > 0$. *This essentially corresponds to the limiting case of the construction in Theorem 6.20 as* $j_\alpha \to \infty$.

6.4.2 Two-Electron Coulomb Potentials

In what follows, for $i = (i_1, i_2) \in \mathbb{Z}^2$, we use the notation $\max i = \max\{i_1, i_2\}$ and $\min i = \min\{i_1, i_2\}$. Note that if $\{2^{-|\nu|}\psi_\nu\}_{\nu\in\nabla}$ is a Riesz basis of $\mathrm{H}^1(\mathbb{R})$, then by (3.23), $\{2^{-\max|\nu|}\Psi_\nu\}_{\nu\in\nabla^2}$ is a Riesz basis of $\mathrm{H}^1(\mathbb{R}^2)$.

For the statement of the following theorem, recall the definition of h_α in (6.21). In addition, for $i, j \in \mathbb{Z}^2$ we introduce the abbreviation

$$m(i,j) := \max\{i_1, i_2, j_1, j_2\} - \max\bigl(\{i_1, i_2, j_1, j_2\} \setminus \max\{i_1, i_2, j_1, j_2\}\bigr) ,$$

that is, the difference between the largest and the second largest value in i and j.

Theorem 6.27. *Let* $\alpha > 0$ *and* $\psi \in \mathrm{W}^p_\infty(\mathbb{R})$ *for a* $p \in \mathbb{N}$, *then for* $(a_{\nu\mu})_{\nu,\mu\in\nabla^2}$ *with entries*

$$a_{\nu\mu} = \int e^{-\alpha(x_1-x_2)^2}\, \Psi_\mu(x)\, \Psi_\nu(x)\, \mathrm{d}x , \quad \nu, \mu \in \nabla^2 , \tag{6.49}$$

we have

$$\|(|a_{\nu\mu}|)_{\nu,\mu\in\nabla^2}\|_{\ell_2(\nabla^2)\to\ell_2(\nabla^2)} \lesssim (\max\{1, j_\alpha - j_0\})^2\,, \tag{6.50}$$

and for $\ell > 0$ *there exists a symmetric infinite matrix* $(\tilde a^{(\ell)}_{\nu\mu})$ *satisfying*

$$\Big\|\big(\sqrt{\alpha}2^{-\max|\mu|-\max|\nu|}|a_{\nu\mu} - \tilde a^{(\ell)}_{\nu\mu}|\big)_{\nu,\mu\in\nabla^2}\Big\|_{\ell_2(\nabla^2)\to\ell_2(\nabla^2)} \lesssim 2^{-\ell}\,, \tag{6.51}$$

where the number of entries in row and column corresponding to $\nu\in\nabla^2$ *can be estimated by*

$$C\big(1+\sqrt{\ell+(\ln\alpha)_+}\big)\min\big\{\big(1+(\ln\alpha)_+\big)2^{2(\ell-\max|\nu|)-||\nu_1|-|\nu_2||}, \max\{1, 2^{-\max|\nu|}\sqrt{\alpha}\}2^{(p+\frac14)^{-1}\ell}\big\}\,, \tag{6.52}$$

and hence the maximum number of entries per row and column is bounded by

$$\tilde C\big(1+\sqrt{\ell+(\ln\alpha)_+}\big)\min\big\{\big(1+(\ln\alpha)_+\big)2^{2\ell}, \big(1+\sqrt{\alpha}\big)2^{(p+\frac14)^{-1}\ell}\big\}\,, \tag{6.53}$$

with $C, \tilde C > 0$ *independent of* ℓ *and* α*. In particular,* $\tilde a^{(\ell)}_{\nu\mu} = 0$ *for* $\nu,\mu\in\nabla^2$ *if*

$$\begin{aligned}\max|\nu| + \max|\mu| - \tfrac12(\min|\nu| + \min|\mu|)&\\ + p\max\big\{m(|\mu|,|\nu|)\,,\ \big(h_\alpha(|\nu_1|,|\mu_1|)\big)_+ + \big(h_\alpha(|\mu_2|,|\nu_2|)\big)_+\big\} &> \ell\,.\end{aligned} \tag{6.54}$$

Remark 6.28. *Theorem 6.27 can be applied to the compression of terms in exponential sum approximations in the same manner as described in Remark 6.21, which yields*

$$\Big\|\Big(\sqrt{\alpha}\,2^{-\max|\mu|-\max|\nu|}\Big(\prod_{i=1}^3 a_{\nu_i\mu_i} - \prod_{i=1}^3 \tilde a_{\nu_i\mu_i}\Big)\Big)_{\mu,\nu\in(\nabla^2)^3}\Big\|_{\ell_2(\nabla^6)\to\ell_2(\nabla^6)} \lesssim \max\{1, j_\alpha - j_0\}^4\,2^{-\ell}\,.$$

This type of estimate is relevant for the methods considered in Chapter 5.

Remark 6.29. *In the proof of the theorem, we restrict ourselves to an integral-order differentiability assumption of* ψ*. Analogously to the one-electron case treated in Remark 6.24, the result can be extended by interpolation theory to also make use of fractional-order differentiability of* ψ*.*

Proof of Theorem 6.27. For given $\nu,\mu\in\nabla^2$, let $S_\nu, S_{\nu\mu}\subset\mathbb{R}^2$ be the smallest Cartesian products of closed intervals such that $\operatorname{supp}\Psi_\nu\subseteq S_\nu$ and $\operatorname{supp}\Psi_\nu\Psi_\mu\subseteq S_{\nu\mu}$. In addition, we introduce $\beta(\nu,\mu),\gamma(\nu,\mu)\in\nabla^2$ with

$$\beta_i(\nu,\mu) = \begin{cases}\mu_i\,, & |\mu_i| < |\nu_i|\\ \nu_i\,, & |\mu_i| \geq |\nu_i|\,,\end{cases} \qquad \gamma_i(\nu,\mu) = \begin{cases}\nu_i\,,\ \beta_i = \mu_i\\ \mu_i\,,\ \beta_i = \nu_i\,,\end{cases} \qquad i = 1,2\,, \tag{6.55}$$

which we will abbreviate as β,γ in what follows; in other words, γ comprises the wavelet indices on the higher levels, β those on the lower levels for each coordinate direction.

Estimates for matrix entries: By Remark 3.4, ψ has at least $p+1$ vanishing moments. We thus obtain, for $0\leq p_1,p_2\leq p$,

$$|a_{\nu\mu}| \lesssim \|\Psi_\gamma\|_{\mathrm{L}_\infty}\,2^{-p_1|\gamma_1|-p_2|\gamma_2|}\int_{S_\gamma}\big|\mathrm{D}^{p_1}_{x_1}\mathrm{D}^{p_2}_{x_2}e^{-\alpha(x_1-x_2)^2}\Psi_\beta(x_1,x_2)\big|\,\mathrm{d}x\,. \tag{6.56}$$

Using Lemma 6.23 we can estimate (6.56) by

$$\begin{aligned}2^{-p_1|\gamma_1|-p_2|\gamma_2|}2^{\frac{1}{2}(|\gamma_1|+|\gamma_2|)}\sum_{i=0}^{p_1}\sum_{j=0}^{p_2}(2\alpha)^{(i+j)/2}\sqrt{(i+j)!}\,2^{(p_1+\frac{1}{2}-i)|\beta_1|}2^{(p_2+\frac{1}{2}-j)|\beta_2|}\int_{S_\gamma} e^{-\frac{\alpha}{2}(x_1-x_2)^2}\,\mathrm{d}x \\ \lesssim\ 2^{-p_1(|\gamma_1|-|\beta_1|)-p_2(|\gamma_2|-|\beta_2|)}2^{\frac{1}{2}(|\gamma_1|+|\gamma_2|+|\beta_1|+|\beta_2|)} \\ \times\sqrt{(p_1+p_2)!}\int_{S_\gamma} e^{-\frac{\alpha}{2}(x_1-x_2)^2}\,\mathrm{d}x\prod_{d=1}^{2}\sum_{i=0}^{m_d}(2\alpha)^{i/2}\,2^{-|\beta_d|i}\,.\end{aligned}$$

Furthermore,

$$\sum_{i=0}^{p_1}(2\alpha)^{i/2}\,2^{-|\beta_1|i}\lesssim\max\{p_1,(2\alpha)^{p_1/2}2^{-|\beta_1|p_1}\}\,, \tag{6.57}$$

$$\int_{S_\gamma} e^{-\frac{\alpha}{2}(x_1-x_2)^2}\,\mathrm{d}x\lesssim 2^{-\max|\gamma|}\min\bigl\{2^{-j_\alpha},2^{-\min|\gamma|}\sup_{x\in S_\gamma}e^{-\frac{\alpha}{2}(x_1-x_2)^2}\bigr\}\,. \tag{6.58}$$

In summary, with constants depending on ψ and p, similarly to the proof of Theorem 6.20 we obtain

$$|a_{\nu\mu}|\lesssim 2^{-\max|\gamma|}\min\bigl\{2^{-j_\alpha},2^{-\min|\gamma|}\sup_{x\in S_{\nu\mu}}e^{-\frac{\alpha}{2}(x_1-x_2)^2}\bigr\}\prod_{d=1}^{2}2^{-p_d\,h_\alpha(|\nu_d|,|\mu_d|)}2^{\frac{1}{2}(|\nu_d|+|\mu_d|)}$$

and by the same argument as for (6.33), for $j\in\mathbb{Z}^2_{j_0}$ we have

$$\sum_{\mu\in\nabla_j^2}|a_{\nu\mu}|\lesssim 2^{-\max|\nu|}\min\bigl\{2^{-j_\alpha},2^{-\min|\nu|}\sup_{x\in S_\nu}e^{-\frac{\alpha}{2}(x_1-x_2)^2}\bigr\}\prod_{d=1}^{2}2^{-p_d\,h_\alpha(|\nu_d|,j_d)}2^{\frac{1}{2}(|\nu_d|+j_d)}\,. \tag{6.59}$$

Note that without the use of vanishing moments, a direct application of Hölder's inequality leads to

$$\sum_{\mu\in\nabla_j^2}|a_{\nu\mu}|\lesssim 2^{-\max|\nu|}\min\bigl\{2^{-j_\alpha},2^{-\min|\nu|}\sup_{x\in S_\nu}e^{-\alpha(x_1-x_2)^2}\bigr\}\prod_{d=1}^{2}2^{\frac{1}{2}(|\nu_d|+j_d)}\,. \tag{6.60}$$

In case that $h_\alpha(|\nu_d|,j_d)\geq 0$ for $d=1,2$, we use the estimate (6.59) with $p_1=p_2=p$. If $h_\alpha(|\nu_1|,j_1)<0$, but $h_\alpha(|\nu_2|,j_2)\geq 0$, we take $p_1=0$, $p_2=p$, and vice versa. If $h_\alpha(|\nu_d|,j_d)<0$ for $d=1,2$, we instead use (6.60). Combining this, we obtain

$$\sum_{\mu\in\nabla_j^2}|a_{\nu\mu}|\lesssim 2^{-\max|\nu|}2^{-\max\{j_\alpha,\min|\nu|\}}\prod_{d=1}^{2}2^{-p(h_\alpha(|\nu_d|,j_d))_+}2^{\frac{1}{2}(|\nu_d|+j_d)}\,. \tag{6.61}$$

A further estimate can be derived from the observation that

$$a_{\nu\mu}=\int\psi_{\nu_1}\psi_{\mu_1}\bigl(e^{-\alpha(\cdot)^2}*\psi_{\nu_2}\psi_{\mu_2}\bigr)\,\mathrm{d}x_1=\int\psi_{\nu_2}\psi_{\mu_2}\bigl(e^{-\alpha(\cdot)^2}*\psi_{\nu_1}\psi_{\mu_1}\bigr)\,\mathrm{d}x_2\,.$$

Without loss of generality, let us assume for the moment that $|\nu_1|=\max\{|\nu_1|,|\nu_2|,|\mu_1|,|\mu_2|\}$. Then

$$|a_{\nu\mu}|\lesssim\|\psi_{\nu_1}\|_{\mathrm{L}_1}2^{-p|\nu_1|}\bigl\|\mathrm{D}^p\bigl(\psi_{\mu_1}(e^{-\alpha(\cdot)^2}*\psi_{\nu_2}\psi_{\mu_2})\bigr)\bigr\|_{\mathrm{L}_\infty}\,,$$

which, using properties of the convolution, can be estimated further by

$$\lesssim 2^{-(p+\frac{1}{2})|\nu_1|}\sum_{i=0}^{p} 2^{(p-i+\frac{1}{2})|\mu_1|}\big\|e^{-\alpha(\cdot)^2} * \mathrm{D}^i(\psi_{\nu_2}\psi_{\mu_2})\big\|_{\mathrm{L}_\infty(S_{\nu_2\mu_2})}\,.$$

Note that

$$\sup_{x_1\in S_{\nu_1\mu_1}}\left|\int e^{-\alpha(x_1-x_2)^2}\mathrm{D}^i(\psi_{\nu_2}\psi_{\mu_2})\,\mathrm{d}x_2\right| \lesssim 2^{\frac{1}{2}(|\mu_2|+|\nu_2|)}2^{i\max\{|\mu_2|,|\nu_2|\}}\sup_{x_1\in S_{\nu_1\mu_1}}\int_{S_{\nu_2\mu_2}} e^{-\alpha(x_1-x_2)^2}\,\mathrm{d}x_2\,,$$

and since by our assumption on $|\nu_1|$, we have $|S_{\nu_1\mu_1}| \lesssim |S_{\nu_2\mu_2}|$ if $\operatorname{supp}\Psi_\nu\Psi_\mu \neq \emptyset$, we obtain

$$\sum_{\nu_2\in\nabla}\sup_{x_1\in S_{\nu_1\mu_1}}\int_{S_{\nu_2\mu_2}} e^{-\alpha(x_1-x_2)^2}\,\mathrm{d}x_2 \lesssim \alpha^{-\frac{1}{2}}\,.$$

In summary, for $j\in\mathbb{Z}^2_{j_0}$ we obtain the additional estimate

$$\sum_{\mu\in\nabla^2}|a_{\nu\mu}| \lesssim 2^{-\max|\nu|}2^{-j_\alpha}2^{\frac{1}{2}(|\nu_1|+|\nu_2|+j_1+j_2)}2^{-p\,m(|\nu|,|\mu|)}\,, \tag{6.62}$$

which complements (6.61).

Proof of (6.50): Let $\omega_j = 2^{-\frac{1}{2}(j_1+j_2)}$ for $j\in\mathbb{Z}^2_{j_0}$. Expanding the different cases in (6.61) similarly to step 2 in the proof of Theorem 6.20, we find

$$\omega_{|\nu|}^{-1}\sum_{\mu}\omega_\mu|a_{\nu\mu}| \lesssim (\max\{1, j_\alpha - j_0\})^2\,. \tag{6.63}$$

Construction of compressed matrices and proof of (6.51): Let $\Theta\in W_2$, and for $i,j\in\mathbb{Z}^2_{j_0}$ and $S\subseteq\mathbb{R}^2$, let

$$F^{(i,j)}_{\mathrm{s}}(S) := \begin{cases}\sup_{x\in S} e^{-\alpha(x_1-x_2)^2}\,, & i_1,i_2,j_1,j_2\le j_\alpha\,,\\ \sup_{x\in S} e^{-\frac{\alpha}{2}(x_1-x_2)^2}\,, & \text{otherwise.}\end{cases}$$

For $t\in\mathbb{R}$, we define

$$\hat{\Lambda}_{\mathrm{s}}(t) := \big\{(\nu,\mu)\in(\nabla^2)^2\colon\; F^{(|\nu|,|\mu|)}_{\mathrm{s}}(S_{\nu\mu}) < \Theta_{|\nu|,|\mu|}2^{-t}\big\}\,. \tag{6.64}$$

For $i,j\in\mathbb{Z}^2$, we define the abbreviations

$$g(i,j) := \max i + \max j - \frac{1}{2}(\min i + \min j)$$

as well as

$$\begin{aligned} c_{\mathrm{s}}(i,j) &:= g(i,j) + p\big((h_\alpha(j_1,i_1))_+ + (h_\alpha(j_2,i_2))_+\big)\,,\\ \bar{c}_{\mathrm{s}}(i,j) &:= g(i,j) + p\max\{m(i,j)\,,\;(h_\alpha(j_1,i_1))_+ + (h_\alpha(j_2,i_2))_+\}\,.\end{aligned}$$

Note that $\bar{c}_{\mathrm{s}}$ is precisely the expression appearing in (6.54). In addition, we define the index sets

$$\hat{\Lambda}^{(\ell)}_{\mathrm{s},i,j} := \hat{\Lambda}_{\mathrm{s}}\big(\ell - c_{\mathrm{s}}(i,j) + (j_\alpha - \min\{\min i, \min j\})_+\big)\,.$$

With this notation, for $\ell > 0$, the compressed matrix is defined by

$$\tilde{a}^{(\ell)}_{\nu\mu} = \begin{cases}0\,, & \bar{c}_{\mathrm{s}}(|\nu|,|\mu|) > \ell \quad\text{or}\quad (\nu,\mu)\in\hat{\Lambda}^{(\ell)}_{\mathrm{s},|\nu|,|\mu|}\,,\\ a_{\nu\mu}\,, & \text{otherwise.}\end{cases} \tag{6.65}$$

In other words, entries are dropped from $(a_{\nu\mu})$ if it can be ensured that their modulus is small enough either due to the combination of the wavelet levels, or because the Gaussian coefficient function is sufficiently small on the support of the wavelet product. In what follows, we use the simplified notation $\tilde{a}_{\nu\mu}$ for $\tilde{a}^{(\ell)}_{\nu\mu}$.

Let now $\omega_j = 2^{-\frac{1}{2}\max j}$ for $j \in \mathbb{Z}^2_{j_0}$. From (6.61) and (6.62), we obtain on the one hand

$$2^{j_\alpha}\omega^{-1}_{|\nu|}\omega_j \sum_{\mu\in\nabla^2_j} 2^{-\max|\nu|-\max j}|a_{\mu\nu}| \lesssim 2^{-g(|\nu|,j)}2^{-p\max\{m(|\nu|,j),\sum_d h_\alpha(|\nu_d|,j_d)_+\}} = 2^{-\bar{c}_\mathrm{s}(|\nu|,j)}$$

for $\nu \in \nabla^2$, $j \in \mathbb{Z}^2_{j_0}$. On the other hand, using (6.59),

$$\begin{aligned}2^{j_\alpha}\omega^{-1}_{|\nu|}\omega_j &\sum_{\{\mu\in\nabla^2_j\colon (\nu,\mu)\in\hat{\Lambda}^{(\ell)}_{\mathrm{s},|\nu|,|\mu|}\}} 2^{-\max|\nu|-\max j}|a_{\mu\nu}| \\ &\lesssim 2^{j_\alpha-\min|\nu|}2^{-c_\mathrm{s}(|\nu|,j)}\Theta_{|\nu|,j}2^{-\ell+c_\mathrm{s}(|\nu|,j)-(j_\alpha-\min\{\min|\nu|,\min j\})_+} \;\leq\; \Theta_{|\nu|,j}2^{-\ell}\,.\end{aligned}$$

Combining these estimates and proceeding as for (6.41) in the proof of Theorem 6.20 yields

$$\begin{aligned}2^{j_\alpha}\omega^{-1}_{|\nu|}&\sum_{\mu\in\nabla^2}\omega_{|\mu|}2^{-\max|\nu|-\max j}|a_{\nu\mu}-\tilde{a}_{\nu\mu}| \\ &\lesssim \sum_{\{j\colon \bar{c}_\mathrm{s}(|\nu|,j)>\ell\}} 2^{-\bar{c}_\mathrm{s}(|\nu|,j)} + \sum_{j\in\mathbb{Z}^2_{j_0}}\Theta_{|\nu|,j}2^{-\ell} \;\leq\; C_\Theta 2^{-\ell}\,,\end{aligned}$$

which by Lemma 6.8 implies (6.51).

Estimates for the number of matrix entries: We shall use the abbreviation $d_\alpha := (j_\alpha - j_0)_+$. For $\nu \in \nabla^2$, let

$$n_\ell(\nu,j) := \#\bigl\{\mu\in\nabla^2\colon |\mu| = (j_1,j_2)\,,\ \tilde{a}_{\nu\mu}\neq 0\bigr\}\,.$$

Without loss of generality, for what follows we assume $|\nu_1| \geq |\nu_2|$.

By considering only the support sizes of the basis functions, we immediately obtain

$$n_\ell(\nu,j) \lesssim 2^{(j_1-|\nu_1|)_+}2^{(j_2-|\nu_2|)_+}\,.$$

In the case $j_2 > |\nu_2|$, we improve this estimate by taking the second compression condition in (6.65) into account, which is related to the decay of the Gaussian coefficient. This is done similarly as in the derivation of the condition (6.43) in the proof of Theorem 6.20.

Recall the definition of L in (6.20) as a bound on the support size of the basis functions on level zero. In addition to ν, we fix a $\mu_1 \in \nabla$ with $|\mu_1| = j_1$ and $S_{\nu_1\mu_1} \neq \emptyset$. Let $j_2 > |\nu_2|$. We now estimate the number of $\mu_2 \in \nabla$ with $|\mu_2| = j_2$ such that $(\nu,\mu) \notin \hat{\Lambda}^{(\ell)}_{\mathrm{s},|\nu|,|\mu|}$.

To this end, note that for $\varepsilon > 0$, the condition $\sup_{x\in S_{\nu\mu}} e^{-\alpha(x_1-x_2)^2} < \varepsilon$ is ensured by

$$\begin{aligned}\max\bigl\{&\bigl||2^{-j_2}|\mathrm{k}(\mu_2)| - 2^{-j_1}|\mathrm{k}(\mu_1)|| - (2^{-j_1}+2^{-j_2})L\bigr|, \\ &\qquad\bigl||2^{-j_2}|\mathrm{k}(\mu_2)| - 2^{-|\nu_1|}|\mathrm{k}(\nu_1)|| - (2^{-|\nu_1|}+2^{-j_2})L\bigr|\bigr\} \gtrsim 2^{-j_\alpha}\sqrt{|\ln\varepsilon|}\,.\end{aligned}$$

Consequently, the number of such μ_2 can be estimated up to a constant by

$$2^{j_2-j_\alpha}\sqrt{|\ln\varepsilon|} + (1+\min\{2^{j_2-j_1}, 2^{j_2-|\nu_1|}\})L\,.$$

In summary, we arrive at

$$n_\ell(\nu,j) \lesssim 2^{(j_1-|\nu_1|)_+}\min\bigl\{1 + 2^{j_2-j_\alpha}\sqrt{\ell+d_\alpha} + 2^{j_2-\max\{j_1,|\nu_1|\}}, 2^{(j_2-|\nu_2|)_+}\bigr\}\,. \tag{6.66}$$

It remains to estimate the sum over all $n_\ell(\nu, j)$ with $j = (j_1, j_2)$ satisfying $\bar c_{\mathrm{s}}(|\nu|, j) \le \ell$ by a constant multiple of (6.52).

For given $\mathcal{J} \subset \mathbb{Z}^2_{j_0}$, we introduce the abbreviation

$$N(\mathcal{J}) := \sum_{j\in\mathcal{J}} n_\ell(|\nu|, j)\,.$$

At several points we will make use of the fact that for any $\tilde c\colon \mathbb{Z}^2_{j_0} \times \mathbb{Z}^2_{j_0} \to \mathbb{Z}$ with $\tilde c \le c_{\mathrm{s}} \le \bar c_{\mathrm{s}}$ and any $\mathcal{J} \subset \mathbb{Z}^2_{j_0}$,

$$N\bigl(\{j \in \mathcal{J}\colon \tilde c(|\nu|, j) < \ell\}\bigr) \;\ge\; N\bigl(\{j \in \mathcal{J}\colon c_{\mathrm{s}}(|\nu|, j) < \ell\}\bigr) \;\ge\; N\bigl(\{j \in \mathcal{J}\colon \bar c_{\mathrm{s}}(|\nu|, j) < \ell\}\bigr)\,.$$

In particular, from (6.66) it can be seen that replacing $\bar c_{\mathrm{s}}$ by the lower bound c_{s} does not change the asymptotic behaviour of the estimate for the number of nonzero entries. As illustrated by Example 6.30 below, the quantitative difference is of practical importance. In the following estimates for the asymptotics, however, we only consider c_{s}.

We first treat the case $|\nu_1| \ge |\nu_2| > j_\alpha$, where (6.66) implies

$$n_\ell(\nu, j) \lesssim 2^{(j_1-|\nu_1|)_+ + (j_2-|\nu_2|)_+}\,. \tag{6.67}$$

We consider first the summation over the corresponding subset of $\mathcal{J}_1 = \{j \in \mathbb{Z}^2_{j_0}\colon j_1, j_2 > j_\alpha\}$. Note that for $j \in \mathcal{J}_1$, we have $c_{\mathrm{s}}(|\nu|, j) = \max j - \frac{1}{2}\min j + |\nu_1| - \frac{1}{2}|\nu_2| + p(||\nu_1| - j_1| + ||\nu_2| - j_2|)$. We subdivide the summation further into

$$\begin{aligned} N(\mathcal{J}_1) = N(\mathcal{J}_1 \cap \{j_1 < |\nu_1|, j_2 < |\nu_2|\}) + N(\mathcal{J}_1 \cap \{j_1 \ge |\nu_1|, j_2 < |\nu_2|\}) \\ + N(\mathcal{J}_1 \cap \{j_1 < |\nu_1|, j_2 \ge |\nu_2|\}) + N(\mathcal{J}_1 \cap \{j_1 \ge |\nu_1|, j_2 \ge |\nu_2|\})\,, \end{aligned} \tag{6.68}$$

and treat each term on the right hand side separately. By (6.66),

$$N(\mathcal{J}_1 \cap \{j_1 < |\nu_1|, j_2 < |\nu_2|\}) \lesssim (\ell/p)^2\,.$$

For $j \in \mathcal{J}_1 \cap \{j_1 < |\nu_1|, j_2 \ge |\nu_2|\}$, we have $c_{\mathrm{s}}(|\nu|, j) \ge (p+\frac{1}{2})(j_2 - |\nu_2|) + |\nu_1| \ge (p+\frac{1}{2})(j_2 - |\nu_2|) + j_0$ as well as $c_{\mathrm{s}}(|\nu|, j) \ge p(|\nu_1| - j_1) + j_0$ and thus

$$N(\mathcal{J}_1 \cap \{j_1 < |\nu_1|, j_2 \ge |\nu_2|\}) \lesssim \ell\, 2^{(p+\frac{1}{2})^{-1}(\ell - j_0)}\,.$$

Similarly, for $j \in \mathcal{J}_1 \cap \{j_1 \ge |\nu_1|, j_2 < |\nu_2|\}$, we have $c_{\mathrm{s}}(|\nu|, j) \ge (p + \frac{1}{2})(j_1 - |\nu_1|) + |\nu_1|$ and $c_{\mathrm{s}}(|\nu|, j) \ge p(|\nu_2| - j_2) + j_0$, and consequently also

$$N(\mathcal{J}_1 \cap \{j_1 \ge |\nu_1|, j_2 < |\nu_2|\}) \lesssim \ell\, 2^{(p+\frac{1}{2})^{-1}(\ell - j_0)}\,.$$

Finally, for $j \in \mathcal{J}_2 := \mathcal{J}_1 \cap \{j_1 \ge |\nu_1|, j_2 \ge |\nu_2|\}$, we have $c_{\mathrm{s}}(|\nu|, j) \ge (p+\frac{1}{2})(j_1 - |\nu_1|) + p(j_2 - |\nu_2|) =: \tilde c_1(|\nu|, j)$ if $j_1 \ge j_2$, and $c_{\mathrm{s}}(|\nu|, j) \ge p(j_1 - |\nu_1|) + (p + \frac{1}{2})(j_2 - |\nu_2|) =: \tilde c_2(|\nu|, j)$ if $j_1 < j_2$. Hence we obtain

$$\begin{aligned} N(\mathcal{J}_2) &\lesssim \sum_{\substack{j \in \mathcal{J}_2 \cap \{j_1 \ge j_2\} \\ \tilde c_1(|\nu|, j) \le \ell}} 2^{j_1 - |\nu_1|} 2^{j_2 - |\nu_2|} + \sum_{\substack{j \in \mathcal{J}_2 \cap \{j_1 < j_2\} \\ \tilde c_2(|\nu|, j) \le \ell}} 2^{j_1 - |\nu_1|} 2^{j_2 - |\nu_2|} \\ &\lesssim \sum_{j_1 = |\nu_1|}^{s_1} \sum_{j_2 = |\nu_2|}^{s_2(j_1)} 2^{j_1 - |\nu_1|} 2^{j_2 - |\nu_2|} \lesssim 2^{(p+\frac{1}{4})^{-1}\ell}\,, \end{aligned}$$

where $s_1 := \lfloor (2p + \frac{1}{2})^{-1}(\ell + p|\nu_1| + (p + \frac{1}{2})|\nu_2|) \rfloor$, $s_2(j_1) := \lfloor (p + \frac{1}{2})^{-1}\bigl(\ell - p(j_1 - |\nu_1|)\bigr) + |\nu_2| \rfloor$.

We have thus already completely covered the case $j_\alpha < j_0$, and therefore assume for the following that $j_\alpha \geq j_0$.

If $|\nu_1| \geq |\nu_2| > j_\alpha$ and $j_\alpha \geq j_0$, we additionally need to sum over $\mathcal{J}_3 := \{j \in \mathbb{Z}^2_{j_0} \colon j_1, j_2 \leq j_\alpha, c_{\mathrm{s}}(|\nu|, j) \leq \ell\}$, which is empty unless $\ell \geq (j_\alpha + j_0)/2$; since for $j \in \mathcal{J}_3$ we have $n_\ell(|\nu|, j) \lesssim 1$, we obtain $N(\mathcal{J}_3) \lesssim \ell^2$. By estimates completely analogous to those for (6.68), we also find

$$N(\{j_1 > j_\alpha, j_2 \leq j_\alpha, c_{\mathrm{s}}(|\nu|, j) \leq \ell\}),\, N(\{j_2 \leq j_\alpha, j_2 > j_\alpha, c_{\mathrm{s}}(|\nu|, j) \leq \ell\}) \lesssim \ell 2^{(p+1)^{-1}\ell}\,,$$

which concludes the treatment of the case $|\nu_1| \geq |\nu_2| > j_\alpha$.

We next consider the case $|\nu_1| > j_\alpha \geq |\nu_2|$, where we have $c_{\mathrm{s}}(|\nu|, j) = g(|\nu|, j) + p\big||\nu_1| - \max\{j_1, j_\alpha\}\big| + p(j_2 - j_\alpha)_+$ and $n_\ell(|\nu|, j) \lesssim 2^{(j_1 - |\nu_1|)_+} 2^{(j_2 - j_\alpha)_+}(1 + \sqrt{\ell + d_\alpha}) + 2^{j_2 - |\nu_1|}$. Noting that $j_2 - |\nu_1| < j_2 - j_\alpha$, we can proceed analogously to the case of $|\nu_1| \geq |\nu_2| > j_\alpha$ above, by distinguishing cases depending on the signs of $j_1 - |\nu_1|$ and $j_2 - j_\alpha$, to likewise obtain

$$N(\{j \in \mathbb{Z}^2_{j_0} \colon\, c_{\mathrm{s}}(|\nu|, j) \leq \ell\}) \lesssim 2^{(p+\frac{1}{4})^{-1}\ell}(1 + \sqrt{\ell + d_\alpha})$$

for $|\nu_1| > j_\alpha \geq |\nu_2|$.

If $|\nu_1|, |\nu_2| \leq j_\alpha$, the number of nonzero entries can be estimated by

$$N(\mathcal{J}_4) \lesssim \sum_{j \in \mathcal{J}_4} (2^{j_1 - |\nu_1|} + 2^{j_2 - |\nu_1|} + 2^{j_1 + j_2 - |\nu_1| - j_\alpha} \sqrt{\ell + d_\alpha})\,, \tag{6.69}$$

where $\mathcal{J}_4 = \big\{j \in \mathbb{Z}^2_{j_0} \colon\, \max j + |\nu_1| - \frac{1}{2}(\min j + |\nu_2|) + p(j_1 - j_\alpha)_+ + p(j_2 - j_\alpha)_+ \leq \ell\big\}$.

For estimating the right hand side of (6.69) further, we consider two cases: First, if $\ell \leq \frac{1}{2} j_\alpha + |\nu_1| - \frac{1}{2}|\nu_2|$, the summation extends only over certain $j_1, j_2 \leq j_\alpha$, and (6.69) can be estimated by

$$\begin{aligned}\sum_{\substack{j \colon \max j - \frac{1}{2}\min j \\ \leq \ell - |\nu_1| + \frac{1}{2}|\nu_2|}} 2^{\max j - |\nu_1|}(2 + 2^{\min j - j_\alpha}\sqrt{\ell + d_\alpha}) &\lesssim \sum_{j_2 = j_0}^{s_2} (1 + 2^{j_2 - j_\alpha}\sqrt{\ell + d_\alpha}) \sum_{j_1 = j_0}^{s_1(j_2)} 2^{j_1 - |\nu_1|} \\ &\lesssim 2^{2\ell - 3|\nu_1| + |\nu_2|}(1 + \sqrt{\ell + d_\alpha} 2^{2\ell - j_\alpha - 2|\nu_1| + |\nu_2|}) \\ &\leq 2^{2\ell - 3|\nu_1| + |\nu_2|}(1 + \sqrt{\ell + d_\alpha})\,,\end{aligned}$$

where $s_2 := \lfloor 2\ell - 2|\nu_1| + |\nu_2| \rfloor$, $s_1(j_2) := \lfloor \ell + \frac{1}{2} j_2 - |\nu_1| + \frac{1}{2}|\nu_2| \rfloor$; note that by the assumption on ℓ, we have $2^{2\ell - 3|\nu_1| + |\nu_2|} \leq 2^{j_\alpha - |\nu_1|}$, and we thus have the sought estimate of the number of matrix entries by (6.52) in this case.

Second, in case that $\ell > \frac{1}{2} j_\alpha + |\nu_1| - \frac{1}{2}|\nu_2|$, the partial sum for $j_1, j_2 \leq j_\alpha$ can be estimated similarly by

$$(d_\alpha + \sqrt{\ell + d_\alpha}) 2^{j_\alpha - |\nu_1|} \leq (d_\alpha + \sqrt{\ell + d_\alpha}) 2^{\frac{4}{4p+1}\ell - \frac{4p+5}{4p+1}|\nu_1| + \frac{2}{4p+1}|\nu_2| + \frac{4p-1}{4p+1} j_\alpha}\,,$$

where we have added $(p + \frac{1}{4})^{-1}(\ell - \frac{1}{2} j_\alpha + |\nu_1| - \frac{1}{2}|\nu_2|) > 0$ in the exponent to obtain the right hand side, which in turn can be bounded by a constant multiple of (6.53), that is,

$$\lesssim (1 + \sqrt{\ell + d_\alpha}) \min\big\{(1 + d_\alpha) 2^{2\ell - 3|\nu_1| + |\nu_2|}, 2^{j_\alpha} 2^{(p+\frac{1}{4})^{-1}\ell - |\nu_1|}\big\}\,.$$

For the partial sum over $\max j > j_\alpha$, $\min j \le j_\alpha$, we obtain

$$\begin{aligned}\sum_{\substack{j:\,\max j - \frac12 \min j \\ + p(\max j - j_\alpha) \\ \le \ell - |\nu_1| + \frac12 |\nu_2|}} 2^{\max j - |\nu_1|}(1 + 2^{\min j - j_\alpha}\sqrt{\ell + d_\alpha}) &= \sum_{j_2 = j_0}^{\lfloor j_\alpha \rfloor} (1 + 2^{j_2 - j_\alpha}\sqrt{\ell + d_\alpha}) \sum_{j_1 = j_\alpha}^{s_1(j_2)} 2^{j_1 - |\nu_1|} \\ &\lesssim 2^{(p+1)^{-1}\ell + \frac{2p+1}{2p+2} j_\alpha - \frac{p+2}{p+1}|\nu_1| + \frac{1}{2(p+1)}|\nu_2|}(1 + \sqrt{\ell + d_\alpha}) \\ &\lesssim 2^{j_\alpha} 2^{(p+\frac14)^{-1}\ell - |\nu_1|}(1 + \sqrt{\ell + d_\alpha})\end{aligned}$$

with $s_1(j_2) := \lfloor (p+1)^{-1}(\ell + \frac12 j_2 + p j_\alpha - |\nu_1| + \frac12 |\nu_2|)\rfloor$. Note that in this case, because $j_\alpha < 2\ell - 2|\nu_1| + |\nu_2|$ we still have

$$2^{\frac{\ell}{p+1} + \frac{2p+1}{2p+2} j_\alpha - \frac{p+2}{p+1}|\nu_1| + \frac{1}{2(p+1)}|\nu_2|} < 2^{2\ell - 3|\nu_1| + |\nu_2|}\,.$$

For the partial sum over $j_1, j_2 > j_\alpha$, the condition on c_s reads $(p+1)\max j + (p - \frac12)\min j \le \ell - |\nu_1| + \frac12|\nu_2| + 2p j_\alpha$, which leads to an estimate by

$$\begin{aligned}(1 + \sqrt{\ell + d_\alpha}) \sum_{j_2 = j_\alpha}^{s_2} \sum_{j_1 = j_2}^{s_1(j_2)} 2^{j_1 - |\nu_1|} 2^{j_2 - j_\alpha} &\le 2^{(p+\frac14)^{-1}\ell - \frac{4p+5}{4p+1}|\nu_1| + \frac{2}{4p+1}|\nu_2| + \frac{4p-1}{4p+1} j_\alpha}(1 + \sqrt{\ell + d_\alpha}) \\ &\lesssim 2^{j_\alpha} 2^{(p+\frac14)^{-1}\ell - |\nu_1|}(1 + \sqrt{\ell + d_\alpha})\end{aligned}$$

with $s_1(j_2) := \lfloor (p+1)^{-1}(\ell - |\nu_1| + \frac12 |\nu_2| + 2p j_\alpha - (p - \frac12) j_2)\rfloor$, $s_2 := \lfloor (2p + \frac12)^{-1}(\ell - |\nu_1| + \frac12|\nu_2| + 2p j_\alpha)\rfloor$. Again, from $\ell > \frac12 j_\alpha + |\nu_1| - \frac12 |\nu_2|$ it follows that

$$2^{\frac{4}{4p+1}\ell - \frac{4p+5}{4p+1}|\nu_1| + \frac{2}{4p+1}|\nu_2| + \frac{4p-1}{4p+1} j_\alpha} < 2^{2\ell - 3|\nu_1| + |\nu_2|}\,,$$

which completes our analysis for the case $|\nu_1|, |\nu_2| \le j_\alpha$. Note that the maximum number of entries arises in the case $|\nu| = (j_0, j_0)$. □

Example 6.30. As in Example 6.25, we compare the estimates for matrix entries in the proof of Theorem 6.27 to the numerical observation. We consider

$$L_{j_1, j_2} := \sqrt{\alpha}\, 2^{-\max\{j_1, j_2\}} \sum_{\mu \in \nabla^2_{(j_1, j_2)}} \left| \int e^{-\alpha(x_1 - x_2)^2} \Psi_\mu \, \Psi_{\nu_0} \, \mathrm{d}x \right|$$

with $\nu_0 = ((0,0,0),(0,0,0)) \in \nabla^2$ and $\alpha = 10^2, 10^4$, corresponding to $j_\alpha = 3.82, 7.14$.

In view of the estimates in the proof of Theorem 6.20, for $j_1, j_2 \ge 0$ we expect

$$L_{j_1, j_2} \le C 2^{-\frac12 |j_1 - j_2|}\, 2^{-p \max\{|j_1 - j_2|, (j_1 - j_\alpha)_+ + (j_2 - j_\alpha)_+\}} \tag{6.70}$$

with some $C > 0$ and with p depending on the wavelet basis. Here we use the same wavelet as in Example 6.30.

As can be seen from Figures 6.4 and 6.5, the estimate (6.70) captures the essential qualitative behaviour. However, similarly to Example 6.25, the predicted values for j_α and p yield an overestimate. The lines with markers show the actual values of L_{j_1, j_2} for the two values of α. The dashed grey lines show the right hand side of (6.48) with $C = 80$, $p = 4.3$, and j_α as above, whereas the dashed black lines show these reference values with $C = 350$, $p = 5.4$, and $j_\alpha = 2.5, 6.0$. The latter reproduce the observed decay more accurately.

Remark 6.31. *There is a similar interpretation for the resulting compressibility as in Remark*

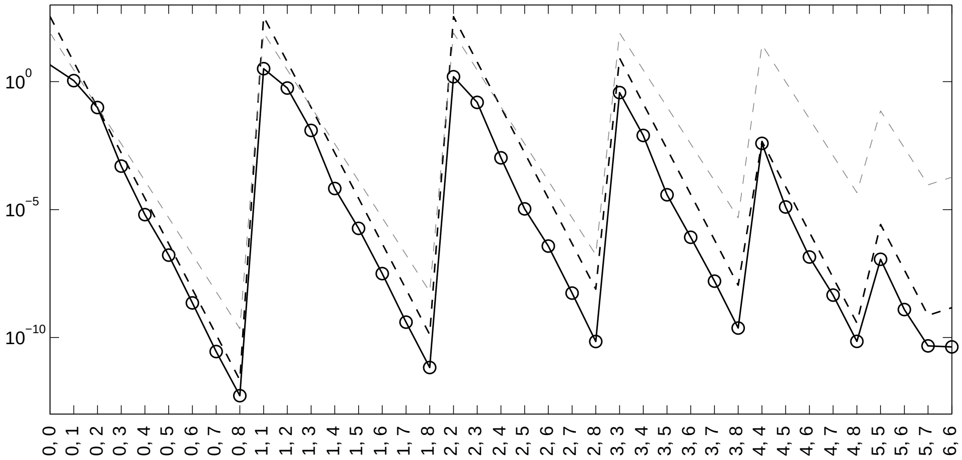

Figure 6.4. Actual values and estimates of L_{j_1,j_2} as in Example 6.30 with $\alpha = 10^2$.

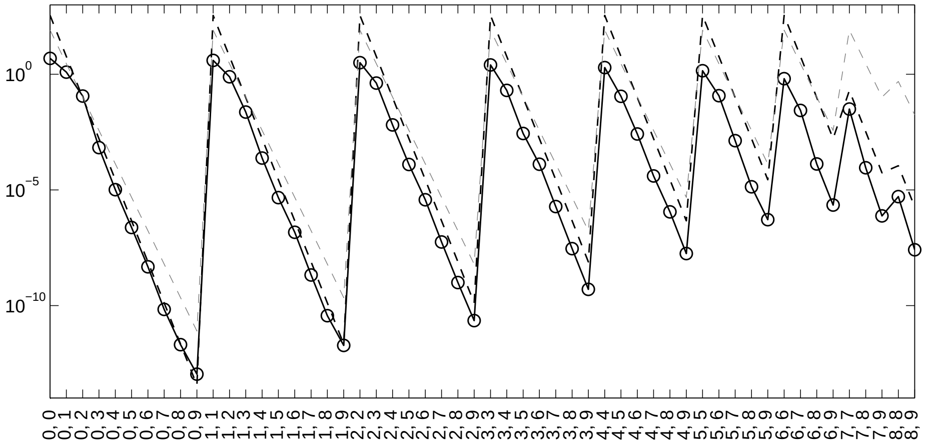

Figure 6.5. Actual values and estimates of L_{j_1,j_2} as in Example 6.30 with $\alpha = 10^4$.

6.26. For large α,

$$\sqrt{\pi^{-1}\alpha}\int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\,\Psi_\mu(x)\,\Psi_\nu(x)\,\mathrm{d}x \approx \int_{\mathbb{R}} \Psi_\mu(x,x)\,\Psi_\nu(x,x)\,\mathrm{d}x =: m_{\nu\mu}\,.$$

Let $\nu \in \nabla^2$ *and* $j \in \mathbb{Z}^2_{j_0}$*, then* $\sum_{\mu\in\nabla^2_j} |m_{\nu\mu}| \lesssim 2^{-\max|\nu|}2^{\frac{1}{2}(|\nu_1|+|\nu_2|+j_1+j_2)}$*, and the total number of nonzero entries for the level combination* $(|\nu|, j)$*, with this fixed* ν*, is of order* $2^{(\max j - \max|\nu|)_+}$.

If we now compress $M := (2^{-\max|\nu|-\max|\mu|}m_{\nu\mu})$ *by setting to zero all entries for which* $\max|\mu| + \max|\nu| - \frac{1}{2}(\min|\mu| + \min|\nu|) > \ell$*, we thus find with Lemma 6.8, using the weight sequence* $\omega_j = 2^{-\frac{1}{2}\max j}$*, that* M *is* s^**-compressible with* $s^* = \frac{1}{2}$*. This value corresponds to the first term in the minimum in* (6.53)*; the second term, however, can yield a better compressibility depending on* α*, which will be considered next.*

From Theorem 6.27, we can derive a result concerning the compressibility of the full six-dimensional Coulomb interaction potential as well. To this end, we additionally estimate the arising parameters α.

Corollary 6.32. *For a tensor product wavelet basis* $\{\Psi_\nu\}_{\nu\in\nabla^6}$ *constructed from a univariate wave-*

let $\psi \in \mathrm{W}^p_\infty(\mathbb{R})$*, the representation matrix*

$$\left(\Big(\sum_{i=1}^{6} 2^{2|\nu_i|}\Big)^{-\frac{1}{2}} \Big(\sum_{i=1}^{6} 2^{2|\mu_i|}\Big)^{-\frac{1}{2}} \int_{\mathbb{R}^6} \frac{1}{|x-y|} \Psi_\nu(x,y)\, \Psi_\mu(x,y)\, \mathrm{d}(x,y) \right)_{\nu,\mu\in\nabla^6}$$

of the two-electron Coulomb potential considered as a multiplication operator $\mathrm{H}^1(\mathbb{R}^6) \to \mathrm{H}^{-1}(\mathbb{R}^6)$ *is* s^**-compressible with*

$$s^* = \left(\frac{4p+1}{4p+5}\right)\frac{1}{3}\,.$$

Proof. In this proof, let C denote a generic positive constant. For given $\delta > 0$, Theorem 4.17 yields an exponential sum approximation of $t \mapsto t^{-1/2}$ with error in supremum norm on $[1,\infty)$ bounded by δ, with $N \lesssim |\ln\delta|^2$ terms. Let $\omega_{\delta,k}$, $\alpha_{\delta,k}$, $k = 1,\ldots,N$, denote the corresponding coefficients. Using Theorem 6.9, which here can be applied with $R = \infty$, we obtain an exponential sum approximation with coefficients $\hat\omega_k := r^{-1}\omega_{\delta,k}$, $\hat\alpha_k := r^{-2}\alpha_{\delta,k}$ for the two-electron Coulomb potential $|x-y|^{-1}$ with error in operator norm $\mathrm{H}^1 \to \mathrm{H}^{-1}$ bounded by $C(r + r^{-1}\delta)$. We thus choose $r = 2^{-\ell}$ and $\delta = r^2$. By Corollary 4.20, the corresponding coefficients $\hat\omega_k$, $\hat\alpha_k$ satisfy $\hat\omega_k \lesssim \ell^{-1}\sqrt{\hat\alpha_k}$. Furthermore, by Corollary 4.21, we have $\hat\alpha_k \lesssim \sqrt{\ell}2^{2\ell}$ and thus $j_{\hat\alpha_k} \lesssim \ell$. Combining Theorem 6.27 with Remark 6.28, we obtain an approximation for each term in the exponential sum approximation with error bounded by $C(\hat\omega_k/\sqrt{\hat\alpha_k}) j^4_{\hat\alpha_k} 2^{-\ell} \lesssim \ell^{-1}\ell^4 2^{-\ell} = \ell^3 2^{-\ell}$, and a number of nonzero entries per row and column bounded by $C(\sqrt{\ell + \ln\hat\alpha_k}\sqrt{\hat\alpha_k}2^{(p+\frac{1}{4})^{-1}\ell})^3 \lesssim \ell^{3/2}2^{3(1+(p+\frac{1}{4})^{-1})\ell}$. Using $N \lesssim \ell^2$, the assertion follows. ☐

Remark 6.33 (Resulting compressibility of factor matrices for relevant choices of α)**.** *Taking the maximum size of the parameter* α *required for a certain error in the exponential sum approximation of the Coulomb potential into account, Theorem 6.27 can yield better compressibility than* $s^* = \frac{1}{2}$ *for the factor matrices* $(\sqrt{\alpha}2^{-\max|\mu|-\max|\nu|}a_{\nu\mu})_{\nu,\mu\in\nabla^2}$*, with* $a_{\nu\mu}$ *as in* (6.49)*. For an exponential sum approximation based on Theorem 4.17, the same argument as in the proof of Corollary 6.32 yields* $s^* = (4p+1)/(4p+5)$ *for these lower-dimensional components – in other words, one can come arbitrarily close to* $s^* = 1$ *for large* p*. Note that this is substantially better than the worst case, for general* α*, as considered in Remark 6.31.*

6.4.3 Nonsymmetric Two-Electron Operators

Theorem 6.34. *Let* $\alpha > 0$ *and* $\psi \in \mathrm{W}^p_\infty(\mathbb{R})$ *for an integer* $p \geq 2$*, then* $(a_{\nu\mu})_{\nu,\mu\in\nabla^2}$ *and* $(b_{\nu\mu})_{\nu,\mu\in\nabla^2}$ *with entries*

$$a_{\nu\mu} = \int e^{-\alpha(x_1-x_2)^2}\Psi_\mu(x)\,\Psi_\nu(x)\,\mathrm{d}x\,, \tag{6.71a}$$

$$b_{\nu\mu} = \int (x_1-x_2)e^{-\alpha(x_1-x_2)^2}\big((\mathrm{D}_{x_1}-\mathrm{D}_{x_2})\Psi_\mu(x)\big)\,\Psi_\nu(x)\,\mathrm{d}x \tag{6.71b}$$

satisfy

$$\|(|a_{\nu\mu}|)\|_{\ell_2(\nabla^2)\to\ell_2(\nabla^2)} \lesssim (\max\{1, j_\alpha - j_0\})^2\,, \tag{6.72}$$

$$\sqrt{\alpha}\|(2^{-\max|\mu|}|b_{\nu\mu}|)\|_{\ell_2(\nabla^2)\to\ell_2(\nabla^2)} \lesssim (\max\{1, j_\alpha - j_0\})^2\,, \tag{6.73}$$

and for $\ell > 0$ *there exist infinite matrices* $(\tilde a^{(\ell)}_{\nu\mu})$*,* $(\tilde b^{(\ell)}_{\nu\mu})$ *for which*

$$\big\|\big(2^{-\max|\nu|}|a_{\nu\mu} - \tilde a^{(\ell)}_{\nu\mu}|\big)\big\|_{\ell_2(\nabla^2)\to\ell_2(\nabla^2)} \lesssim (\max\{1, j_\alpha - j_0\})^{\frac{1}{2}}2^{-\ell}\,, \tag{6.74a}$$

$$\big\|\big(\sqrt{\alpha}2^{-\max|\mu|-\max|\nu|}|b_{\nu\mu} - \tilde b^{(\ell)}_{\nu\mu}|\big)\big\|_{\ell_2(\nabla^2)\to\ell_2(\nabla^2)} \lesssim (\max\{1, j_\alpha - j_0\})^{\frac{1}{2}}2^{-\ell}\,, \tag{6.74b}$$

where the number of entries in the column corresponding to $\mu \in \nabla^2$ *is bounded by*

$$C\big(1+\sqrt{\ell}\big)\min\big\{\big(1+(\ln\alpha)_+\big)2^{\ell-\max|\mu|}, \max\{1, 2^{-\max|\mu|}\sqrt{\alpha}\}2^{\tilde{p}^{-1}\ell}\big\}\,, \tag{6.75}$$

and hence the maximum number of entries per column is bounded by

$$\tilde{C}\big(1+\sqrt{\ell}\big)\min\big\{\big(1+(\ln\alpha)_+\big)2^{\ell}, (1+\sqrt{\alpha})2^{\tilde{p}^{-1}\ell}\big\}\,, \tag{6.76}$$

where $\tilde{p} = p+\frac{1}{2}$ *in the case of* $(\tilde{a}^{(\ell)}_{\nu\mu})$ *and* $\tilde{p} = p-\frac{1}{2}$ *in the case of* $(\tilde{b}^{(\ell)}_{\nu\mu})$, *and* $C, \tilde{C} > 0$ *are independent of* ℓ *and* α.

Remark 6.35. *The application of Theorem 6.34 to terms in exponential sum approximations of* $|x-y|^{-1}(x-y)\cdot(\mathrm{D}_x - \mathrm{D}_y)$ *deviates slightly from Remarks 6.21 and 6.28; we obtain*

$$\begin{aligned}
&\Big\|\Big(\sqrt{\alpha}2^{-\max|\mu|-\max|\nu|}\Big(b_{\nu_1\mu_1}a_{\nu_2\mu_2}a_{\nu_3\mu_3} - \tilde{b}_{\nu_1\mu_1}\tilde{a}_{\nu_2\mu_2}\tilde{a}_{\nu_3\mu_3}\Big)\Big)_{\mu,\nu\in(\nabla^2)^3}\Big\| \\
&\qquad \lesssim \big\|(|a_{\nu_1\mu_1}|)_{\nu_1,\mu_1\in\nabla^2}\big\|^2\Big(\sqrt{\alpha}\big\|(2^{-\max|\nu_1|-\max|\mu_1|}|b_{\nu_1\mu_1} - \tilde{b}_{\nu_1\mu_1}|)_{\nu_1,\mu_1\in\nabla^2}\big\|\Big) \\
&\qquad\qquad + \Big(\sqrt{\alpha}\big\|(2^{-\max|\mu_1|}|b_{\nu_1\mu_1}|)_{\nu_1,\mu_1\in\nabla^2}\big\|\Big)\,\big\|(|a_{\nu_1\mu_1}|)_{\nu_1,\mu_1\in\nabla^2}\big\| \\
&\qquad\qquad\qquad \times \big\|(2^{-\max|\nu_1|}|a_{\nu_1\mu_1} - \tilde{a}_{\nu_1\mu_1}|)_{\nu_1,\mu_1\in\nabla^2}\big\| \;\lesssim\; \max\{1, j_\alpha - j_0\}^{\frac{9}{2}}\,2^{-\ell}\,.
\end{aligned} \tag{6.77}$$

It should also be noted that in contrast to Theorems 6.20 and 6.27, for reasons that will become clear in the proof, in Theorem 6.34 we do not obtain useful compressibility estimates for the transposed matrices.

Proof of Theorem 6.34. For given $\nu, \mu \in \nabla^2$, let β_i, γ_i be defined as in (6.55), and let $S_\nu, S_{\nu\mu} \subset \mathbb{R}^2$ be the smallest Cartesian products of closed intervals such that $\operatorname{supp}\Psi_\nu \subseteq S_\nu$ and $\operatorname{supp}\Psi_\nu\Psi_\mu \subseteq S_{\nu\mu}$.

Estimates for matrix entries: For any integers $0 \le p_1, p_2 \le p-1$,

$$\begin{aligned}
|b_{\nu\mu}| &\lesssim 2^{-j_\alpha}2^{\max|\nu|}2^{\frac{1}{2}(|\nu_1|+|\nu_2|+|\mu_1|+|\mu_2|)}2^{-p_1|\gamma_1|-p_2|\gamma_2|} \\
&\qquad \times \sum_{i_1=0}^{p_1}\sum_{i_2=0}^{p_2} 2^{(p_1-i_1)|\beta_1|}2^{(p_2-i_2)|\beta_2|}\int_{S_\gamma}|\mathrm{D}^{i_1}_{x_1}\mathrm{D}^{i_2}_{x_2}\sqrt{\alpha}(x_1-x_2)e^{-\alpha(x_1-x_2)^2}|\,\mathrm{d}x\,;
\end{aligned} \tag{6.78}$$

note the multiplication by $2^{-j_\alpha}2^{j_\alpha} \sim 2^{-j_\alpha}\sqrt{\alpha}$. Combining the estimate

$$\begin{aligned}
|\mathrm{D}^{i_1}_{x_1}\mathrm{D}^{i_2}_{x_2}\sqrt{\alpha}(x_1-x_2)e^{-\alpha(x_1-x_2)^2}| &\le |\sqrt{\alpha}\mathrm{D}^{i_1-1}_{x_1}\mathrm{D}^{i_2}_{x_2}e^{-\alpha(x_1-x_2)^2}| + |\sqrt{\alpha}(x_1-x_2)\partial^{i_1}_{x_1}\partial^{i_2}_{x_2}e^{-\alpha(x_1-x_2)^2}| \\
&\le C_{p_1,p_2}(2\alpha)^{\frac{1}{2}(i_1+i_2)}\big(e^{-\frac{\alpha}{2}(x_1-x_2)^2} + \sqrt{\alpha}|x_1-x_2|\,e^{-\frac{\alpha}{2}(x_1-x_2)^2}\big)
\end{aligned}$$

with the definition

$$F^{(i,j)}_{\mathrm{ns}}(S) := \begin{cases} \sup_{x\in S}\sqrt{\alpha}|x_1-x_2|e^{-\alpha(x_1-x_2)^2}\,, & i_1, i_2, j_1, j_2 \le j_\alpha\,, \\ \sup_{x\in S}\max\{1, \sqrt{\alpha}|x_1-x_2|\}e^{-\frac{\alpha}{2}(x_1-x_2)^2}\,, & \text{otherwise} \end{cases}$$

for $i, j \in \mathbb{Z}^2_{j_0}$ and $S \subseteq \mathbb{R}^2$, we obtain in the same manner as in the proof of Theorem 6.27 that

$$\int_{S_\gamma}\sqrt{\alpha}|x_1-x_2|\,e^{-\frac{\alpha}{2}(x_1-x_2)^2}\,\mathrm{d}x \lesssim 2^{-\max|\gamma|}\min\big\{2^{-j_\alpha}, 2^{-\min|\gamma|}F^{(|\nu|,|\mu|)}_{\mathrm{ns}}(S_\gamma)\big\}\,.$$

Hence, using (6.57) and (6.58),

$$|b_{\nu\mu}| \lesssim 2^{-j_\alpha} 2^{\max|\mu|} 2^{-\max|\gamma|} \min\bigl\{2^{-j_\alpha}, 2^{-\min|\gamma|} F_{\mathrm{ns}}^{(|\nu|,|\mu|)}(S_\gamma)\bigr\} \\ \times \prod_{d=1}^{2} 2^{\frac{1}{2}(|\mu_d|+|\nu_d|)} 2^{-(p-1)h_\alpha(|\nu_d|,|\mu_d|)} \,.$$

Estimating $|b_{\nu\mu}|$ directly by Hölder's inequality, we also obtain

$$|b_{\nu\mu}| \lesssim 2^{-j_\alpha} 2^{\max|\mu|} 2^{-\max|\gamma|} \min\bigl\{2^{-j_\alpha}, 2^{-\min|\gamma|} F_{\mathrm{ns}}^{(|\nu|,|\mu|)}(S_\gamma)\bigr\} \prod_{d=1}^{2} 2^{\frac{1}{2}(|\mu_d|+|\nu_d|)} \,.$$

We combine these estimates in the same manner as in the proof of Theorem 6.27. However, as to be expected, summations over rows and columns of $(b_{\nu\mu})$ yield different results. Using compact support of the wavelets as in (6.33), we obtain

$$\sum\nolimits_{\mu\in\nabla^2_j} |b_{\nu\mu}| \lesssim 2^{-j_\alpha} 2^{\max j} 2^{-\max|\nu|} \min\bigl\{2^{-j_\alpha}, 2^{-\min|\nu|} F_{\mathrm{ns}}^{(|\nu|,j)}(S_\nu)\bigr\} \\ \times \prod_{d=1}^{2} 2^{\frac{1}{2}(j_d+|\nu_d|)} 2^{-(p-1)(h_\alpha(|\nu_d|,j_d))_+} \,, \tag{6.79}$$

$$\sum\nolimits_{\nu\in\nabla^2_j} |b_{\nu\mu}| \lesssim 2^{-j_\alpha} \min\bigl\{2^{-j_\alpha}, 2^{-\min|\mu|} F_{\mathrm{ns}}^{(j,|\mu|)}(S_\mu)\bigr\} \prod_{d=1}^{2} 2^{\frac{1}{2}(|\mu_d|+j_d)} 2^{-(p-1)(h_\alpha(j_d,|\mu_d|))_+} \,. \tag{6.80}$$

Proof of (6.72), (6.73): The estimate for $\|(|a_{\nu\mu}|)\|$ has been shown in the proof of Theorem 6.27. Setting $\omega_j = 2^{-\frac{1}{2}(j_1+j_2)}$ and using (6.79) and (6.80), we find

$$2^{j_\alpha}\omega_{|\nu|}^{-1} \sum_{\mu\in\nabla^2} \omega_\mu 2^{-\max|\mu|} |b_{\nu\mu}| \,, \quad 2^{j_\alpha}\omega_{|\mu|}^{-1} \sum_{\nu\in\nabla^2} \omega_\nu 2^{-\max|\mu|} |b_{\nu\mu}| \quad \lesssim \bigl(\max\{1, j_\alpha - j_0\}\bigr)^2 \,,$$

and thus obtain (6.73) by Lemma 6.8.

Construction of compressed matrices and proof of (6.74): We fix $\Theta \in W_2$ and define, for $\nu,\mu \in \nabla^2$,

$$\hat\Lambda_{\mathrm{ns}}(t) := \bigl\{(\nu,\mu) \in (\nabla^2)^2 \colon\; F_{\mathrm{ns}}^{(|\nu|,|\mu|)}(S_{\nu\mu}) < \Theta_{|\nu|,|\mu|} 2^{-t}\bigr\} \,.$$

Furthermore, let $c_{\mathrm{ns},q}(i,j) := \max i + q((h_\alpha(i_1,j_1))_+ + (h_\alpha(i_2,j_2))_+)$ for $i,j \in \mathbb{Z}^2$ and $q > 0$. We define the compressed matrices for $(b_{\nu\mu})$ as

$$\tilde b_{\nu\mu}^{(\ell)} = \begin{cases} 0\,, & c_{\mathrm{ns},p-1}(|\nu|,|\mu|) > \ell \quad\text{or}\quad (\nu,\mu) \in \hat\Lambda_{\mathrm{ns}}(\ell - c_{\mathrm{ns},p-1}(|\nu|,|\mu|))\,, \\ b_{\nu\mu}\,, & \text{otherwise,} \end{cases} \tag{6.81}$$

where the superscript is suppressed in what follows.

The error is estimated by Lemma 6.8 with $\omega_j = 2^{-\frac{1}{2}(j_1+j_2)}$. On the one hand, using (6.79),

$$2^{j_\alpha}\omega_{|\nu|}^{-1} \sum_{\mu\in\nabla^2} \omega_{|\mu|} 2^{-\max|\nu|-\max|\mu|} |b_{\nu\mu} - \tilde b_{\nu\mu}| \\ \lesssim \sum_{j\in\mathbb{Z}^2_{j_0}} \Theta_{|\nu|,j} 2^{-\ell} + 2^{-\max|\nu|} \sum_{\substack{j\in\mathbb{Z}^2_{j_0} \\ c_{\mathrm{ns},p-1}(|\nu|,j)>\ell}} \prod_{d=1}^{2} 2^{-(p-1)(h_\alpha(|\nu_d|,j_d))_+} \lesssim \bigl(1 + \max\{1, j_\alpha - j_0\}\bigr) 2^{-\ell} \,. \tag{6.82}$$

On the other hand, by (6.80),

$$
\begin{aligned}
&2^{j_\alpha}\omega_{|\mu|}^{-1}\sum_{\nu\in\nabla^2}\omega_{|\nu|}2^{-\max|\nu|-\max|\mu|}|b_{\nu\mu}-\tilde{b}_{\nu\mu}| \\
&\qquad\qquad \lesssim \sum_{j\in\mathbb{Z}^2_{j_0}}\Theta_{|\nu|,j}2^{-\ell} + \sum_{\substack{j\in\mathbb{Z}^2_{j_0}\\ c_{\mathrm{ns},p-1}(j,|\mu|)>\ell}} 2^{-\max j}\prod_{d=1}^{2}2^{-(p-1)(h_\alpha(j_d,|\mu_d|))_+} \lesssim 2^{-\ell}\,, \qquad (6.83)
\end{aligned}
$$

which together shows (6.74b).

From (6.59), (6.61) we see that $(2^{-\max|\nu|}|a_{\nu\mu}|)$ satisfies the estimates that have been used above for $(\sqrt{\alpha}2^{-\max|\nu|-\max|\mu|}|b_{\nu\mu}|)$ as well, with the exception that F_{ns} is replaced by F_{s} and $p-1$ by p. The compressed matrices for $(a_{\nu\mu})$ are therefore defined as

$$
\tilde{a}^{(\ell)}_{\nu\mu} = \begin{cases} 0\,, & c_{\mathrm{ns},p}(|\nu|,|\mu|) > \ell \quad \text{or} \quad (\nu,\mu)\in\hat{\Lambda}_{\mathrm{s}}(\ell - c_{\mathrm{ns},p}(|\nu|,|\mu|)) \\ a_{\nu\mu}\,, & \text{otherwise,} \end{cases} \qquad (6.84)
$$

with $\hat{\Lambda}_{\mathrm{s}}$ defined as in (6.64). Using again $\omega_j = 2^{-\frac{1}{2}(j_1+j_2)}$, we obtain the estimates

$$
\omega_{|\nu|}^{-1}\sum_{\mu\in\nabla^2}\omega_{|\mu|}2^{-\max|\nu|}|a_{\nu\mu}-\tilde{a}_{\nu\mu}| \lesssim \max\{1, j_\alpha - j_0\}2^{-\ell}\,, \qquad (6.85)
$$

$$
\omega_{|\mu|}^{-1}\sum_{\nu\in\nabla^2}\omega_{|\nu|}2^{-\max|\nu|}|a_{\nu\mu}-\tilde{a}_{\nu\mu}| \lesssim 2^{-\ell} \qquad (6.86)
$$

as in (6.82), (6.83).

Estimates for the number of matrix entries: Let $\mu\in\nabla^2$ with $|\mu_1|\geq|\mu_2|$, then

$$
\begin{aligned}
n_\ell(|\mu|,j) &:= \#\{\nu\in\nabla^2\colon |\nu| = (j_1,j_2)\,,\ \tilde{b}_{\nu\mu}\neq 0\} \\
&\lesssim 2^{(j_1-|\mu_1|)_+}\min\{1 + 2^{j_2-j_\alpha}\sqrt{\ell} + 2^{j_2-\max\{j_1,|\mu_1|\}}, 2^{(j_2-|\mu_2|)_+}\}\,.
\end{aligned}
$$

We need to sum this expression over all $j=(j_1,j_2)$ with $c_{\mathrm{ns}}(|\mu|,j)\leq\ell$.

We treat here the case $|\mu_1|,|\mu_2|\leq j_\alpha$ with $j_\alpha\geq j_0$ that leads to the asymptotic upper bound for the number of nonzero entries per column; the remaining cases can be treated analogously to the proof of (6.52).

Let $\mu\in\nabla^2$ with $|\mu_1|\geq|\mu_2|$ and $|\mu_1|,|\mu_2|\leq j_\alpha$. We obtain

$$
\sum_{j\in\mathbb{Z}^2_{j_0}} n_\ell(|\mu|,j) \lesssim \sum_{j\in L_\ell}(2^{j_1-\max|\mu|} + 2^{j_2-\max|\mu|} + 2^{j_1+j_2-\max|\mu|-j_\alpha}\sqrt{\ell})\,, \qquad (6.87)
$$

where $L_\ell := \bigl\{j\in\mathbb{Z}^2_{j_0}\colon \max j + (p-1)(j_1-j_\alpha)_+ + (p-1)(j_2-j_\alpha)_+ \leq \ell\bigr\}$. Note that $\ell\leq j_\alpha$ implies $j_1,j_2\leq j_\alpha$. In the latter case, (6.87) can be estimated further by

$$
\begin{aligned}
\sum_{j\colon\max j\leq\ell} 2^{\max j-\max|\mu|}(1+2^{\min j-j_\alpha}\sqrt{\ell}) &\leq \sum_{j_1=j_0}^{\lfloor\ell\rfloor}\sum_{j_2=j_0}^{j_1}2^{j_1-\max|\mu|}(1+2^{j_2-j_\alpha}\sqrt{\ell}) \\
&\lesssim \bigl((j_\alpha-j_0)_+ + \sqrt{\ell}\bigr)2^{\ell-\max|\mu|}\,.
\end{aligned}
$$

In case that $\ell > j_\alpha$, the partial sum over $j_1,j_2\leq j_\alpha$ can be estimated by $(j_\alpha-j_0)_+2^{j_\alpha-\max|\mu|}$. If

$\max j > j_\alpha$, $\min j \leq j_\alpha$, we obtain

$$\sum_{\substack{j\colon \max j + \\ (p-1)(\max j - j_\alpha) \leq \ell}} 2^{\max j - \max|\mu|}(1 + 2^{\min j - j_\alpha}\sqrt{\ell}) \leq \sum_{j_1 = j_\alpha}^{\lfloor p^{-1}(\ell + (p-1)j_\alpha)\rfloor} \sum_{j_2 = j_0}^{\lfloor j_\alpha \rfloor} 2^{j_1 - \max|\mu|}(1 + 2^{j_2 - j_\alpha}\sqrt{\ell})$$
$$\lesssim \bigl((j_\alpha - j_0)_+ + \sqrt{\ell}\bigr) 2^{\frac{\ell}{p} + \frac{p-1}{p} j_\alpha - \max|\mu|} \,.$$

Note that in this case, because of $\ell > j_\alpha$, we still have

$$2^{\frac{\ell}{p} + \frac{p-1}{p} j_\alpha - \max|\mu|} < 2^{\ell - \max|\mu|} \,.$$

If $j_1, j_2 > j_\alpha$, the condition in the summation reads $p \max j + (p-1)\min j \leq \ell + 2(p-1)j_\alpha$, which leads to the estimate

$$(1 + \sqrt{\ell}) \sum_{j_2 = j_\alpha}^{s_2} \sum_{j_1 = j_2}^{s_1(j_2)} 2^{j_1 - \max|\mu|} 2^{j_2 - j_\alpha} \lesssim (1 + \sqrt{\ell}) 2^{\frac{2}{2p-1}\ell + \frac{2p-3}{2p-1} j_\alpha - \max|\mu|}$$

with $s_2 = \lfloor (2p-1)^{-1}(\ell + 2(p-1)j_\alpha)\rfloor$, $s_1(j_2) = \lfloor p^{-1}(\ell + 2(p-1)j_\alpha - (p-1)j_2)\rfloor$. Again, $\ell > j_\alpha$ implies that

$$2^{\frac{2}{2p-1}\ell + \frac{2p-3}{2p-1} j_\alpha - \max|\mu|} < 2^{\ell - \max|\mu|} \,.$$

The maximum number of entries arises in the case $\mu = (j_0, j_0)$. Altogether, we obtain the estimates (6.75), (6.76) for $(\tilde{b}_{\nu\mu})$; the very same line of arguments leads to the estimate for $(\tilde{a}_{\nu\mu})$. ☐

6.5 Evaluation of Basic Integrals of Wavelets

For the numerical realization of adaptive wavelet schemes, the use of piecewise polynomial basis functions is beneficial in a number of ways. As mentioned in Section 6.2, the compression of a large class of operators, including in particular the Laplacian relevant in our case, can be done more efficiently for piecewise polynomial wavelets. Furthermore, for such wavelets the computation of integrals can be carried out by standard quadrature schemes.

As discussed in Section 6.1, however, in our setting an orthonormal basis is required. Since orthonormal spline multiwavelets of higher approximation order will generally lead to a large number of active basis functions, it may thus be preferable to use compactly supported orthonormal wavelets from the Daubechies family. These are given only implicitly via the compactly supported coefficient sequences $(h_k)_{k\in\mathbb{Z}}$ and $(g_k)_{k\in\mathbb{Z}}$ in the scaling relations

$$\varphi = \sqrt{2}\sum_k h_k\,\varphi(2\cdot - k)\,, \qquad \psi = \sqrt{2}\sum_k g_k\,\varphi(2\cdot - k)\,. \tag{6.88}$$

In principle, these scaling relations can be used to approximate point values of the wavelets via the cascade algorithm (see e.g. [38]), but the convergence of this procedure depends rather unfavorably on the Hölder smoothness of the wavelets. Since we are mainly interested in wavelet bases of fairly limited smoothness, we therefore do not rely on standard quadrature procedures that require point evaluations for such wavelets, but instead consider integration schemes that directly use the scaling relations (6.88).

It should be noted that for general wavelet bases, we cannot expect to achieve an integration scheme that is as efficient as in the piecewise polynomial case, where it is typically possible to compute arbitrary discretization matrix entries using $\mathcal{O}(1)$ operations. However, as illustrated by the numerical experiments in Section 6.6, we do obtain schemes that allow to compute the integrals required for our purposes with reasonable complexity. Before turning to the integrals required for the approximate potential terms in Section 6.6, in this section we discuss the computation of basic integrals of wavelets as arising, for instance, in the representation of the Laplacian.

Certain basic integrals of products of wavelets, for instance

$$\int \psi_\nu\,\psi_\mu\,\mathrm{d}x\,,\qquad \int \psi'_\nu\,\psi'_\mu\,\mathrm{d}x\,,\qquad \int \psi_\lambda\,\psi_\mu\,\psi_\nu\,\mathrm{d}x\,,$$

can be obtained recursively from the corresponding integrals with scaling functions, in the above examples

$$\int \varphi\,\varphi(\cdot-k)\,\mathrm{d}x\,,\qquad \int \varphi'\,\varphi'(\cdot-k)\,\mathrm{d}x\,,\qquad \int \varphi\,\varphi(\cdot-k)\,\varphi(\cdot-l)\,\mathrm{d}x\,. \tag{6.89}$$

For instance, for $j_1,k_1,j_2,k_2\in\mathbb{Z}$ with $j_2\geq j_1$ we obtain, with the aid of (6.88),

$$\int \psi'_{j_1,k_1}\,\psi'_{j_2,k_2}\,\mathrm{d}x = 2^{2(j_1+1)}\sum_{l_1,l_2} g_{l_1}g_{l_2}\int \varphi'_{0,0}\,\varphi_{j_2-j_1,l_2+2k_2-2^{j_2-j_1}(l_1+2k_1)}\,\mathrm{d}x\,.$$

For the integrals of the form as on the right hand side, for $j,k\in\mathbb{Z}$ we have

$$\int \varphi'\,\varphi'_{j,k}\,\mathrm{d}x = 4\sum_l h_l\int \varphi'\,\varphi'_{j-1,k-2^{j-1}l}\,\mathrm{d}x\,. \tag{6.90}$$

In this manner, we obtain a recursive reduction to the corresponding integrals in (6.89).

As shown in [11, 35], the basic scaling function integrals in (6.89) can be computed as the solutions of constrained eigenvalue problems derived from the scaling relations (6.88). For instance, assuming that $\varphi\in\mathrm{H}^2(\mathbb{R})$, we have $\int\varphi'\,\varphi'_{0,k}\,\mathrm{d}x = -\int\varphi\,\varphi''_{0,k}\,\mathrm{d}x$ and from (6.88) we obtain

$$\int \varphi\,\varphi''_{0,k}\,\mathrm{d}x = 4\sum_{l_1,l_2} h_{l_1-2k+l_2}h_{l_2}\int \varphi\,\varphi''_{0,l_1}\,\mathrm{d}x\,. \tag{6.91}$$

In addition, by Remark 3.4, the translates of φ can exactly represent polynomials of degree two; from this, one derives the additional condition

$$\sum_k k^2\int \varphi\,\varphi''_{0,k}\,\mathrm{d}x = 2\,. \tag{6.92}$$

The system of equations given by (6.91) and (6.92) can be solved for the required integrals. A detailed analysis of this approach in a more general setting is given in [35].

The approximations to basic integrals obtained in this way are highly accurate, but cannot be computed independently of each other, which would be desirable for adaptive wavelet methods. Recall that $\int\varphi'\,\varphi'_{j,k}\,\mathrm{d}x$, for arbitrary j,k, can be computed from the values $\int\varphi\,\varphi'_{0,l}\,\mathrm{d}x$, $l\in\mathbb{Z}$, by repeated application of (6.90). Counting the number of intermediate values required for carrying this out, one finds that the work and storage required for any integral of the form $\int\psi'_\nu\,\psi'_\mu\,\mathrm{d}x$ is of order $\mathcal{O}(||\nu|-|\mu||)$, where the constant depends quadratically on the support length of the wavelets.

For the Laplacian, the overhead incurred by the recursive evaluation of integrals therefore does not pose a problem in practice. As we shall see in the following section, however, an approach of this type becomes too expensive for integrals arising in the wavelet representation of approximate potentials.

6.6 Integrals of Wavelets with Gaussians

In what follows, we consider algorithms for evaluating the integrals

$$\int_{\mathbb{R}} e^{-\alpha x^2}\, \psi_{\nu_1}\, \psi_{\mu_1}\, \mathrm{d}x \tag{6.93}$$

$$\int_{\mathbb{R}^2} e^{-\alpha (x_1-x_2)^2}\, (\psi_{\nu_1}\otimes\psi_{\nu_2})\, (\psi_{\mu_1}\otimes\psi_{\mu_2})\, \mathrm{d}x\,, \tag{6.94}$$

as well as

$$\int (x_1-x_2) e^{-\alpha (x_1-x_2)^2} \big[(\mathrm{D}_{x_1}-\mathrm{D}_{x_2})(\psi_{\nu_1}\otimes\psi_{\nu_2})\big] (\psi_{\mu_1}\otimes\psi_{\mu_2})\, \mathrm{d}x\,, \tag{6.95}$$

where $\nu_1,\mu_1,\nu_2,\mu_2\in\nabla$, with a possibly large parameter $\alpha>0$.

The integration scheme we propose here is based on rewriting the integrals of interest as integrals in Fourier domain. Recall that by Plancherel's theorem, for $f,g\in \mathrm{L}_2(\mathbb{R})$ we have

$$\int_{\mathbb{R}} f\, g\, \mathrm{d}x = \int_{\mathbb{R}} \hat f\, \overline{\hat g}\, \mathrm{d}\xi\,. \tag{6.96}$$

For the convolution defined for $x\in\mathbb{R}$ a.e. by

$$(f*g)(x) = \int_{\mathbb{R}} f(y)\, g(x-y)\, dy\,,$$

we have the identity

$$(f*g)^\wedge = \sqrt{2\pi}\hat f \hat g\,. \tag{6.97}$$

We shall also need the Fourier transforms

$$\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} e^{-\alpha x^2}\, e^{-ix\xi}\, \mathrm{d}x = (2\alpha)^{-\frac12}\, e^{-\frac{\xi^2}{4\alpha}}\,, \tag{6.98}$$

$$\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} x\, e^{-\alpha x^2}\, e^{-ix\xi}\, \mathrm{d}x = -i\xi(2\alpha)^{-\frac32}\, e^{-\frac{\xi^2}{4\alpha}}\,. \tag{6.99}$$

As an immediate consequence of (6.96) and (6.98), for $f\in \mathrm{L}_1(\mathbb{R})$ we obtain

$$\int_{\mathbb{R}} e^{-\alpha x^2}\, f(x)\, \mathrm{d}x = (2\alpha)^{-\frac12}\int_{\mathbb{R}} e^{-\xi^2/(4\alpha)}\, \hat f(\xi)\, \mathrm{d}\xi\,. \tag{6.100}$$

In particular, for $f=\psi_\nu\psi_\mu$,

$$\int_{\mathbb{R}} e^{-\alpha x^2}\, \psi_\nu(x)\, \psi_\mu(x)\, \mathrm{d}x = (2\alpha)^{-\frac12}\int_{\mathbb{R}} e^{-\xi^2/(4\alpha)} \big(\psi_\nu\, \psi_\mu\big)^\wedge(\xi)\, \mathrm{d}\xi\,. \tag{6.101}$$

Similarly for $f,g\in\mathrm{L}_2(\mathbb{R})$, using (6.96),

$$\int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\, f(x_1)\, g(x_2)\, \mathrm{d}x = \int_{\mathbb{R}} f(x)\big(e^{-\alpha(\cdot)^2}*g\big)(x)\, \mathrm{d}x = \int_{\mathbb{R}} \overline{\hat f(\xi)}\big(e^{-\alpha(\cdot)^2}*g\big)^\wedge(\xi)\, \mathrm{d}\xi\,,$$

and by (6.97) and (6.98),

$$\int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\, f(x_1)\, g(x_2)\, \mathrm{d}x = \sqrt{\frac{\pi}{\alpha}}\int_{\mathbb{R}} e^{-\xi^2/(4\alpha)}\overline{\hat f(\xi)}\, \hat g(\xi)\, \mathrm{d}\xi\,. \tag{6.102}$$

Note that the integrands on the right hand sides of (6.100), (6.102) are conjugate-symmetric about zero, i.e., it suffices to compute an integral over $[0,\infty)$ for the real part. For the case of interest

$f = \psi_{\nu_1}\psi_{\mu_1}$, $g = \psi_{\nu_2}\psi_{\mu_2}$, (6.102) yields

$$\begin{aligned}\int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\, \psi_{\nu_1}(x_1)\, \psi_{\nu_2}(x_2)\, \psi_{\mu_1}(x_1)\, \psi_{\mu_2}(x_2)\, \mathrm{d}x \qquad\qquad& \\ = \sqrt{\frac{\pi}{\alpha}} \int_{\mathbb{R}} e^{-\xi^2/(4\alpha)}\, \overline{\bigl(\psi_{\nu_1}\,\psi_{\mu_1}\bigr)^\wedge(\xi)}\, \bigl(\psi_{\nu_2}\,\psi_{\mu_2}\bigr)^\wedge(\xi)\, \mathrm{d}\xi\,. & \quad (6.103)\end{aligned}$$

In (6.101), (6.103), we have thus obtained representations of (6.93), (6.94) as integrals over the real line of certain Fourier transforms.

For the case (6.95), one additionally needs the following variant that can be derived similarly to (6.102), making use of (6.99): for $f, g \in \mathrm{L}_2(\mathbb{R})$,

$$\int_{\mathbb{R}^2} (x_1 - x_2) e^{-\alpha(x_1-x_2)^2}\, f(x_1)\, g(x_2)\, \mathrm{d}x = -\frac{i}{2}\sqrt{\frac{\pi}{\alpha^3}} \int_{\mathbb{R}} \xi e^{-\xi^2/(4\alpha)}\, \overline{\hat f(\xi)}\, \hat g(\xi)\, \mathrm{d}\xi\,,$$

and as a consequence,

$$\begin{aligned}\int_{\mathbb{R}^2} (x_1 - x_2) e^{-\alpha(x_1-x_2)^2} \bigl[(\mathrm{D}_{x_1} - \mathrm{D}_{x_2})\psi_{\nu_1}(x_1)\, \psi_{\nu_2}(x_2)\bigr] \psi_{\mu_1}(x_1)\, \psi_{\mu_2}(x_2)\, \mathrm{d}x \qquad& \\ = -\frac{i}{2}\sqrt{\frac{\pi}{\alpha^3}} \int_{\mathbb{R}} \xi e^{-\xi^2/(4\alpha)} \Bigl(\overline{\bigl(\psi'_{\nu_1}\,\psi_{\mu_1}\bigr)^\wedge(\xi)}\, \bigl(\psi_{\nu_2}\,\psi_{\mu_2}\bigr)^\wedge(\xi) \qquad& \\ - \overline{\bigl(\psi_{\nu_1}\,\psi_{\mu_1}\bigr)^\wedge(\xi)}\, \bigl(\psi'_{\nu_2}\,\psi_{\mu_2}\bigr)^\wedge(\xi)\Bigr)\, \mathrm{d}\xi\,. & \quad (6.104)\end{aligned}$$

On the basis of this representation, one can proceed similarly as for (6.101) and (6.103).

Recall that in our context, the integrals (6.93), (6.94) arise in particular from approximations of Coulomb potentials by sums of separable functions of the form

$$\frac{1}{|x|} \approx \sum_k \omega_k e^{-\alpha_k |x|^2}\,, \qquad \frac{1}{|x-y|} \approx \sum_k \omega_k e^{-\alpha_k |x-y|^2}\,, \qquad x, y \in \mathbb{R}^3 \tag{6.105}$$

as discussed in Sections 4.3.1 and 6.3; analogous approximations of $(x-y)/|x-y| \cdot (\mathrm{D}_x - \mathrm{D}_y)$ lead to integrals of the forms (6.95) and (6.94).

For the construction of such separable approximations based on sinc approximation as in Theorem 4.17, by Corollary 4.20 we have $\omega_k \lesssim \sqrt{\alpha_k}$. We shall assume such an estimate to hold in our error analysis for the integration scheme. Taking this scaling into account, it suffices to estimate quadrature errors for the scaled integrals

$$\sqrt{\alpha} \int_{\mathbb{R}} e^{-\alpha x^2}\, \psi_{\nu_1}\, \psi_{\mu_1}\, \mathrm{d}x\,, \quad \sqrt{\alpha} \int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\, (\psi_{\nu_1} \otimes \psi_{\nu_2})\, (\psi_{\mu_1} \otimes \psi_{\mu_2})\, \mathrm{d}x\,. \tag{6.106}$$

For our purposes, the potentials approximated in (6.105) are considered as multiplication operators, that is, as mappings from H^1 to H^{-1}. Based on the error estimates in the corresponding operator norm as in Section 6.3, one finds that an error $\varepsilon_0 > 0$ in the approximation (6.105), with respect to the norm $\|\cdot\|_{\mathrm{H}^1 \to \mathrm{H}^{-1}}$, requires a separable expansion with $\max_k \alpha_k \sim \varepsilon_0^{-2}$.

Recall from Section 3.1 that provided $\varphi \in \mathrm{H}^{1+\varepsilon}(\mathbb{R})$ for some $\varepsilon > 0$, we have that $\{2^{-|\nu|}\psi_\nu\}_{\nu\in\nabla}$ is a Riesz basis of $\mathrm{H}^1(\mathbb{R})$, and $\{(2^{2|\nu_1|} + 2^{2|\nu_2|})^{-1/2}(\psi_{\nu_1} \otimes \psi_{\nu_2})\}_{(\nu_1,\nu_2)\in\nabla^2}$ is a Riesz basis of $\mathrm{H}^1(\mathbb{R}^2)$. In order to ensure a certain accuracy in the full separable representations (6.105) in operator norm

$\mathrm{H}^1 \to \mathrm{H}^{-1}$, it suffices to control the quadrature error in the rescaled matrices

$$\begin{gathered} 2^{-|\nu_1|-|\mu_1|}\sqrt{\alpha}\int_{\mathbb{R}} e^{-\alpha x^2}\,\psi_{\nu_1}\,\psi_{\mu_1}\,\mathrm{d}x\,, \\ (2^{2|\nu_1|}+2^{2|\nu_2|})^{-\frac{1}{2}}(2^{2|\mu_1|}+2^{2|\mu_2|})^{-\frac{1}{2}}\sqrt{\alpha}\int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\,(\psi_{\nu_1}\otimes\psi_{\nu_2})\,(\psi_{\mu_1}\otimes\psi_{\mu_2})\,\mathrm{d}x\,. \end{gathered} \tag{6.107}$$

In view of Lemmas 6.7 and 6.8, integrals corresponding to higher wavelet levels thus require lower accuracy. In our error estimates, we shall not explicitly take advantage of this and formulate the estimates for the integrals scaled as in (6.106) instead. We shall, however, make use of the practically relevant rescaling (6.107) in the numerical tests later in this section.

Before turning to the description and analysis of the integration scheme, we briefly review a straightforward quadrature scheme that has been used previously in a similar form by other authors.

6.6.1 A Reference Scheme: Integration Using Triple Products

A basic approach for evaluating integrals of products of wavelets with a sufficiently smooth coefficient consists in replacing the coefficient by a suitable wavelet approximation. Although we shall see in this section that such an approach is too expensive in the case of the two-dimensional integrals (6.94), it will serve as a reference scheme in our numerical tests in Subsection 6.6.5.

For the following discussion, we assume θ, $\tilde\theta$ to be compactly supported, biorthogonal scaling functions. Then the integrals in (6.106) can be approximated by expansions

$$\sum_{k\in\mathbb{Z}}\int\sqrt{\alpha}\,e^{-\alpha x^2}\tilde\theta_{J_1,k}(x)\,\mathrm{d}x\int_{\mathbb{R}}\theta_{J_1,k}\,\psi_\nu\,\psi_\mu\,\mathrm{d}x\,, \tag{6.108}$$

and

$$\sum_{k\in\mathbb{Z}^2}\int\sqrt{\alpha}\,e^{-\alpha(x_1-x_2)^2}\tilde\theta_{J_2,k_1}\otimes\tilde\theta_{J_2,k_2}\,\mathrm{d}x\int_{\mathbb{R}}\theta_{J_2,k_1}\,\psi_{\nu_1}\,\psi_{\mu_1}\,\mathrm{d}x\int_{\mathbb{R}}\theta_{J_2,k_2}\,\psi_{\nu_2}\,\psi_{\mu_2}\,\mathrm{d}x\,, \tag{6.109}$$

respectively, with sufficiently large levels $J_1, J_2 \in \mathbb{Z}$. This approach has been mentioned for general integrals arising in wavelet-Galerkin methods in [35], and has been used similarly to our present setting in [49]. The advantage of such an expansion is that all arising coefficients can be evaluated only on the basis of the refinement relations (6.88); before discussing this point, we consider the error incurred by such an expansion.

We first consider the error in dependence on J_1, J_2 in the approximation of the integrals (6.93), (6.94) by the expansions (6.108), (6.109), where we assume for the moment that all coefficients in these expansions are given exactly. A proof of the following proposition is given in Appendix A.4.

Proposition 6.36. *Let θ and $\tilde\theta$ have orders of polynomial reproduction $p-1$ and $\tilde p-1$, respectively, let $\varphi,\psi\in\mathrm{C}^\tau(\mathbb{R})$ for a $\tau>0$, and let $q:=\min\{\lfloor\tau\rfloor,\tilde p\}$. Then there exist $C_1, C_2 > 0$ such that for ε sufficiently small, the following hold: for $J_1\in\mathbb{Z}$ such that*

$$J_1 \geq \min\Bigl\{\tfrac{1}{p}\log_2\varepsilon^{-1}+\tfrac{1}{2}\bigl(1+\tfrac{1}{p}\bigr)\log_2\alpha,\ \tfrac{1}{q}\log_2\varepsilon^{-1}+\max\{|\nu_1|,|\mu_1|\}+\tfrac{1}{2q}(|\nu_1|+|\mu_1|)\Bigr\}$$

and

$$\mathcal{K}^{(1)}_{J_1,\varepsilon} := \Bigl\{k\in\mathbb{Z}\colon\ |x|\leq\alpha^{-\frac{1}{2}}|\ln\varepsilon|^{\frac{1}{2}}\ \textit{for all } x\in\operatorname{supp}\tilde\theta_{J_1,k}\Bigr\}\,,$$

we have

$$\left|\int_{\mathbb{R}} e^{-\alpha x^2}\,\psi_{\nu_1}\,\psi_{\mu_1}\,\mathrm{d}x-\sum_{k\in\mathcal{K}^{(1)}_{J_1,\varepsilon}}\int\sqrt{\alpha}e^{-\alpha x^2}\tilde\theta_{J_1,k_1}\,\mathrm{d}x\int_{\mathbb{R}}\theta_{J_1,k_1}\,\psi_{\nu_1}\,\psi_{\mu_1}\,\mathrm{d}x\right|\leq C_1\varepsilon\,,$$

and for $J_2 \in \mathbb{Z}$ *such that*

$$J_2 \geq \min\Bigl\{\tfrac{1}{p}\log_2 \varepsilon^{-1} + \tfrac{1}{2}\bigl(1+\tfrac{1}{p}\bigr)\log_2 \alpha,\\ \tfrac{1}{q}\log_2 \varepsilon^{-1} + \max\{|\nu_1|, |\mu_1|, |\nu_2|, |\mu_2|\} + \tfrac{1}{2q}(|\nu_1| + |\mu_1| + |\nu_2| + |\mu_2|)\Bigr\} \qquad (6.110)$$

and

$$\mathcal{K}^{(2)}_{J_2,\varepsilon} := \Bigl\{k \in \mathbb{Z}^2 \colon\; |x_1 - x_2| \leq \alpha^{-\frac{1}{2}}(\max\{\tfrac{1}{4}, \ln \varepsilon^{-1}\})^{\frac{1}{2}} \;\textit{ for all } (x_1,x_2) \in \operatorname{supp} \tilde\theta_{J_2,k_1} \otimes \tilde\theta_{J_2,k_2}\Bigr\},$$

we have

$$\Bigl| \int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\,(\psi_{\nu_1} \otimes \psi_{\nu_2})\,(\psi_{\mu_1} \otimes \psi_{\mu_2})\,\mathrm{d}x \\ - \sum_{k \in \mathcal{K}_{J_2,\varepsilon}} \int \sqrt{\alpha} e^{-\alpha(x_1-x_2)^2} \tilde\theta_{J_2,k_1} \otimes \tilde\theta_{J_2,k_2}\,\mathrm{d}x \int_{\mathbb{R}} \theta_{J_2,k_1}\,\psi_{\nu_1}\,\psi_{\mu_1}\,\mathrm{d}x \int_{\mathbb{R}} \theta_{J_2,k_2}\,\psi_{\nu_2}\,\psi_{\mu_2}\,\mathrm{d}x \Bigr| \leq C_2 \varepsilon\,.$$

We next consider the numerical evaluation of the coefficients in the expansions (6.108), (6.109). As mentioned above, the advantage of this approach is that all required coefficients can be evaluated by methods which use only the refinement coefficients for φ, ψ, and θ.

The arising integrals over triple products can be evaluated by computing $\int \theta_{0,k}\,\varphi_{0,l}\,\varphi\,\mathrm{d}x$ from a constrained eigenvalue problem derived from the scaling relations (6.88), and recursively applying the scaling relations to reduce all further integrals to this case, cf. [35].

One possible approach for evaluating the required coefficients of Gaussian functions is to use an auxiliary scaling function $\tilde\theta$ with sufficiently many vanishing moments. In our case, we now additionally assume

$$\int x^n \tilde\theta\,\mathrm{d}x = 0\,, \quad 0 < n < p\,. \qquad (6.111)$$

For such $\tilde\theta$, the simple approximation of the wavelet coefficients of a sufficiently smooth function by its point values satisfies an error estimate with the same convergence rate as the corresponding wavelet expansion; in other words, for $f \in C^s$ with $s \leq p$ we have

$$\Bigl| \int_{\mathbb{R}} f\,\tilde\theta_{\tilde J,k}\,\mathrm{d}x - 2^{-\tilde J/2} f(2^{-\tilde J}k) \Bigr| \lesssim 2^{-s\tilde J} |f|_{C^s}\,, \quad \tilde J \in \mathbb{Z}\,.$$

The property (6.111) is satisfied, for instance, by Coiflets [38] and by Deslaurier-Dubuc-Sweldens wavelets [40, 136]. For the error in the coefficients, using Taylor expansion, (6.111), and Lemma 6.23, we thus obtain

$$\Bigl| \int \sqrt{\alpha} e^{-\alpha(x_1-x_2)^2} \tilde\theta_{\tilde J,k_1}(x_1)\,\tilde\theta_{\tilde J,k_2}(x_2)\,\mathrm{d}x - 2^{-\tilde J}\sqrt{\alpha} e^{-\alpha 2^{-2\tilde J}(k_1-k_2)^2} \Bigr| \lesssim 2^{-p\tilde J} \alpha^{\frac{1}{2}(1+p)}\,,$$

and an analogous estimate for the one-dimensional case. Due to the compact support of θ, the same estimate holds, with a different constant depending on the support size of θ, for the total error in the expansion due to the approximate coefficients. Note that depending on the choice of J_2 in (6.110), it may be necessary to choose $\tilde J > J_2$, and to subsequently obtain the coefficients of the Gaussian term on level J_2 by downsampling.

On the basis of Proposition 6.36, estimates for the number of summands required in the expansions (6.108), (6.109) can be obtained. A more detailed consideration can be found in Appendix A.4; at this point, we briefly summarize the conclusions at which one arrives.

In the case of the one-dimensional integrals (6.93) it can be seen from (A.12) and (A.13) that, for the values of $\alpha \lesssim \varepsilon^{-2}$ of interest, arbitrarily high convergence orders with respect to the number of summands can be achieved for sufficiently large p. Choosing a high order p for the auxiliary basis functions $\theta, \tilde{\theta}$ does not pose a major problem.

In the case of the two-dimensional integrals (6.94), the situation is different: Regardless of p, the complexity will in general always be worse than $\mathcal{O}(\varepsilon^{-1/q})$, and hence the regularity of ψ, which enters via q, becomes a limiting factor. It is a different problem, however, that renders the scheme infeasible in practical discretization methods even for fairly smooth ψ: As can be seem from (A.11), for large values of α, a factor $2^{\max\{|\nu_1|,|\nu_2|,|\mu_1|,|\mu_2|\}}$ enters in the number of triple products that need to be computed. Since these triple products need to be generated recursively, recomputing them only when required is impractical, and thus for higher accuracies a prohibitively large number of coefficients needs to be held in memory.

The crucial difference between the cases of the one- and the two-dimensional integrals is essentially that in the one-dimensional case, for large α the Gaussian coefficients are concentrated at a point, and therefore only triple products involving basis functions with support close to this point are actually needed, whereas in the two-dimensional case, for large α the Gaussian coefficients are concentrated along a diagonal line, and therefore a large subset of all triple products for the corresponding levels needs to be available.

In summary, we may conclude that for the one-dimensional integrals (6.93), the approach considered above yields a potentially quite efficient method. However, it becomes unacceptably expensive for the two-dimensional integrals as in (6.94) or (6.95). This shortcoming is a main motivation for the alternative scheme proposed in this section.

For the one-dimensional integrals, if a large p is used, the scheme discussed above can in general be asymptotically advantageous over the scheme proposed in this work. An interesting additional feature of the alternative scheme that we consider in the next section, however, is that individual integrals for certain wavelet coefficients can be computed largely independently of each other, but many required quantities can still be precomputed. This is in contrast to the rather tightly coupled evaluation of triple products by recursions required by the approach considered above.

6.6.2 Relation to Previous Work

Quadrature rules for products of arbitrary functions with wavelets, which use the wavelets only in terms of their refinement relations, have been studied for instance in [137] and [85]. This approach, where wavelets are treated as weight functions, is not suitable in our situation, since it is sensitive to large derivatives in the integrands arising for large exponents in the Gaussian terms. In our context, it would also require a different quadrature rule for each combination of wavelets, or a recursive reduction, based on the scaling relations, to certain combinations of scaling functions; this would both be prohibitively expensive in our case, particularly for (6.94).

Several quadrature schemes have been devised for related problems of integrating products of wavelets with certain potential terms in electronic structure calculations. In the scheme proposed in [114] smoothness, or more specifically, small high-order derivatives of the involved potentials terms are required. This method is therefore suitable for computations involving pseudopotentials, but not in our setting.

In [49], the computation of discretization matrix entries for the full singular three- and six-dimensional Coulomb potentials has been considered in detail. This aim is different from our setting, since here we are most interested in the direct use of lower-dimensional factor matrices as in (6.93), (6.94) in a computational scheme. The quadrature developed in [49] is related to the one discussed in the previous subsection in that it also uses a more sophisticated variant of an expansion with triple products to reduce the problem to the computation of wavelet coefficients of Coulomb potentials. These coefficients are approximated based on a separable approximation of the type (6.106), and subsequently an approach via Fourier transforms based on identities similar to (6.101) and (6.103) is used to compute wavelet coefficients of Gaussians. In this case, it is not necessary to evaluate Fourier transforms of products of wavelets as in our case, but only Fourier transforms of the wavelets themselves, which can be done using their infinite product expansion. It should be noted that in contrast to this scheme, in our approach we avoid the use of triple products corresponding to higher wavelet levels.

Observations similar to the identities (6.101) and (6.103) concerning the representation in terms of Fourier transforms of related integrals can also be found in [65] in the context of a direct treatment of three- and six-dimensional Coulomb potentials. There such an approach was suggested for integrals of products of globally supported Meyer wavelets with the full higher-dimensional potentials. The Fourier transforms of Meyer wavelets have a closed-form representation, but the Fourier transforms of the Coulomb potentials are singular. The situation here is different in that the resulting integrands in Fourier domain do not have a closed-form representation, but are analytic functions.

For piecewise polynomial wavelets, the computation of integrals of the form (6.93), (6.94) has been considered in [154]. In the particular case of spline wavelets, the approach given there is potentially more efficient than the scheme considered here, and the method developed in this section is therefore of interest mainly in the case of wavelets that do not have this additional structure, such as Daubechies wavelets.

6.6.3 Convergence Analysis for the Trapezoidal Rule in Fourier Domain

We now come to the description and analysis of the basic quadrature scheme. When using compactly supported wavelets, the integrands in the transformed integrals

$$\frac{1}{\sqrt{2}}\int_{\mathbb{R}} e^{-\xi^2/(4\alpha)}\,(\psi_\nu\,\psi_\mu)^\wedge(\xi)\,d\xi\,,\qquad \sqrt{\pi}\int_{\mathbb{R}} e^{-\xi^2/(4\alpha)}\,\overline{(\psi_{\nu_1}\,\psi_{\mu_1})^\wedge(\xi)}\,(\psi_{\nu_2}\,\psi_{\mu_2})^\wedge(\xi)\,d\xi$$

and

$$-i\frac{\sqrt{\pi}}{2\alpha}\int_{\mathbb{R}} \xi e^{-\xi^2/(4\alpha)}\Bigl(\overline{(\psi'_{\nu_1}\,\psi_{\mu_1})^\wedge(\xi)}\,(\psi_{\nu_2}\,\psi_{\mu_2})^\wedge(\xi) - \overline{(\psi_{\nu_1}\,\psi_{\mu_1})^\wedge(\xi)}\,(\psi'_{\nu_2}\,\psi_{\mu_2})^\wedge(\xi)\Bigr)\,d\xi\,,$$

obtained by the identities (6.101), (6.103), (6.104), and rescaled as in (6.106), are restrictions to $\mathbb{R}$ of analytic functions. This makes the trapezoidal rule an interesting option for approximating these integrals. More precisely, for an integrand $u\colon \mathbb{C}\to\mathbb{C}$ we approximate the integral over the real line by

$$\int_{\mathbb{R}} u(\xi)\,\mathrm{d}\xi \approx h\sum_{k=-N}^{N} u(kh)\,,$$

where the error is estimated by

$$\Bigl|\int_{\mathbb{R}} u(\xi)\,\mathrm{d}\xi - h\sum_{k\in\mathbb{Z}} u(kh)\Bigr| + \Bigl|h\sum_{|k|>N} u(kh)\Bigr|\,. \tag{6.112}$$

For given h, the behaviour of the second term in (6.112) is determined by the decay towards infinity of u on $\mathbb{R}$. The appropriate choice of h depends on the first term, for which the crucial aspect, as the general statement in Theorem 4.19 shows, is the growth of the integrand on strips in the complex plane that contain the real line. The following lemma provides this connection in our particular situation.

Lemma 6.37. *Let* $u(\xi)=(8\sqrt{\pi})^{-1}\alpha^{-(n+\frac{1}{2})}\xi^n e^{-(4\alpha)^{-1}\xi^2}\phi(\xi)$ *with* $\alpha>0$, $|\phi(\xi)|\le e^{\kappa|\operatorname{Im}\xi|}$, $\kappa>0$, *and* $n\in\{0,1\}$. *For any* $d>0$, *if*

$$h=\frac{2\pi d}{\ln\delta^{-1}+n\ln(\alpha^{-1}d+2(\pi\alpha)^{-1/2})+(4\alpha)^{-1}d^2+\kappa d} \tag{6.113}$$

for $\delta > 0$ *with* $\delta \leq \frac{1}{2}(\alpha^{-1}d + 2(\pi\alpha)^{-1/2})^n e^{(4\alpha)^{-1}d^2+\kappa d}$, *then*

$$\left|\int_{\mathbb{R}} u(\xi)\,\mathrm{d}\xi - h\sum_{k\in\mathbb{Z}} u(hk)\right| \leq \delta\,. \tag{6.114}$$

Remark 6.38. *Note that if* $n = 0$ *and* $\delta < 1$, *then* h *as in* (6.113) *is maximal for the choice* $d = 2(\alpha|\ln\delta|)^{\frac{1}{2}}$, *and the condition on* δ *in Lemma 6.37 is ensured by* $\delta \leq 2^{-1/2}$. *In the case* $n = 1$, $\delta < 1$, *with the same choice of* d *this condition holds for* $\delta \leq (\pi\alpha)^{-1/4}$.

For the proof of Lemma 6.37, we again invoke Theorem 4.19; to this end, recall the definitions of $\mathcal{D}_d \subset \mathbb{C}$ for $d > 0$ and $N_1(u, \mathcal{D}_d)$ for u analytic in $\mathcal{D}_d$ as in Definition 4.18.

Proof of Lemma 6.37. Note first that for $\xi_1, \xi_2 \in \mathbb{R}$ such that $\xi_1 + i\xi_2 \in \mathcal{D}_d$,

$$\left|(\xi_1 + i\xi_2)^n e^{-(4\alpha)^{-1}(\xi_1+i\xi_2)^2}\right| \leq (|\xi_1| + d)^n e^{-(4\alpha)^{-1}\xi_1^2} e^{(4\alpha)^{-1}d^2}\,,$$

for $n = 0, 1$, and as a consequence

$$\begin{aligned} N_1(u, \mathcal{D}_d) &\leq 2(8\sqrt{\pi})^{-1}\alpha^{-\frac{1}{2}-n} e^{(4\alpha)^{-1}d^2} e^{\kappa d} \int_{\mathbb{R}} (|\xi| + d)^n e^{-(4\alpha)^{-1}\xi^2}\, d\xi \\ &= 2(8\sqrt{\pi})^{-1}\big(2\sqrt{\pi}(\alpha^{-1}d)^n + 4n\alpha^{-\frac{1}{2}}\big)\, e^{(4\alpha)^{-1}d^2} e^{\kappa d} \\ &= \tfrac{1}{2}\big(\alpha^{-1}d + 2(\pi\alpha)^{-\frac{1}{2}}\big)^n e^{(4\alpha)^{-1}d^2+\kappa d}\,, \qquad n = 0, 1\,. \end{aligned} \tag{6.115}$$

By Theorem 4.19, if $e^{-2\pi d/h} \leq \frac{1}{2}$,

$$\left|\int_{\mathbb{R}} u(x)\,\mathrm{d}x - h\sum_{k\in\mathbb{Z}} u(kh)\right| \leq 2e^{-2\pi d/h} N_1(u, \mathcal{D}_d)\,, \tag{6.116}$$

and combining this with (6.115), we see that if h is chosen as in the assertion, the upper bound on the right hand side of (6.116) equals δ, provided that $\delta \leq \frac{1}{2}(\alpha^{-1}d + 2(\pi\alpha)^{-1/2})^n e^{(4\alpha)^{-1}d^2+\kappa d}$, which ensures both that $e^{-2\pi d/h} \leq \frac{1}{2}$ and that the denominator in (6.113) is positive. □

We now return to the second error term in (6.112), where we consider two qualitatively different types of decay of the integrand separately: exponential decay due to the α–dependent Gaussian term, and algebraic decay depending on the smoothness of the wavelet basis. We begin with a result concerning the former.

Lemma 6.39. *Let* $|u(\xi)| \leq c|\xi|^n e^{-(4\alpha)^{-1}\xi^2}$ *for* $\xi \in \mathbb{R}$, $n \in \{0, 1\}$. *Then for any* $h > 0$ *and* $N \in \mathbb{N}$,

$$h\sum_{|k|>N} |u(kh)| \leq \begin{cases} 4c\,\alpha\,(Nh)^{-1}\,e^{-(4\alpha)^{-1}(Nh)^2}\,, & n = 0\,, \\ 8\sqrt{2}\,c\,\alpha^{3/2}\,(Nh)^{-1}\,e^{-(8\alpha)^{-1}(Nh)^2}\,, & n = 1\,. \end{cases}$$

Proof. In the case $n = 0$, proceeding similarly as in [59, Lemma 2.4], we obtain

$$h\sum_{|k|>N} |u(kh)| \leq 2ch \sum_{k=N+1}^{\infty} e^{-(4\alpha)^{-1}(kh)^2} \leq 2ch \int_N^\infty e^{-(4\alpha)^{-1}(xh)^2}\,\mathrm{d}x$$

by monotonicity, and furthermore

$$\leq 2ch \int_N^\infty \frac{2(4\alpha)^{-1}h^2 x}{2(4\alpha)^{-1}h^2 N} e^{-(4\alpha)^{-1}h^2x^2}\,\mathrm{d}x = 4c\alpha(Nh)^{-1}e^{-(4\alpha)^{-1}(Nh)^2}\,.$$

For $n = 1$,

$$h \sum_{|k|>N} |u(kh)| \le 2ch \sum_{k=N+1}^{\infty} kh e^{-(4\alpha)^{-1}(kh)^2} \le 2^{\frac{3}{2}} ch\alpha^{\frac{1}{2}} \sum_{k=N+1}^{\infty} e^{-(8\alpha)^{-1}(kh)^2} , \tag{6.117}$$

where we have used that $xe^{-(4\alpha)^{-1}x^2} \le (2\alpha)^{1/2} e^{-(8\alpha)^{-1}x^2}$ for $x > 0$. Again using monotonicity, the right hand side in (6.117) can be estimated further by

$$2^{\frac{3}{2}} ch\alpha^{\frac{1}{2}} \int_N^\infty \frac{2(8\alpha)^{-1}h^2 x}{2(8\alpha)^{-1}h^2 N} e^{-(8\alpha)^{-1}(xh)^2} \,\mathrm{d}x = 8\sqrt{2}\, c\, \alpha^{\frac{3}{2}} \,(Nh)^{-1} e^{-(8\alpha)^{-1}(Nh)^2} . \qquad \square$$

If the parameter α is very large, the algebraic decay of integrands due to the smoothness of the basis functions becomes important. Provided that a corresponding decay estimate is available, this can be exploited via the following lemma.

Lemma 6.40. *Let $|u(\xi)| \le c(1 + \beta|\xi|)^{-\kappa}$ for $\xi \in \mathbb{R}$ with $\kappa > 1$ and $\beta > 0$. Then for any $h > 0$ and $N \in \mathbb{N}$,*

$$h \sum_{|k|>N} |u(kh)| \le 2c\beta^{-1}(\kappa - 1)^{-1}(1 + \beta N h)^{-(\kappa-1)} .$$

Proof. Similarly to Lemma 6.39, this follows with

$$h \sum_{|k|>N} |u(kh)| \le 2ch \sum_{k=N+1}^{\infty} (1 + \beta kh)^{-\kappa} \le 2ch \int_N^\infty (1 + \beta xh)^{-\kappa} \,\mathrm{d}x . \qquad \square$$

For the specific integrands we are interested in, a decay estimate as required for Lemma 6.40 can be established on the basis of the decay of the Fourier transform of the scaling function from which the wavelets are derived.

Proposition 6.41. *Let φ be a scaling function such that*

$$|\hat{\varphi}(\xi)| \lesssim C(1 + |\xi|)^{-\eta} ,$$

where $\eta > 1$, $C > 0$, then for the corresponding wavelet basis $\{\psi_\nu\}_{\nu\in\nabla}$ there exists $c_{\psi,\eta} > 0$ such that

$$\big|(\psi_\nu \psi_\mu)^\wedge(\xi)\big| \le c_{\psi,\eta}\, 2^{\frac{1}{2}||\nu|-|\mu||} \big(1 + 2^{-\max\{|\nu|,|\mu|\}} |\xi|\big)^{-\eta} .$$

If additionally $\eta > 2$, there exists $\tilde{c}_{\psi,\eta} > 0$ with

$$\big|(\psi'_\nu \psi_\mu)^\wedge(\xi)\big| \le \tilde{c}_{\psi,\eta}\, 2^{|\nu|} 2^{\frac{1}{2}||\nu|-|\mu||} \big(1 + 2^{-\max\{|\nu|,|\mu|\}} |\xi|\big)^{-(\eta-1)} .$$

Proof. Note first that $|\hat{\psi}_\nu(\xi)| = 2^{-|\nu|/2} |\hat{\psi}(2^{-|\nu|}\xi)| \lesssim 2^{-|\nu|/2}(1 + 2^{-|\nu|}|\xi|)^{-\eta}$. It thus remains to estimate

$$\big|(\psi_\nu \psi_\mu)^\wedge(\xi)\big| = \frac{\big|(\hat{\psi}_\nu * \hat{\psi}_\mu)(\xi)\big|}{\sqrt{2\pi}} \lesssim 2^{-\frac{1}{2}(|\nu|+|\mu|)} \int_{\mathbb{R}} (1 + 2^{-|\nu|}|\xi - \tau|)^{-\eta} (1 + 2^{-|\mu|}|\tau|)^{-\eta} \,\mathrm{d}\tau ,$$

which can be done by the argument in [62, Proposition 2.2.7]: On the one hand,

$$\int_{\{|\xi-\tau|\ge\frac{1}{2}|\xi|\}} (1 + 2^{-|\nu|}|\xi - \tau|)^{-\eta} (1 + 2^{-|\mu|}|\tau|)^{-\eta} \,\mathrm{d}\tau \le (1 + 2^{-|\nu|-1}|\xi|)^{-\eta} \int_{\mathbb{R}} (1 + 2^{-|\mu|}|\tau|)^{-\eta} \,\mathrm{d}\tau ,$$

on the other hand, since $|\xi - \tau| \le \frac{1}{2}|\xi|$ implies $|\tau| \ge \frac{1}{2}|\xi|$,

$$\int_{\{|\xi-\tau|\le\frac{1}{2}|\xi|\}} (1 + 2^{-|\nu|}|\xi - \tau|)^{-\eta} (1 + 2^{-|\mu|}|\tau|)^{-\eta} \,\mathrm{d}\tau \le (1 + 2^{-|\mu|-1}|\xi|)^{-\eta} \int_{\mathbb{R}} (1 + 2^{-|\nu|}|\tau|)^{-\eta} \,\mathrm{d}\tau .$$

In summary, this yields the first part of the assertion; the second part follows in the same way with $|(\psi'_\nu)^\wedge(\xi)| = 2^{|\nu|/2}|(\psi')^\wedge(2^{-|\nu|}\xi)| \lesssim 2^{|\nu|/2}(1+2^{-|\nu|}|\xi|)^{-(\eta-1)}$. ☐

Corollary 6.42. *Let $\{\psi_\nu\}_{\nu\in\nabla}$ be a Daubechies wavelet basis with N vanishing moments, then we have*

$$\big|(\psi_\nu\psi_\mu)^\wedge(\xi)\big| \leq C_N 2^{\frac{1}{2}||\nu|-|\mu||}\big(1+2^{-\max\{|\nu|,|\mu|\}}|\xi|\big)^{-\eta(N)},$$

where

$$\eta(N) := N - \frac{\ln 3}{2\ln 2}(N-1)\,.$$

Proof. From [38, eq. (7.1.23)], we obtain $|\hat\varphi(\xi)| \lesssim (1+|\xi|)^{-N+(2\ln 2)^{-1}\ln 3^{N-1}}$, and the claim follows with Proposition 6.41. ☐

Remark 6.43. *More generally, for any wavelet family such that $\psi \in \mathrm{H}^k(\mathbb{R})$, $k \in \mathbb{N}$, one finds by integration by parts*

$$|\hat\varphi(\xi)| \lesssim \min\big\{1, |\xi|^{-k}\big\} \lesssim (1+|\xi|)^{-k}\,. \tag{6.118}$$

For Daubechies wavelets, however, Proposition 6.42 yields substantially faster decay for given N than (6.118) *combined with Sobolev regularity estimates as provided, e.g., in [119].*

For putting the above results together for the particular integrals of interest, we introduce the following additional notation: for $\nu,\mu\in\nabla$, let

$$l_{\mu\nu} := \sup\big\{|x| :\ x \in \operatorname{supp}\psi_\nu\psi_\mu\big\}$$

and for $\nu,\mu\in\nabla^2$,

$$L_{\mu\nu} := \sup\big\{|x-y| :\ x\in\operatorname{supp}\psi_{\nu_1}\psi_{\mu_1},\ y\in\operatorname{supp}\psi_{\nu_2}\psi_{\mu_2}\big\}\,.$$

We estimate quadrature errors for the integrals (6.93) and (6.94) in Theorem 6.44. An analogous result for (6.95) is provided by Theorem 6.49. In each case, we consider the integrands scaled by a factor $\sqrt{\alpha}$, which corresponds to the scaling of terms in the exponential sum approximations (6.105).

Theorem 6.44 below explicitly gives an appropriate choice of the integration step size h. Here, the required number of integration points N is determined by the minimum of two types of bounds. The first bounds in (6.119) and (6.120) are related to the decay of the Fourier transform of the Gaussian coefficient, whereas the remaining bounds result from the decay of the Fourier transforms of wavelet products.

Theorem 6.44. *Let $\alpha > 0$ and let $\{\psi_\nu\}_{\nu\in\nabla}$ be a wavelet basis with scaling function φ satisfying $|\hat\varphi(\xi)| \lesssim (1+|\xi|)^{-\eta}$ for $\eta > 1$, and with the normalization $\|\psi_\nu\|_{\mathrm{L}_2} = 1$. Let $\varepsilon > 0$ with $\varepsilon \leq \sqrt{\alpha}$, then the following holds:*

(i) *Let $\nu,\mu\in\nabla$. If $h = 2\pi\big(\alpha^{-\frac{1}{2}}\big|\ln(8\sqrt{\alpha})^{-1}\varepsilon\big| + l_{\nu\mu}\big)^{-1}$ and, with $\tilde\eta_1 := \eta - 1$,*

$$N \geq \min\Big\{\pi^{-1}\big(\big|\ln(8\sqrt{\alpha})^{-1}\varepsilon\big| + \sqrt{\alpha}\,l_{\nu\mu}\big|\ln(8\sqrt{\alpha})^{-1}\varepsilon\big|^{\frac{1}{2}}\big)\,,\\ C_{\psi,\eta}\big(\alpha^{-\frac{1}{2}}\big|\ln(8\sqrt{\alpha})^{-1}\varepsilon\big|^{\frac{1}{2}} + l_{\nu\mu}\big)2^{(2\tilde\eta_1)^{-1}||\nu|-|\mu||}2^{(1+\tilde\eta_1^{-1})\max\{|\nu|,|\mu|\}}\,\varepsilon^{-\tilde\eta_1^{-1}}\Big\}, \tag{6.119}$$

where $C_{\psi,\eta} > 0$, then we have the estimate

$$\Big|\sqrt{\alpha}\int_{\mathbb{R}} e^{-\alpha x^2}\psi_\nu\psi_\mu\,\mathrm{d}x - \frac{h}{\sqrt{2}}\sum_{k=-N}^{N} e^{-(4\alpha)^{-1}(kh)^2}(\psi_\nu\psi_\mu)^\wedge(kh)\Big| \leq \varepsilon\,.$$

(ii) *Let* $\nu, \mu \in \nabla^2$*. If* $h = 2\pi\big(\alpha^{-\frac{1}{2}} \ln(8\sqrt{\alpha}/\varepsilon) + L_{\nu\mu}\big)^{-1}$ *and, with* $\tilde\eta_1 := \eta - 1$ *and* $\tilde\eta_2 := 2\eta - 1$*,*

$$\begin{aligned} N \geq \min\Big\{ &\pi^{-1}\big(\big|\ln(8\sqrt{\alpha})^{-1}\varepsilon\big| + \sqrt{\alpha}\, L_{\nu\mu}\big|\ln(8\sqrt{\alpha})^{-1}\varepsilon\big|^{\frac{1}{2}}\big)\ , \\ &\tilde C_{\psi,\eta}\big(\alpha^{-\frac{1}{2}}\big|\ln(8\sqrt{\alpha})^{-1}\varepsilon\big|^{\frac{1}{2}} + L_{\nu\mu}\big)2^{(2\tilde\eta_1)^{-1}(||\nu_1|-|\mu_1||+||\nu_2|-|\mu_2||)} \\ &\qquad \times 2^{(1+\tilde\eta_1^{-1})\min\{\max\{|\nu_1|,|\mu_1|\},\max\{|\nu_2|,|\mu_2|\}\}}\,\varepsilon^{-\tilde\eta_1^{-1}}\ , \\ &\tilde C_{\psi,\eta}\big(\alpha^{-\frac{1}{2}}\big|\ln(8\sqrt{\alpha})^{-1}\varepsilon\big|^{\frac{1}{2}} + L_{\nu\mu}\big)2^{(2\tilde\eta_2)^{-1}(||\nu_1|-|\mu_1||+||\nu_2|-|\mu_2||)} \\ &\qquad\qquad \times 2^{\frac{1}{2}(1+\tilde\eta_2^{-1})(\max\{|\nu_1|,|\mu_1|\}+\max\{|\nu_2|,|\mu_2|\})}\,\varepsilon^{-\tilde\eta_2^{-1}}\Big\}, \end{aligned} \tag{6.120}$$

where $\tilde C_{\psi,\eta} > 0$*, then we have the estimate*

$$\begin{aligned} \Big|\sqrt{\alpha}\int_{\mathbb{R}^2} &e^{-\alpha(x-y)^2}\psi_{\nu_1}(x)\,\psi_{\nu_2}(y)\,\psi_{\mu_1}(x)\,\psi_{\mu_2}(y)\,\mathrm{d}(x,y) \\ &- h\sqrt{\pi}\sum_{k=-N}^{N} e^{-(4\alpha)^{-1}(kh)^2}\overline{(\psi_{\nu_1}\psi_{\mu_1})^\wedge(kh)}(\psi_{\nu_2}\psi_{\mu_2})^\wedge(kh)\Big| \leq \varepsilon\,. \end{aligned}$$

Before coming to the proof, we discuss the intepretation of the result of Theorem 6.44. From the first bounds on N in the conditions (6.119), (6.120), it can be seen that for any fixed α, we obtain exponential convergence with respect to N. However, in exponential sum approximations as in (6.105), the maximum required value of α is related to the expansion error. More specifically, assuming that we aim for a quadrature error of the same order as this expansion error, in the example (6.105) we obtain $\sqrt{\alpha} \sim \varepsilon^{-1}$. For the largest values of α required in combination with a certain ε, we may therefore in general obtain better estimates using the further bounds on N in (6.119), (6.120). These yield algebraic convergence with respect to N, with rate depending on η and hence on the smoothness of the wavelet basis.

Remark 6.45. *In order to interpret the result of Theorem 6.44 in more detail, we need to estimate* $l_{\mu\nu}$ *and* $L_{\mu\nu}$*.*

Note first that in the case of the one-dimensional integrals, if for all $x \in \operatorname{supp}\psi_\mu\psi_\nu$ *we have* $\sqrt{\alpha}\, e^{-\alpha x^2} \leq C\varepsilon$ *with a suitable fixed* $C > 0$*, then the value of the integral is bounded by the error tolerance and can be approximated by zero. Similarly, for the two-dimensional integrals this is the case provided that for all* $(x_1, x_2) \in \operatorname{supp}\psi_{\mu_1}\psi_{\nu_1} \times \operatorname{supp}\psi_{\mu_2}\psi_{\nu_2}$ *it holds that* $\sqrt{\alpha}\, e^{-\alpha(x_1-x_2)^2} \leq C\varepsilon$*.*

Taking the support size of the wavelets for a given level and the estimate $\ln\alpha \lesssim |\ln\varepsilon|$ *into account, for the indices for which an approximation of the integral actually need to be computed we find the conditions*

$$\begin{aligned} l_{\mu\nu} &\lesssim \alpha^{-\frac{1}{2}}|\ln\varepsilon|^{\frac{1}{2}} + 2^{-\max\{|\nu|,|\mu|\}}\,, \\ L_{\mu\nu} &\lesssim \alpha^{-\frac{1}{2}}|\ln\varepsilon|^{\frac{1}{2}} + 2^{-\min\{\max\{|\nu_1|,|\mu_1|\},\,\max\{|\nu_2|,|\mu_2|\}\}}\,. \end{aligned}$$

Remark 6.46. *By Remark 6.45 and* $\ln\alpha \lesssim |\ln\varepsilon|$*, Theorem 6.44 leads to a number of integration points* N *for the one-dimensional integral of point (i) that is of order*

$$\begin{aligned} N \lesssim \min\big\{&|\ln\varepsilon| + \alpha^{\frac{1}{2}}\,2^{-\max\{|\nu|,|\mu|\}}|\ln\varepsilon|^{\frac{1}{2}}\,, \\ &\big(1 + \alpha^{-\frac{1}{2}}2^{\max\{|\nu|,|\mu|\}}|\ln\varepsilon|\big)2^{(2\tilde\eta_1)^{-1}||\nu|-|\mu||}2^{\tilde\eta_1^{-1}\max\{|\nu|,|\mu|\}}\,\varepsilon^{-\tilde\eta_1^{-1}}\big\}\,. \end{aligned} \tag{6.121}$$

For the two-dimensional integral of point (ii), with the notations $m_i := \max\{|\nu_i|, |\mu_i|\}$*,* $d_i :=$

$||\nu_i| - |\mu_i||$ *for* $i = 1, 2$, *we obtain*

$$\begin{aligned} N \lesssim \min\bigl\{ &|\ln\varepsilon| + \alpha^{\frac{1}{2}}\, 2^{-\min\{m_1,m_2\}} |\ln\varepsilon|^{\frac{1}{2}}\,, \\ &\bigl(1 + \alpha^{-\frac{1}{2}} 2^{\min\{m_1,m_2\}} |\ln\varepsilon|\bigr) 2^{\tilde\eta_1^{-1}(\min\{m_1,m_2\} + \frac{1}{2}(d_1+d_2))}\, \varepsilon^{-\tilde\eta_1^{-1}}\,, \\ &\bigl(2^{\frac{1}{2}|m_1-m_2|} + \alpha^{-\frac{1}{2}} 2^{\frac{1}{2}(m_1+m_2)} |\ln\varepsilon|\bigr) 2^{(2\tilde\eta_2)^{-1}(m_1+m_2+d_1+d_2)}\, \varepsilon^{-\tilde\eta_2^{-1}} \bigr\}\,. \end{aligned} \tag{6.122}$$

Recall that $\eta_2 = \eta_1 + \eta$. *In* (6.122), *the estimate of order* $\varepsilon^{-\tilde\eta_2^{-1}}$ *deteriorates as* $|m_1 - m_2|$ *grows; in this case, the estimate of order* $\varepsilon^{-\tilde\eta_1^{-1}}$ *as in the one-dimensional case may determine the quantitative behaviour of* N *for relevant accuracies.*

Remark 6.47. *The estimates in Theorem 6.44 refer to the integrals* (6.106). *Estimates for the rescaled integrals* (6.107) *can be obtained by replacing* ε *by* $2^{|\nu|+|\mu|}\varepsilon$ *in* (6.121), *and by* $(2^{2|\nu_1|} + 2^{2|\nu_2|})^{\frac{1}{2}}(2^{2|\mu_1|}+2^{2|\mu_2|})^{\frac{1}{2}}\varepsilon \sim 2^{\max|\nu|+\max|\mu|}\varepsilon$ *in* (6.122). *This yields an improvement in the dependence of the estimates on the wavelet levels. In the case of the estimate* (6.121) *for the one-dimensional integrals, for instance, with this modification we arrive at*

$$\begin{aligned} N \lesssim \min\bigl\{ &|\ln\varepsilon| + \alpha^{\frac{1}{2}}\, 2^{-\max\{|\nu|,|\mu|\}} |\ln\varepsilon|^{\frac{1}{2}}\,, \\ &\bigl(1 + \alpha^{-\frac{1}{2}} 2^{\max\{|\nu|,|\mu|\}} |\ln\varepsilon|\bigr) 2^{(2\tilde\eta_1)^{-1}(\max\{|\mu|,|\nu|\} - 3\min\{|\mu|,|\nu|\})}\, \varepsilon^{-\tilde\eta_1^{-1}} \bigr\}\,. \end{aligned}$$

Proof of Theorem 6.44. For part (i), note that by (6.101),

$$\sqrt{\alpha} \int_{\mathbb{R}} e^{-\alpha x^2} \psi_\nu \psi_\mu \,\mathrm{d}x = \int_{\mathbb{R}} u_1(\xi)\,\mathrm{d}\xi\,, \quad u_1(\xi) := 2^{-\frac{1}{2}} e^{-(4\alpha)^{-1}\xi^2} (\psi_\nu\psi_\mu)^\wedge(\xi)\,.$$

Since $|(\psi_\nu\psi_\mu)^\wedge(\xi_1 + i\xi_2)| \le (2\pi)^{-\frac{1}{2}} e^{l_{\nu\mu} d}$ for $\xi_1, \xi_2 \in \mathbb{R}$ with $|\xi_2| \le d$, and by our assumption $\varepsilon \le \sqrt{\alpha}$ and Remark 6.38, we can apply Lemma 6.37 with $\delta = (8\sqrt{\alpha})^{-1}\varepsilon$, $\kappa = l_{\nu\mu}$, $n = 0$, and $d = 2(\alpha \ln \delta^{-1})^{1/2}$ to obtain

$$\Bigl| \int_{\mathbb{R}} u_1(\xi)\,\mathrm{d}\xi - h \sum_{k\in\mathbb{Z}} u_1(kh) \Bigr| \le \frac{\varepsilon}{2}$$

for h as in the hypothesis. Now on the one hand, for $\xi \in \mathbb{R}$, $|u_1(\xi)| \le (2\sqrt{\pi})^{-1} e^{-(4\alpha)^{-1}\xi^2}$, and hence by Lemma 6.39,

$$h \sum_{|k|>N} |u_1(kh)| \le 2\pi^{-\frac{1}{2}} \alpha\, (Nh)^{-1} e^{-(4\alpha)^{-1}(Nh)^2} \tag{6.123}$$

for $N \in \mathbb{N}$. On the other hand, by Proposition 6.41, $|u_1(\xi)| \lesssim 2^{\frac{1}{2}||\nu|-|\mu||}(1 + 2^{-\max\{|\nu|,|\mu|\}}|\xi|)^{-\eta}$ and hence

$$h \sum_{|k|>N} |u_1(kh)| \lesssim 2^{\frac{1}{2}||\nu|-|\mu||} 2^{\max\{|\nu|,|\mu|\}} (1 + 2^{-\max\{|\nu|,|\mu|\}} Nh)^{-(\eta-1)} \tag{6.124}$$

with constants depending on η and the wavelet basis, which determine $C_{\psi,\eta}$ in (6.119). Using (6.119) in conjunction with (6.123), (6.124), we obtain

$$h \sum_{|k|>N} |u_1(kh)| \le \frac{\varepsilon}{2}\,,$$

completing the proof of part (i).

For part (ii), we obtain $|\overline{(\psi_{\nu_1}\psi_{\mu_1})^\wedge(\xi_1 + i\xi_2)}(\psi_{\nu_2}\psi_{\mu_2})^\wedge(\xi_1 + i\xi_2)| \le (2\pi)^{-1} e^{L_{\nu\mu} d}$ for $\xi_1, \xi_2 \in \mathbb{R}$ with $|\xi_2| \le d$. Lemma 6.37 can therefore be applied exactly as before, but with $\kappa = L_{\nu\mu}$, to the integrand

$$u_2(\xi) := \sqrt{\pi}\, e^{-(4\alpha)^{-1}\xi^2} \overline{(\psi_{\nu_1}\psi_{\mu_1})^\wedge(\xi)} (\psi_{\nu_2}\psi_{\mu_2})^\wedge(\xi)\,. \tag{6.125}$$

The estimate (6.123) holds with u_1 replaced by u_2 as well, which yields the first condition on N in (6.120). Concerning an analogue of (6.124) for u_2, we have

$$|u(\xi)| \lesssim 2^{\frac{1}{2}(||\nu_1|-|\mu_1||+||\nu_2|-|\mu_2||)}(1+2^{-\max\{|\nu_1|,|\mu_1|\}}|\xi|)^{-\eta}(1+2^{-\max\{|\nu_2|,|\mu_2|\}}|\xi|)^{-\eta}$$

by Proposition 6.41. On the one hand, the right hand side can be estimated by

$$2^{\frac{1}{2}(||\nu_1|-|\mu_1||+||\nu_2|-|\mu_2||)}(1+2^{-\min\{\max\{|\nu_1|,|\mu_1|\},\max\{|\nu_2|,|\mu_2|\}\}}|\xi|)^{-\eta}\,, \tag{6.126}$$

corresponding to the second condition on N. On the other hand, we have

$$\begin{aligned}(1+2^{-\max\{|\nu_1|,|\mu_1|\}}|\xi|)^{-\eta}&(1+2^{-\max\{|\nu_2|,|\mu_2|\}}|\xi|)^{-\eta}\\ &\leq (1+2^{-\max\{|\nu_1|,|\mu_1|\}}2^{-\max\{|\nu_2|,|\mu_2|\}}|\xi|^2)^{-\eta}\\ &\qquad\leq 2^{\eta}(1+2^{-\frac{1}{2}(\max\{|\nu_1|,|\mu_1|\}+\max\{|\nu_2|,|\mu_2|\})}|\xi|)^{-2\eta}\,,\end{aligned}$$

leading to the third condition on N; in the latter case, Lemma 6.40 gives

$$\begin{aligned}h\sum_{|k|>N}|u_2(kh)| \lesssim 2^{\frac{1}{2}(||\nu_1|-|\mu_1||+||\nu_2|-|\mu_2||)}&2^{\frac{1}{2}(\max\{|\nu_1|,|\mu_1|\}+\max\{|\nu_2|,|\mu_2|\})}\\ &\times(1+2^{-\frac{1}{2}(\max\{|\nu_1|,|\mu_1|\}+\max\{|\nu_2|,|\mu_2|\})}Nh)^{-\tilde\eta_2}\,,\end{aligned}$$

and analogously with (6.126). The assertion thus follows by the assumption (6.120) on the choice of N. □

Remark 6.48. *Additionally, one could consider changes of variable that lead to faster decay of the integrand. For instance, by the standard substitution $\xi = \tau\sinh t$ (see e.g. [148]) with a suitably chosen $\tau > 0$, one obtains from* (6.102) *the integral*

$$\frac{\tau\sqrt{\pi}}{\sqrt{\alpha}}\int_{\mathbb{R}} e^{-(\tau\sinh t)^2/(4\alpha)}\,\overline{\hat f(\tau\sinh t)}\,\hat g(\tau\sinh t)\,\cosh t\,\mathrm{d}t\,. \tag{6.127}$$

The faster decay, however, comes at the price of increased $N_1(\cdot,\mathcal{D}_d)$, which in case of (6.127) *remains finite only for $d < \pi/4$; all in all, one finds that this substitution does not lead to an improvement. More involved alternative substitutions, for instance as used in [73] in the construction of separable approximations, do not lead to an improvement in our context either: similarly to the case of the simpler substitution* (6.127)*, one finds that the improvement in decay on $\mathbb{R}$ is undone by an increase in $N_1(\cdot,\mathcal{D}_d)$.*

For integrals of the form (6.95) involving derivatives of wavelets, we obtain a result very similar to Theorem 6.44.

Theorem 6.49. *Let $\alpha > 0$ and let $\{\psi_\nu\}_{\nu\in\nabla}$ be a wavelet basis with scaling function φ satisfying $|\hat\varphi(\xi)| \lesssim (1+|\xi|)^{-\eta}$ for $\eta > 2$, and with the normalization $\|\psi_\nu\|_{\mathrm{L}_2} = 1$. Let $\varepsilon > 0$ with $\varepsilon \leq \min\{1, b_\psi\}\min\{1,\sqrt{\alpha}\}$, and let $\nu,\mu \in \nabla^2$. If, with $b_\psi := \max\{\|\varphi'\|_{\mathrm{L}_2}, \|\psi'\|_{\mathrm{L}_2}\}$ and $\delta := (8b_\psi\sqrt{\alpha})^{-1}\varepsilon$,*

$$h = \frac{2\pi\sqrt{\alpha}}{|\ln\delta|^{\frac{1}{2}} + L_{\nu\mu}\sqrt{\alpha} + (4|\ln\delta|)^{-\frac{1}{2}}\bigl(\ln 2\alpha^{-\frac{1}{2}} + \ln(|\ln\delta|^{\frac{1}{2}} + \pi^{-\frac{1}{2}})\bigr)}$$

and with $\tilde\eta_3 := 2\eta - 3$ let

$$\begin{aligned}N \geq h^{-1}\min\Bigl\{&\sqrt{8\alpha}\bigl|\ln(\sqrt{\alpha}\,\delta)\bigr|^{\frac{1}{2}}\,,\\ &\hat C_{\psi,\eta}2^{(2\tilde\eta_3)^{-1}(||\nu_1|-|\mu_1||+||\nu_2|-|\mu_2||)}2^{\frac{1}{2}(1+3\tilde\eta_3^{-1})(\max\{|\nu_1|,|\mu_1|\}+\max\{|\nu_2|,|\mu_2|\})}\,(\alpha\varepsilon)^{-\tilde\eta_3^{-1}}\Bigr\},\end{aligned} \tag{6.128}$$

where $\hat{C}_{\psi,\eta} > 0$*, then we have*

$$\Big|\sqrt{\alpha}\int_{\mathbb{R}^2}(x-y)e^{-\alpha(x-y)^2}[(\mathrm{D}_x-\mathrm{D}_y)\psi_{\nu_1}(x)\,\psi_{\nu_2}(y)]\,\psi_{\mu_1}(x)\,\psi_{\mu_2}(y)\,\mathrm{d}(x,y)$$
$$-h\frac{(-i)\sqrt{\pi}}{2\alpha}\sum_{k=-N}^{N}kh\,e^{-(4\alpha)^{-1}(kh)^2}\Big(\overline{(\psi'_{\nu_1}\psi_{\mu_1})^\wedge(kh)}(\psi_{\nu_2}\psi_{\mu_2})^\wedge(kh)$$
$$-\overline{(\psi_{\nu_1}\psi_{\mu_1})^\wedge(kh)}(\psi'_{\nu_2}\psi_{\mu_2})^\wedge(kh)\Big)\Big|\le\varepsilon\,.$$

Inserting the choice of h into the expression in (6.128), one finds that the corresponding result is quite similar to that of Theorem 6.44, but the presence of derivatives leads to slower decay the involved Fourier transforms.

Proof. In this case, the integrand reads

$$u_3(\xi) := -\frac{i\sqrt{\pi}}{2\alpha}\xi e^{-(4\alpha)^{-1}\xi^2}\left(\overline{(\psi'_{\nu_1}\psi_{\mu_1})^\wedge(\xi)}(\psi_{\nu_2}\psi_{\mu_2})^\wedge(\xi)-\overline{(\psi_{\nu_1}\psi_{\mu_1})^\wedge(\xi)}(\psi'_{\nu_2}\psi_{\mu_2})^\wedge(\xi)\right).$$

For $\xi=\xi_1+i\xi_2$, $\xi_1,\xi_2\in\mathbb{R}$ with $|\xi_2|\le d$, we have

$$\left|\overline{(\psi'_{\nu_1}\psi_{\mu_1})^\wedge(\xi)}(\psi_{\nu_2}\psi_{\mu_2})^\wedge(\xi)\right|+\left|\overline{(\psi_{\nu_1}\psi_{\mu_1})^\wedge(\xi)}(\psi'_{\nu_2}\psi_{\mu_2})^\wedge(\xi)\right|\le\pi^{-1}\,b_\psi\,e^{L_{\nu\mu}d}\,.$$

Note that $\delta<1$ because $\varepsilon\le\sqrt{\alpha}$, and furthermore $\delta\le(8b_\psi)^{-1}\min\{1,b_\psi\}\min\{\alpha^{-1/2},1\}<(\pi\alpha)^{-1/4}$. Hence by Remark 6.38 we can apply Lemma 6.37 with $\delta=(8b_\psi\sqrt{\alpha})^{-1}\varepsilon$, $\kappa=L_{\nu\mu}$, $n=1$, and $d=2(\alpha\ln\delta^{-1})^{1/2}$, to obtain

$$\left|\int_{\mathbb{R}}u_3(\xi)\,\mathrm{d}\xi-h\sum_{k\in\mathbb{Z}}u_3(kh)\right|\le\frac{\varepsilon}{2}$$

for h as in the assertion. For $\xi\in\mathbb{R}$, we have $|u_3(\xi)|\le(2\sqrt{\pi}\alpha)^{-1}b_\psi\,|\xi|e^{-(4\alpha)^{-1}\xi^2}$ and hence by Lemma 6.39,

$$h\sum_{|k|>N}|u_3(kh)|\le\frac{4b_\psi\sqrt{2\alpha}}{\sqrt{\pi}Nh}e^{-(8\alpha)^{-1}(Nh)^2}\,. \tag{6.129}$$

The choice of N as in (6.128) ensures that the right hand side in (6.129) is bounded by $\varepsilon/2$; note that $\sqrt{\alpha}\,\delta<1$ by our assumptions on ε. For the second part of (6.128) related to the decay of $\hat{\varphi}$, we use Proposition 6.41 to obtain

$$|u(\xi)|\lesssim\alpha^{-1}2^{\frac{1}{2}(||\nu_1|-|\mu_1||+||\nu_2|-|\mu_2||)}2^{\max\{|\nu_1|,|\mu_1|\}+\max\{|\nu_2|,|\mu_2|\}}$$
$$\times\left(1+2^{-\frac{1}{2}\max\{|\nu_1|,|\mu_1|\}-\frac{1}{2}\max\{|\nu_2|,|\mu_2|\}}|\xi|\right)^{-2(\eta-1)},$$

with a multiplicative constant depending on η and the wavelet basis, and Lemma 6.40 therefore yields

$$h\sum_{|k|>N}|u_3(kh)|\lesssim\alpha^{-1}2^{\frac{1}{2}(||\nu_1|-|\mu_1||+||\nu_2|-|\mu_2||)}2^{\frac{3}{2}(\max\{|\nu_1|,|\mu_1|\}+\max\{|\nu_2|,|\mu_2|\})}$$
$$\times\left(1+2^{-\frac{1}{2}\max\{|\nu_1|,|\mu_1|\}-\frac{1}{2}\max\{|\nu_2|,|\mu_2|\}}|\xi|\right)^{-\tilde{\eta}_3}.$$

Choosing N such that the latter is bounded by $\varepsilon/2$ leads to the second part of (6.128). □

6.6.4 Evaluating Fourier Transforms of Wavelet Products

The error estimates of the previous section are applicable to fairly general compactly supported basis functions. In order to evaluate the required Fourier transforms of products of wavelets numerically, we consider next a scheme that relies on the particular multilevel structure of the type of wavelet basis of interest, and only requires the scaling coefficients as inputs.

As a prerequisite, we need a means of evaluating integrals of the form $\int x^n \varphi(x)\,\varphi(x-l)\,\mathrm{d}x$ for $n \in \mathbb{N}$ and $l \in \mathbb{Z}$. Let $\eta, \tilde{\eta}$ be a pair of auxiliary biorthogonal scaling functions, where η has degree of polynomial reproduction p, then for any $n < p$, we have

$$\int x^n \varphi(x)\,\varphi(x-l)\,\mathrm{d}x = \sum_m \int x^n \tilde{\eta}(x-m)\,\mathrm{d}x \int \eta(x-m)\,\varphi(x)\,\varphi(x-l)\,\mathrm{d}x\,. \tag{6.130}$$

The moments of $\tilde{\eta}$ can be evaluated by the recursion

$$\int x^n \tilde{\eta}(x-k)\,\mathrm{d}x = \frac{1}{(2^n-1)\sqrt{2}} \sum_{i=0}^{n-1} \binom{n}{i} \int x^i \tilde{\eta}(x-k)\,\mathrm{d}x \sum_m h_m (m+k)^{n-i}\,.$$

The expression on the right hand side can be evaluated independently for each $k \in \mathbb{Z}$. These quantities need to be computed only once for each required n, k.

Note that since scaling function φ and wavelet ψ have compact support, for the corresponding scaling sequences (h_n), (g_n) as in (6.88) we may choose a minimal finite subset $S \subset \mathbb{Z}$ such that $\operatorname{supp}(h_n), \operatorname{supp}(g_n) \subseteq S$ and set $L := \min S$, $U := \max S$.

We first consider the evaluation of Fourier transforms of the form $(\varphi_{0,0}\,\varphi_{0,l})^\wedge(\xi)$, to which all other combinations of scaling functions and wavelets on different levels can be reduced; this expression vanishes for all ξ unless $l \in \{L-U+1, \dots, U-L-1\}$. Using the scaling relation for φ, we obtain the recursion

$$\begin{aligned}\int \varphi(x)\,\varphi(x-l)\,e^{-ix\xi}\,\mathrm{d}x &= \sum_{n,m} h_n h_m e^{-i\xi n/2} \int \varphi(x)\,\varphi(x+n-m-2l)\,e^{-ix\xi/2}\,\mathrm{d}x \\ &= \sum_{m,n} h_{m-n+2l} h_m e^{-i\xi(m-n+2l)/2} \int \varphi(x)\,\varphi(x-n)\,e^{-ix\xi/2}\,\mathrm{d}x\,. \end{aligned} \tag{6.131}$$

For the following, let

$$A_{l,n}(\xi) := \sum_m h_{m-n+2l} h_m e^{-i\xi(m-n+2l)/2}\,,$$

so that

$$\int \varphi(x)\,\varphi(x-l)\,e^{-ix\xi}\,\mathrm{d}x = \sum_n A_{l,n}(\xi) \int \varphi(x)\,\varphi(x-n)\,e^{-ix\xi/2}\,\mathrm{d}x\,. \tag{6.132}$$

For obtaining an approximation of $(\varphi_{0,0}\,\varphi_{0,l})^\wedge(\xi)$ for arbitrary ξ, we still need suitable starting values for the recursion (6.132). For $J \in \mathbb{N}$, let $\xi_J := 2^{-J}\xi$, then for J sufficiently large,

$$\int \varphi(x)\,\varphi(x-l)\,e^{-i\xi_J x}\,\mathrm{d}x \;\approx\; \sum_{n=0}^{N} \frac{(-i\xi_J)^n}{n!} \int x^n \varphi(x)\,\varphi(x-l)\,\mathrm{d}x\,. \tag{6.133}$$

More precisely, if $\kappa > 0$ such that $\operatorname{supp}\varphi \subset [-\kappa, \kappa]$, and J is large enough so that $\xi_J < \kappa^{-1}$, the error in absolute value in (6.133) can be estimated by

$$\frac{\kappa^N}{N!} \max_{|x|\le\kappa} \max\bigl\{\bigl|\mathrm{D}_x^N \cos(|\xi_J|x)\bigr|, \bigl|\mathrm{D}_x^N \sin(|\xi_J|x)\bigr|\bigr\} \le \frac{|\kappa\xi_J|^N}{N!}\,.$$

Recall that, as discussed in the beginning of this section, the quantities $\int x^n \varphi(x)\,\varphi(x-l)\,\mathrm{d}x$ can be precomputed up to any desired value of n. Applying (6.132) J times, with J large enough in relation to N, we can thus obtain approximations for $(\varphi_{0,0}\,\varphi_{0,l})^\wedge(\xi)$ from the approximations of the corresponding $(\varphi_{0,0}\,\varphi_{0,l})^\wedge(\xi_J)$ provided by (6.133).

Similarly, the expressions $(\psi'_\nu\,\psi_\mu)^\wedge(\xi)$, which are required for the modified integrals (6.104), can be obtained from $(\varphi'_{0,0}\,\varphi_{0,l})^\wedge(\xi)$. The latter can be evaluated by the recursion

$$\int \varphi'(x)\,\varphi(x-l)\,e^{-ix\xi}\,\mathrm{d}x = 2\sum_n A_{l,n}(\xi)\int \varphi'(x)\,\varphi(x-n)\,e^{-ix\xi/2}\,\mathrm{d}x \tag{6.134}$$

in place of (6.132). We restrict our following discussion to the computation of $(\psi_\nu\,\psi_\mu)^\wedge(\xi)$, but the evaluation of $(\psi'_\nu\,\psi_\mu)^\wedge(\xi)$ can therefore be done in a completely analogous manner.

We do not attempt a formal stability analysis of the above recursions at this point. This is a rather delicate matter, since the relevant matrix norms of $A(\xi)$ are not bounded by one for all ξ. However, as demonstrated in Section 6.6.5, no problems in this regard are observed in numerical practice, and integration errors close to machine precision can be achieved.

Remark 6.50. *An alternative to the above recursive scheme is to use the identity*

$$\int_{\mathbb{R}} \varphi(x)\,\varphi(x-l)\,e^{-ix\xi}\,\mathrm{d}x = \int_{\mathbb{R}} \hat\varphi(\xi-\eta)\,\hat\varphi(\eta)\,e^{-il\eta}\,\mathrm{d}\eta\,, \tag{6.135}$$

and to apply the trapezoidal rule to the integral on the right hand side, where $\hat\varphi$ can be evaluated approximately based on its infinite product expansion; note that for the numerical evaluation of this product expansion, it is typically advantageous to convert it to a sum by taking its logarithm. The error estimate of Theorem 4.19 applies in this case as well. Due to the algebraic decay of $\hat\varphi$, the resulting convergence is only algebraic in the number of integration points[3]*. Using this approach, the overall asymptotic complexity of the integration scheme would therefore deteriorate substantially.*

The combination of (6.132) and (6.133) enables the evaluation of $(\varphi_{0,0}\,\varphi_{0,l})^\wedge(\xi)$ for any $l \in \mathbb{Z}$ and $\xi \in \mathbb{R}$. For any $j, J, k, l \in \mathbb{Z}$ with $J \geq j$, we also have

$$(\varphi_{j,k}\varphi_{J,l})^\wedge(\xi) = (\varphi_{0,k}\,\varphi_{J-j,l})^\wedge(2^{-j}\xi) = e^{-ik2^{-j}\xi}(\varphi_{0,0}\,\varphi_{J-j,l-2^{J-j}k})^\wedge(2^{-j}\xi)\,.$$

It thus suffices to consider $(\varphi_{0,0}\,\varphi_{j,l})^\wedge(\xi)$ for $j > 0$. By j steps of the recursion

$$\int \varphi(x)\varphi(2^j x - l)\,e^{-ix\xi}\,\mathrm{d}x = \frac{1}{\sqrt{2}}\sum_n h_n e^{-in\xi/2}\int \varphi(x)\varphi(2^{j-1}x + 2^{j-1}n - l)\,e^{-ix\xi/2}\,\mathrm{d}x\,,$$

this case can again be reduced to the evaluation of $(\varphi_{0,0}\,\varphi_{0,n})^\wedge(\xi)$ for $n = L-U+1,\ldots,U-L-1$. The number of intermediate results required in each step stays bounded by $2U-2L-1$: for each $0 \leq \iota < j$, it suffices to compute the intermediate values

$$\int \varphi(x)\,\varphi(2^\iota x - (l_\iota - 2^\iota n_\iota))\,e^{-ix(2^{j-\iota}\xi)}\,\mathrm{d}x\,,$$

where l_ι is defined by $l_\iota = l \mod 2^\iota$, for all $n_\iota = -U + \lceil (L+l_\iota+1)/2^\iota\rceil,\ldots,-L+\lfloor (U+l_\iota-1)/2^\iota\rfloor$. Pairs of wavelets, or of wavelets and scaling functions, can be treated by replacing in the final step of the respective computation the sequence (h_n) by the scaling sequence (g_n) of the wavelets where necessary, for instance

$$\int \psi(x)\,\psi(x-l)\,e^{-ix\xi}\,\mathrm{d}x = \sum_{m,n} g_{m-n+2l}\,g_m\,e^{-i\xi(m-n+2l)/2}\int \varphi(x)\,\varphi(x-n)\,e^{-ix\xi/2}\,\mathrm{d}x\,. \tag{6.136}$$

---

[3] The substitutions mentioned in Remark 6.48 that would guarantee exponential decay turn out to give no improvement in the overall convergence estimate in this case either.

Combining the above recursions, we are therefore able to approximately evaluate $(\psi_\nu\psi_\mu)^\wedge(\xi)$ for any $\xi \in \mathbb{R}$ and $\nu, \mu \in \nabla$.

6.6.5 Numerical Realization

We now turn to the practical realization of the quadrature scheme. For instance, additionally exploiting symmetries, for (6.94) we have a quadrature scheme of the form

$$\begin{aligned}\sqrt{\alpha}\int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}(\psi_{\nu_1}\otimes\psi_{\nu_2})\,(\psi_{\mu_1}\otimes\psi_{\mu_2})\,\mathrm{d}x \;&\approx\; h\sqrt{\pi}\,\overline{(\psi_{\nu_1}\psi_{\mu_1})^\wedge(0)}(\psi_{\nu_2}\psi_{\mu_2})^\wedge(0)\\ &\quad + 2h\sum_{k=1}^{N}\sqrt{\pi}\,e^{-(4\alpha)^{-1}(kh)^2}\overline{(\psi_{\nu_1}\psi_{\mu_1})^\wedge(kh)}(\psi_{\nu_2}\psi_{\mu_2})^\wedge(kh)\,.\end{aligned}$$

The parameters N and h can in practice be chosen adaptively by successively halving the value of h, and appropriately adjusting N, taking into account both the convergence with respect to h as in Theorem 4.19 and the qualitative knowledge about the decay of the integrand. With a dyadic refinement of h, function values computed previously for the same integral for larger values of h can be reused for smaller h. Note furthermore that if the parameters N, h for each integral are stored, the accuracy of computed values can easily be refined later as well.

A major advantage of the simple uniform quadrature grid of the trapezoidal rule is that many quantities required for the comparably expensive evaluation of Fourier transforms can be precomputed. To this end, it makes sense to base the evaluation of *all* integrals on the same dyadic grid of points of the form $2^{-j}k\,\tau_0$, $j,k \in \mathbb{Z}$, with some fixed $\tau_0 > 0$. One may then, for instance, precompute a certain range of values $(\varphi_{0,0}\,\varphi_{0,l})^\wedge(2^{-j}k\,\tau_0)$. This can yield a substantial gain in efficiency because, by the recursions discussed in Section 6.6.4, all other required evaluations of Fourier transforms can be reduced to such values in a few steps. Depending on the underlying discretization scheme, it can of course also be useful to precompute $(\psi_\nu\,\psi_\mu)^\wedge(\xi)$ for further combinations of $\nu, \mu \in \nabla$ and integration points ξ.

The matrix in the recursion (6.131) has the form of a discrete convolution and can thus be evaluated by FFT, which decreases the complexity of one step in the recursion with respect to the scaling sequence length $M := U - L + 1$ from M^2 to $M \log M$. In our numerical tests, however, a direct evaluation by (6.131) was consistently faster for values of M up to 46, even when using the optimized FFT library, FFTW [55].

A further point of practical significance is that except for the optional caching of values of Fourier transforms mentioned above, individual function values and integrals can be computed independently of each other, and the integration scheme we have described is therefore straightforward to parallelize.

Numerical Experiments

For our numerical tests, we again use the orthonormal wavelet from [119] with support length 19 and 6 vanishing moments shown in Figure 6.2, which is in $\mathrm{H}^s(\mathbb{R})$ for $s \approx 4.32$.

We consider, with u_2 as in (6.125), the integrals

$$\sqrt{\alpha}\int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\,(\psi_{\nu_1}\otimes\psi_{\nu_2})\,(\psi_{\mu_1}\otimes\psi_{\mu_2})\,\mathrm{d}x = \int_{\mathbb{R}} u_2(\xi)\,\mathrm{d}\xi\,, \tag{6.137}$$

for the six different combinations of $\nu_1, \nu_2, \mu_1, \mu_2$ which are listed in Table 6.1, and for

$$\alpha = 10^0,\, 10^2,\, 10^4,\, 10^6,\, 10^8,\, 10^{16}\,.$$

	ν_1	ν_2	μ_1	μ_2
1	$(0,0,0)$	$(0,0,0)$	$(0,0,0)$	$(0,0,0)$
2	$(0,9,0)$	$(0,0,0)$	$(0,0,0)$	$(0,0,0)$
3	$(3,0,1)$	$(0,0,1)$	$(0,0,1)$	$(0,0,1)$
4	$(6,0,1)$	$(0,0,1)$	$(6,0,1)$	$(0,0,0)$
5	$(6,0,1)$	$(6,0,1)$	$(6,0,1)$	$(6,0,1)$
6	$(6,1,1)$	$(3,0,1)$	$(0,1,0)$	$(3,0,1)$

Table 6.1. Combinations of wavelet indices $\nu_1, \nu_2, \mu_1, \mu_2 \in \nabla$ used in (6.137) for the numerical experiments; recall that for $\nu \in \nabla$, we have $\nu = (|\nu|, \mathrm{k}(\nu), \mathrm{s}(\nu))$.

α	Integral 1	Integral 2
10^0	$6.445,564,928,603,676 \times 10^{-01}$	$3.087,756,935,213,937 \times 10^{-07}$
10^2	$1.044,688,765,938,243 \times 10^{+00}$	$3.280,482,098,078,684 \times 10^{-08}$
10^4	$1.055,320,499,670,092 \times 10^{+00}$	$3.182,372,092,623,544 \times 10^{-08}$
10^6	$1.055,428,713,601,353 \times 10^{+00}$	$3.181,395,966,734,626 \times 10^{-08}$
10^8	$1.055,429,795,933,709 \times 10^{+00}$	$3.181,386,205,984,803 \times 10^{-08}$
10^{16}	$1.055,429,806,866,383 \times 10^{+00}$	$3.181,386,107,391,438 \times 10^{-08}$
α	Integral 3	Integral 4
10^0	$-4.072,379,711,218,127 \times 10^{-06}$	$1.867,098,215,486,562 \times 10^{-02}$
10^2	$1.798,985,688,973,480 \times 10^{-03}$	$-8.269,936,318,309,225 \times 10^{-03}$
10^4	$2.420,502,335,354,703 \times 10^{-03}$	$-3.494,643,176,839,263 \times 10^{-02}$
10^6	$2.426,105,327,025,463 \times 10^{-03}$	$-3.525,196,817,558,028 \times 10^{-02}$
10^8	$2.426,161,253,646,409 \times 10^{-03}$	$(-3.525,502,876,165,434 \times 10^{-02})$
10^{16}	$2.426,161,818,551,820 \times 10^{-03}$	$(-3.525,505,967,720,674 \times 10^{-02})$
α	Integral 5	Integral 6
10^0	$9.995,156,344,291,690 \times 10^{-01}$	$-8.216,257,535,442,750 \times 10^{-13}$
10^2	$9.556,600,670,183,798 \times 10^{+00}$	$1.876,368,135,997,672 \times 10^{-09}$
10^4	$3.421,268,763,593,881 \times 10^{+01}$	$-1.572,584,027,194,289 \times 10^{-04}$
10^6	$5.377,733,435,130,575 \times 10^{+01}$	$-2.812,674,495,013,307 \times 10^{-04}$
10^8	$(5.557,894,638,574,768 \times 10^{+01})$	$(-2.832,442,081,084,854 \times 10^{-04})$
10^{16}	$(5.559,816,312,094,642 \times 10^{+01})$	$(-2.832,642,840,672,890 \times 10^{-04})$

Table 6.2. Reference values for integrals (6.137) with wavelet indices as in Table 6.1.

For comparing numerical errors, reference values for the integrals were computed using the completely different scheme of Subsection 6.6.1 to accuracy close to machine precision. Due to the extremely large memory requirements for the evaluation of the required triple products, especially in the cases 4, 5, and 6 of Table 6.1, this computation was not feasible for large α in the cases 5 and 6. Substitute values obtained by the Fourier-based scheme with $h = 0.125$ and $h = 0.325$, respectively, are given in brackets for these cases; this corresponds to half the minimum step sizes used in the tests in Figure 6.8.

We first study the numerical errors that can be achieved in principle by the integration of Section 6.6.3 combined with the recursive evaluation of Fourier transforms as in Section 6.6.4. For this first test, we thus take an approach similar to the basic strategy of the convergence analysis: for given h we first approximate

$$\varepsilon(h) = \left| \int_{\mathbb{R}} u_2(\xi)\,\mathrm{d}\xi - h \sum_{k\in\mathbb{Z}} u_2(hk) \right|$$

by choosing a summation range for k such that the error due to truncation of the sum is on the order of the roundoff error; we then choose N_h such that

$$\varepsilon_h(N_h) := h \sum_{|k|>N_h} |u_2(hk)| \leq \varepsilon(h)\,,$$

1	2	3	4	5	6
5.00×10^{-01}	5.00×10^{-01}	8.77×10^{-02}	8.77×10^{-02}	2.44×10^{-04}	1.22×10^{-04}

Table 6.3. Rescaling factors $(2^{2|\nu_1|} + 2^{2|\nu_2|})^{-\frac{1}{2}}(2^{2|\mu_1|} + 2^{2|\mu_2|})^{-\frac{1}{2}}$ for reference values in Table 6.2.

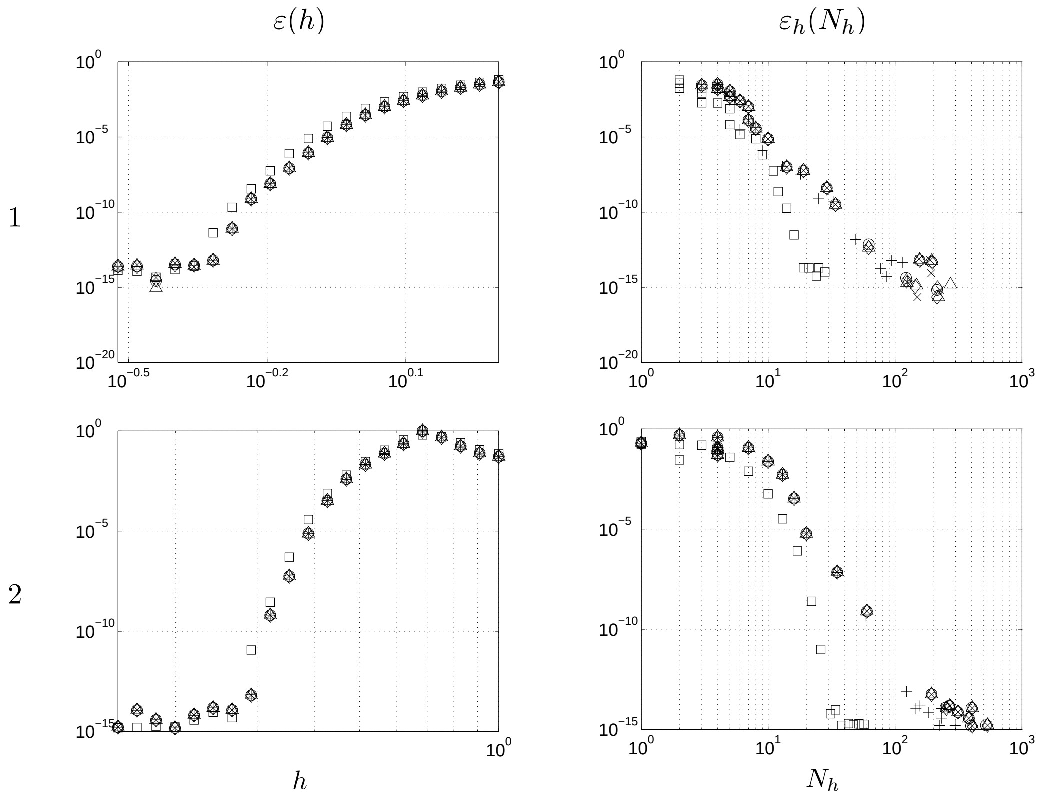

Figure 6.6. Integration error in dependence of given h and corresponding N_h, with markers corresponding to values of α: $\square$ 1, $+$ 10^2, $\circ$ 10^4, $\times$ 10^6, $\diamond$ 10^8, $*$ 10^{16}.

that is, the error is at most doubled by the additional truncation in the summation. The resulting integration errors for the relevant ranges of h, and the error in dependence of the corresponding N_h, are shown for the different test cases in Figures 6.6, 6.7, and 6.8. In each case, errors close to machine precision are achieved; an exception is case 5 in Figure 6.8, where the minimum errors are of order $\approx 10^{-13}$. This is not surprising since, for instance,

$$\int_{\mathbb{R}} e^{-(4\alpha)^{-1}\xi^2} |(\psi_{j,0} \otimes \psi_{j,0})^\wedge|^2 \,\mathrm{d}\xi = 2^j \int_{\mathbb{R}} e^{-(4\alpha)^{-1}2^{2j}\xi^2} |(\psi_{0,0} \otimes \psi_{0,0})^\wedge|^2 \,\mathrm{d}\xi \,,$$

and thus the error in the integral on the right hand side, which is on the order of machine precision, is multiplied by 2^j. However, this is not an issue in practice, since we still need to take the scaling factor as in Table 6.3 into account, which in the present example is 2^{-2j+1}. Therefore, the effective error in the relevant quantities actually decreases for wavelets on higher levels.

The approach taken for these first tests is of course not practically useful. We therefore consider next an adaptive dyadic refinement scheme that exclusively uses function values on a fixed dyadic grid as outlined in the beginning of this section. Here we consider the integrals rescaled by $(2^{2|\nu_1|} + 2^{2|\nu_2|})^{-\frac{1}{2}}(2^{2|\mu_1|} + 2^{2|\mu_2|})^{-\frac{1}{2}}$ as in (6.107), since for the applications we have in mind, we need to control the absolute error in these rescaled quantities; the scaling factors corresponding to the test cases are listed in Table 6.3. The results given in Table 6.4 show that the automatic refinement procedure reliably produces approximate integrals with prescribed error, requiring in each case a number of points only slightly larger than the minimum possible according to the basic tests in Figures 6.6, 6.7, and 6.8.

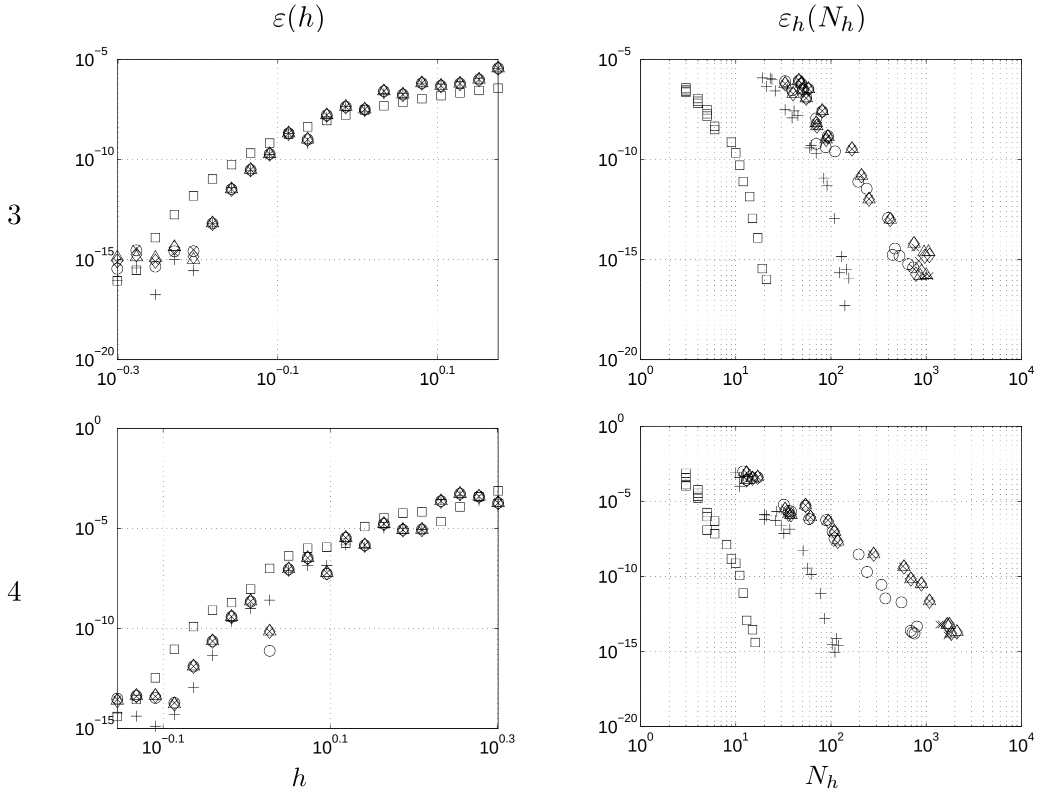

Figure 6.7. Integration error in dependence of given h and corresponding N_h, with markers as in Figure 6.6.

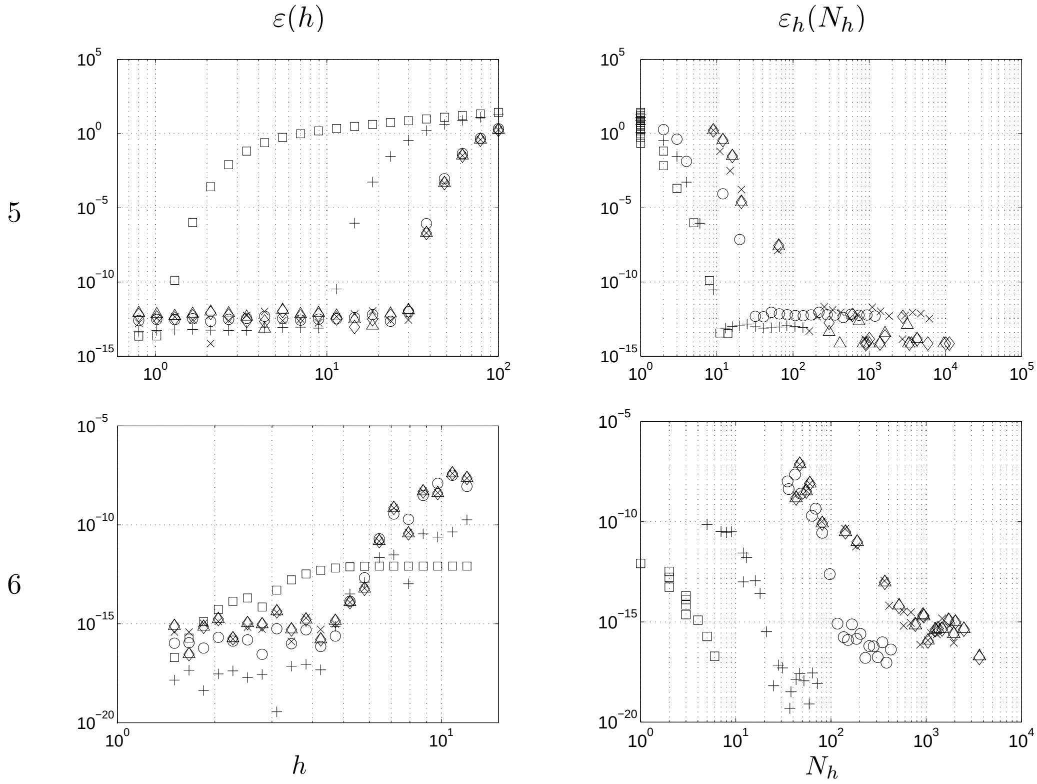

Figure 6.8. Integration error in dependence of given h and corresponding N_h, with markers as in Figure 6.6.

		10^{-6}		10^{-8}		10^{-10}		10^{-12}	
	α	N	error	N	error	N	error	N	error
1	10^0	38	5.44×10^{-15}	42	5.38×10^{-15}	34	5.77×10^{-15}	78	6.11×10^{-15}
	10^2	122	3.73×10^{-13}	114	1.66×10^{-12}	130	1.50×10^{-13}	170	1.68×10^{-14}
	10^4	218	1.05×10^{-13}	250	2.80×10^{-14}	282	1.68×10^{-14}	282	1.68×10^{-14}
	10^6	218	1.16×10^{-13}	250	3.31×10^{-14}	282	2.04×10^{-14}	410	1.88×10^{-14}
	10^8	218	1.12×10^{-13}	250	2.94×10^{-14}	282	1.68×10^{-14}	410	1.50×10^{-14}
	10^{16}	218	1.15×10^{-13}	250	3.15×10^{-14}	282	1.89×10^{-14}	410	1.71×10^{-14}
2	10^0	82	1.03×10^{-15}	90	1.03×10^{-15}	74	1.03×10^{-15}	74	1.03×10^{-15}
	10^2	250	4.10×10^{-15}	202	4.99×10^{-13}	266	2.74×10^{-15}	330	6.94×10^{-16}
	10^4	442	3.77×10^{-15}	506	5.92×10^{-16}	570	5.77×10^{-16}	474	4.68×10^{-16}
	10^6	442	4.02×10^{-15}	506	5.92×10^{-16}	570	5.75×10^{-16}	634	5.68×10^{-16}
	10^8	442	4.03×10^{-15}	506	6.06×10^{-16}	570	5.86×10^{-16}	634	5.72×10^{-16}
	10^{16}	442	4.03×10^{-15}	506	6.03×10^{-16}	570	5.83×10^{-16}	634	5.68×10^{-16}
3	10^0	29	3.79×10^{-10}	54	1.98×10^{-16}	54	1.98×10^{-16}	52	4.87×10^{-15}
	10^2	98	3.01×10^{-10}	202	1.03×10^{-10}	258	3.82×10^{-14}	298	2.80×10^{-16}
	10^4	186	8.02×10^{-12}	474	7.76×10^{-12}	474	7.76×10^{-12}	826	2.84×10^{-14}
	10^6	186	1.32×10^{-11}	474	1.28×10^{-11}	474	1.28×10^{-11}	890	1.37×10^{-13}
	10^8	186	1.32×10^{-11}	474	1.29×10^{-11}	474	1.29×10^{-11}	890	1.39×10^{-13}
	10^{16}	186	1.32×10^{-11}	474	1.29×10^{-11}	474	1.29×10^{-11}	890	1.39×10^{-13}
4	10^0	47	1.01×10^{-12}	55	1.19×10^{-13}	57	1.19×10^{-15}	89	6.01×10^{-20}
	10^2	75	9.93×10^{-13}	172	5.95×10^{-18}	172	5.95×10^{-18}	428	4.59×10^{-18}
	10^4	108	7.76×10^{-11}	268	2.34×10^{-12}	453	7.84×10^{-14}	1210	1.54×10^{-15}
	10^6	108	1.04×10^{-10}	268	5.32×10^{-12}	453	5.03×10^{-13}	1466	1.48×10^{-13}
	10^8	108	1.05×10^{-10}	268	5.37×10^{-12}	453	5.17×10^{-13}	1466	1.56×10^{-13}
	10^{16}	108	1.05×10^{-10}	268	5.38×10^{-12}	453	5.17×10^{-13}	1466	1.56×10^{-13}
5	10^0	108	2.41×10^{-18}	115	2.49×10^{-18}	115	2.49×10^{-18}	131	2.49×10^{-18}
	10^2	42	9.32×10^{-18}	106	9.11×10^{-18}	106	9.11×10^{-18}	106	9.11×10^{-18}
	10^4	74	4.42×10^{-17}	82	4.42×10^{-17}	90	4.42×10^{-17}	90	4.42×10^{-17}
	10^6	98	2.41×10^{-09}	146	4.36×10^{-11}	194	2.50×10^{-13}	222	1.58×10^{-14}
	10^8	98	4.87×10^{-09}	146	1.84×10^{-10}	194	3.80×10^{-12}	274	1.39×10^{-13}
	10^{16}	98	4.90×10^{-09}	146	1.86×10^{-10}	194	3.91×10^{-12}	274	1.49×10^{-13}
6	10^0	43	7.61×10^{-18}	43	7.61×10^{-18}	50	1.01×10^{-20}	50	1.01×10^{-20}
	10^2	18	7.98×10^{-13}	25	1.43×10^{-14}	25	1.43×10^{-14}	40	4.86×10^{-21}
	10^4	11	1.34×10^{-08}	66	4.54×10^{-14}	186	8.39×10^{-19}	218	8.39×10^{-19}
	10^6	11	9.50×10^{-09}	82	1.19×10^{-12}	218	1.42×10^{-13}	474	1.42×10^{-13}
	10^8	11	9.50×10^{-09}	82	1.26×10^{-12}	218	1.89×10^{-13}	474	1.89×10^{-13}
	10^{16}	11	9.50×10^{-09}	82	1.26×10^{-12}	218	1.89×10^{-13}	474	1.89×10^{-13}

Table 6.4. Results of dyadic refinement scheme for different prescribed target errors. The table shows the total number of integration points N and the error with respect to the reference values of Table 6.2, rescaled by the factors given in Table 6.3.

		10^{-6}	10^{-8}	10^{-10}	10^{-12}	# stored values (memory)
$\xi_0 = 1$,	1 thread	4,254.5	6,212.1	9,125.9	14,808.5	865 (501 KB)
$\xi_0 = 1$,	4 threads	1,196.4	1,768.5	2,578.9	4,123.7	
$\xi_0 = 10^3$,	1 thread	95.7	132.2	184.5	276.5	1878 (1086 KB)
$\xi_0 = 10^3$,	4 threads	31.6	44.1	61.1	90.6	

Table 6.5. Times in seconds for evaluation of the 153664 integrals with parameters as in (6.138), run on a Xeon E5450 system at 3 GHz, for different prescribed target accuracies, where values of $(\varphi_{0,l}\,\varphi_{0,0})^\wedge(2^{-j}k)$ for $0 \leq 2^{-j}k \leq \xi_0$ are stored and reused. In addition, in each case 1.57 seconds are spent on preprocessing.

We finally consider CPU times for the evaluation of the integrals (6.137) in the range of parameters

$$\alpha \in \{1, 10^4, 10^8, 10^{12}\}\,, \quad \nu_1, \nu_2, \mu_1, \mu_2 \in \{(0,k,s)\colon\; k = -3, \ldots, 3\,,\; s = 0, 1\}\,. \tag{6.138}$$

This amounts to a total number of 153664 integrals[4]. Here we consider the acceleration of the Fourier-based scheme by two strategies: On the one hand, by storing and reusing computed values of $(\varphi_{0,l}\,\varphi_{0,0})^\wedge(2^{-j}k)$, for certain j and k, and for all l such that this expression does not vanish; these values are not precomputed, but accumulated during the computation for $2^{-j}k \in [0, \xi_0]$, where $\xi_0 > 0$ is a preset bound. On the other hand, we consider the gain by OpenMP parallelization, that is, we compare the performance of the integration scheme using one and four threads.

CPU times are given in Table 6.5 for several target accuracies; integrals are evaluated by the dyadic refinement scheme, and in each case, the resulting error with respect to the reference values is smaller than the listed prescribed bound. The results show in particular that storing more Fourier transform values leads to a very significant reduction of execution time, with only very moderate additional memory requirements. One also obtains the expected speedup by parallelization.

Remark 6.51. *Comparing the results obtained with a practical implementation of the scheme in Table 6.4 to the convergence analysis of Section 6.6.3, one observes that the number of required points N generally remains quite low in the case of small α, with very little variation of N with respect to the error tolerance. This is consistent with the α-dependent exponential convergence estimate corresponding to the first bound in* (6.120) *and* (6.122)*.*

With increasing α, in each test case in Table 6.4, N grows up to a certain limiting value. Here, an algebraic increase of N with decreasing error tolerance can be observed, which is stronger in test cases 3, 4, and 6 than in cases 1, 2, and 5. This is to be expected in view of Remark 6.46. Since $|\max\{|\nu_1|, |\mu_1|\} - \max\{|\nu_2|, |\mu_2|\}|$ *is larger in tests 3, 4, and 6, the third bound in* (6.122) *is larger in these cases than in the remaining tests. We therefore expect the second bound in* (6.122)*, which corresponds to a less favorable algebraic convergence rate, to determine the quantitative behaviour in tests 3, 4, and 6, which is consistent with the results of Table 6.4.*

It can also be observed, however, that for moderate accuracy requirements, the values of N are similar in all cases.

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[4] Note that in practice, due to the symmetries of the integrand, not all of these integrals would need to be evaluated separately.

7 Numerical Realization and Experiments

In this chapter, we summarize how the eigenvalue solver developed in Section 5.4 can be realized in the case of the electronic Schrödinger model problems under consideration, and we discuss the results of our numerical tests. The model problems include the basic one-electron problem of hydrogen, and the two-electron problems of hookium and helium. In addition, we consider simpler model problems with separable solutions in three and six space dimensions.

In Section 4.3, we have obtained tensor approximability results for the ground states of hydrogen and hookium. Concerning the approximability of mode frames, we have seen that an explicitly correlated formulation is advantageous. As shown in the previous chapter, also for the nonsymmetric explicitly correlated Hamiltonians as in (2.16) and (2.19), the necessary ingredients for the approximation of the modified operators are in place. However, since the iterative solution methods for the corresponding nonsymmetric eigenvalue problems require further investigation, we restrict ourselves to the self-adjoint standard formulation in what follows.

Our test problems are thus all of the form

$$Hu := -\tfrac{1}{2}\Delta u + Vu = \lambda u$$

with a potential function V, which is either given explicitly as a sum of separable terms, or needs to be approximated in this form. In each case, we compute approximations to the eigenfunction u_0 corresponding to the lowest eigenvalue λ_0. In the examples with explicit solutions, we give expressions for u_0 normalized to $\|u_0\|_{\mathrm{L}_2} = 1$.

Note that the test problems and their solutions each have certain problem-specific symmetries, which could be exploited to reduce the computational effort. For better comparability of results, however, we do not make use of any such symmetries in our tests. Recall furthermore that antisymmetry constraints do not play a role in the ground states of one- and two-electron systems.

All tests in this chapter are based on orthonormal Daubechies-type wavelets constructed by Ojanen that have already been used for numerical examples in Chapter 6, shown in Figure 6.2. Recall that this wavelet has 6 vanishing moments and, according to the estimates in [119], is contained in $\mathrm{H}^s(\mathbb{R})$ for $s \approx 4.32$. In this chapter, the tensor product wavelet bases $\{\Psi_\nu\}_{\nu\in\nabla^d}$ for $d = 3, 6$ are always constructed from these univariate wavelets.

We use the subdivided tensor representation as defined in Subsection 5.2.3. The wavelet representation of H is thus given by

$$\mathbf{H} := \mathbf{S}_d \bigl(\langle H\Psi_\nu, \Psi_\mu\rangle\bigr)_{\nu,\mu\in\nabla^d} \mathbf{S}_d$$

with the rescaling operator $\mathbf{S}_d$ defined as in (5.31). The corresponding wavelet coefficients of u_0 are

$$\mathbf{u}_0 = \mathbf{S}_d^{-1} \bigl(\langle u_0, \Psi_\nu\rangle\bigr)_{\nu\in\nabla^d} .$$

If u_0 is separable, this separability is by construction inherited by $\mathbf{u}_0|_{\bar\Lambda_{d,n}}$, and by linearity sums of separable terms are preserved on each $\bar\Lambda_{d,n}$ in the same way. Note that this will in general not hold for $\mathbf{u}_0$ itself without this subdivision, which may have unbounded multilinear rank even if u_0 is separable.

For solving the eigenvalue problems, we use the scheme `tensor_evpsolve` given in Algorithm 5.6 with some minor modifications. Recall that this algorithm has an outer iteration, indexed by i, which comprises a sequence of inner iterations indexed by j, with error tolerances η_j, and a coarsening operation. The iterates $\mathbf{v}_i$ produced by each outer iteration step, which approximate

$\mathbf{u}_0$, are of the form

$$\mathbf{v}_i = \sum_n \sum_{k\in\mathcal{K}_3(r_n)} a_{n,k} \bigotimes_{l=1}^{3} \mathbf{U}^{(l)}_{n,k_l}\,,$$

where each $\mathbf{U}^{(l)}_{n,k_l}$ is a compactly supported vector on $\bar\Lambda^{(l)}_{d,n} \subset \nabla^{d/3}$.

The action of operators on expansions of this form is approximated by the routine apply described in Algorithm 5.4, which is performed once per iteration step. Recall that the concrete construction of a partitioning of mode frames into pieces with different operator approximation accuracies as in (5.61) was left unspecified in the description of apply. Here we apply binary binning as described in Subsection 3.6.3 to the coefficients in each mode frame, and use the same approximation of the operator for the elements of each bin.

Since no sufficiently sharp estimates for the constants in the iterations are available, we need to choose these ad hoc for each test case. In the given tests, the parameters are chosen rather conservatively, that is, the error tolerances in the scheme are smaller than necessary for ensuring convergence.

Note that in the presentation of results, unless stated otherwise, we shall always show data for the full sequence of all iterates produced by the inner iterations. We thus introduce a total iteration number that counts the number of calls of apply.

The additional modifications with respect to tensor_evpsolve improve the quantitative performance of the method:

1. Before each call of apply, additional steps of the basic iterative scheme restricted to the current basis coefficients are performed to reduce the residual on this set of indices. Since the corresponding approximation of operators on a given set of output indices is much less expensive than apply, this yields a significant acceleration.

2. Instead of the residual approximation $\mathbf{r}_j$ produced by apply, we use coarsen$(\mathbf{r}_j, c\min\{\eta_j, \|\mathbf{r}_j\|\})$ with a small $c > 0$, and accordingly adjusted tolerance for the computation of $\mathbf{r}_j$. This is advantageous because the approximate application of operators based on wavelet compressibility estimates still tends to produce many negligible entries, which are eliminated from the update to the current iterate by this additional a posteriori step. Note that the norm of the residual, which is used to assess the progress of the iteration, is evaluated before this coarsening step.

3. The approximate evaluation of Rayleigh quotients is done with a specialized routine that does not use tensor recompression operations. Due to the lower numerical costs, it can thus be done with a tighter error tolerance than required for the convergence of the iteration, which yields improved approximate eigenvalues.

The Laplacian term is treated in all tests as described in Sections 6.2 and 6.5. As a consequence of the results in Section 6.2, the representation of the Laplacian in the wavelet basis used here is s^*–compressible with at least $s^* \approx 2.82$.

As noted in Remark 3.16, the constants in the norm equivalences between rescaled wavelet coefficients and H^1–norms depend on the choice of scaling function level j_0 of the wavelet index set ∇. For the condition number of the rescaled operator, an appropriate choice of j_0 is therefore decisive. This has also been discussed in [90], where a choice of j_0 for operator equations on unbounded domains depending on the right hand side was proposed. As we are not aware of a suitable method for finding the j_0 leading to the best condition number in our setting, we resort to a heuristic comparison of different choices.

It needs to be emphasized that the residual values given in the numerical results do not refer to fixed discretizations, but are estimates for the norms of the residuals of the infinite-dimensional eigenvalue problems. Note that by Lemma 3.23(iii), up to a multiplicative constant this residual is an upper bound for the H^1–error in the eigenfunction (provided that the error is sufficiently small).

7.1 Three-Dimensional Problems

In the three-dimensional examples, each tensor factor corresponds to a subset of the one-dimensional wavelet index set ∇. We use the basis with $j_0 = -2$ and start from the index set consisting of the single element $(\bar\nu_0, \bar\nu_0, \bar\nu_0) \in \nabla^3$ with $\bar\nu_0 = (j_0, 0, 0)$.

7.1.1 Delta Potentials

We first consider a model problem with separable solution. The weak formulation reads

$$\tfrac{1}{2}\int_{\mathbb{R}^3} \mathrm{D}u \cdot \mathrm{D}v \,\mathrm{d}x - \sum_{i=1}^{3} \int_{\mathbb{R}^2} (u\,v)|_{x_i=0} \,\mathrm{d}x = \lambda \int_{\mathbb{R}^3} u\,v \,\mathrm{d}x\,, \quad v \in \mathrm{H}^1(\mathbb{R}^3)\,.$$

We shall abbreviate this formally, as customary in physics literature, as

$$H_{\delta 3} := -\tfrac{1}{2}\Delta u - \sum_{i=1}^{3} \delta_{x_i} u = \lambda u\,. \tag{$\delta 3$}$$

Note that this operator can be written as a sum of three separable terms. The lowest eigenvalue is given by $\lambda_0 = -\frac{3}{2}$, with corresponding eigenfunction

$$u_0(x) = \prod_{i=1}^{3} e^{-|x_i|}\,, \quad x \in \mathbb{R}^3\,.$$

Since the solution is separable, on each part $\bar\Lambda_{3,n}$ of the subdivision of the wavelet index set, the coefficients $\mathbf{u}_0$ thus have multilinear rank $(1, 1, 1)$.

For the approximate application of the potential terms, we use the wavelet compression strategy given in Remark 6.26. As noted there, these potential terms are s^*-compressible for any $s^* > 0$. For the one-dimensional operators $-\frac{1}{2}\mathrm{D}^2_{x_i} - \delta_{x_i}$, and by Proposition 6.4 also for $H_{\delta 3}$, we thus have at least $s^* \approx 2.82$.

Figure 7.1 shows the convergence behaviour of the scheme in dependence on the iteration count (with each iteration corresponding to one call to apply). As to be expected, the decrease in the residual is interrupted by a slight increase after each coarsening step. The eigenvalue error stays well below the residual, but is also more sensitive to variations below the current operator approximation tolerance. In the present case, in the beginning of the iteration, the approximate eigenvalues approach the exact value from above and show a rather regular convergence pattern, but begin to oscillate more strongly after crossing the exact value for the first time.

Figure 7.2 shows the convergence of L_2-normalized intermediate solutions (after a coarsening step) to the exact solution on a one-dimensional section. Concerning the complexity of the produced approximations, the dependence of the total number of parameters on the H^1–error is of interest. The direct evaluation of this error for each iterate would be prohibitively expensive. Recall, however, that by Lemma 3.23(iii), the approximate residual norm provides an estimate for the H^1–error, and can therefore be used as a substitute for these complexity considerations. Figure 7.3 thus shows the total number of parameters in the mode frames of the intermediates in dependence on the current residual estimate. As the results show, the best possible rate for the used wavelet basis, which has order of polynomial reproduction 5, is recovered: for H^1–error ε, we can expect the total number of coefficients in the mode frames to grow at best as $\mathcal{O}(\varepsilon^{-\frac{1}{5}})$.

This result is in fact more favorable than what is to be expected on the basis of the available estimates: a stronger growth in the number of coefficients during the inner iterations would be possible due to the limited s^*-compressibility of the Laplacian. The results thus suggest that the compressibility estimate is in fact rather pessimistic.

A point that is particularly remarkable in this example is that over the whole course of the

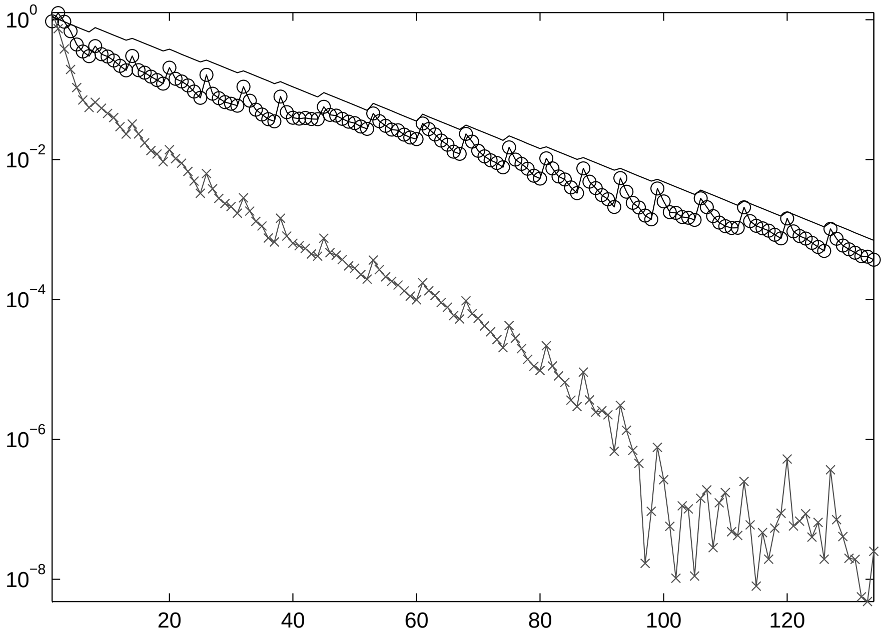

Figure 7.1. Problem ($\delta 3$): ∘ residual, × eigenvalue approximation for each iteration step; the line gives the current error tolerance η.

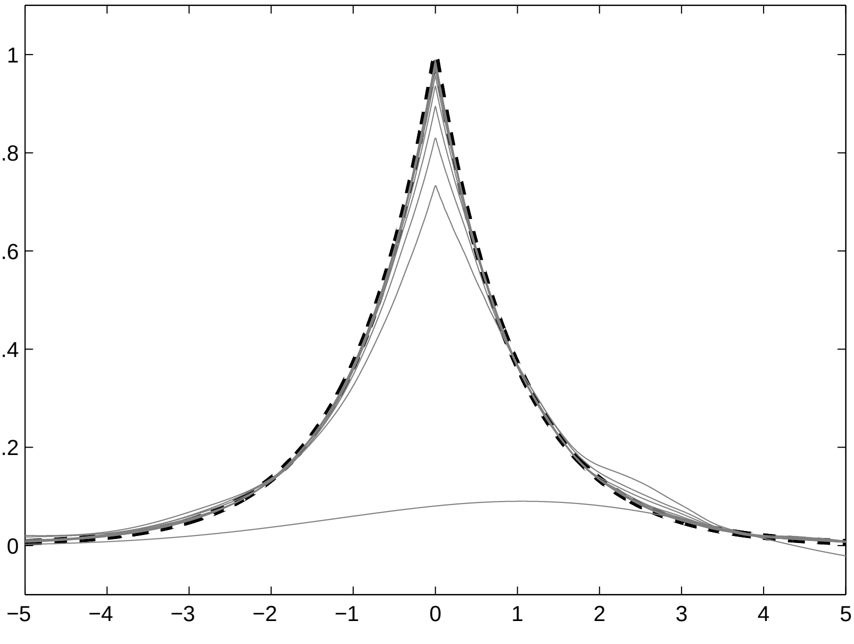

Figure 7.2. Problem ($\delta 3$): convergence of first 10 iterates, including the starting value, on the section $(x_1, 0, 0)$.

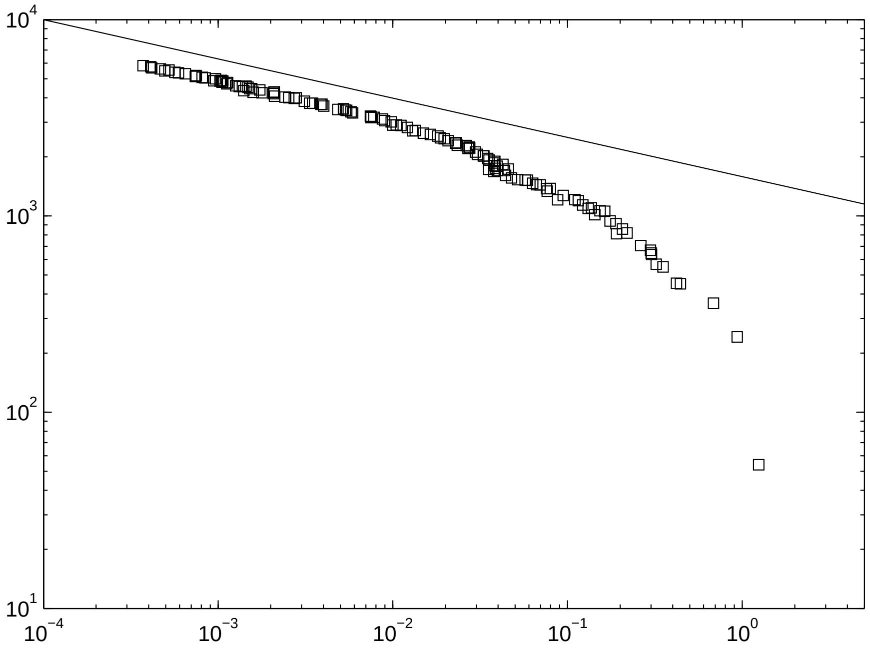

Figure 7.3. Problem ($\delta 3$): total number of nonzero coefficients in mode frames, in dependence on residual estimate. The line has slope $-\frac{1}{5}$.

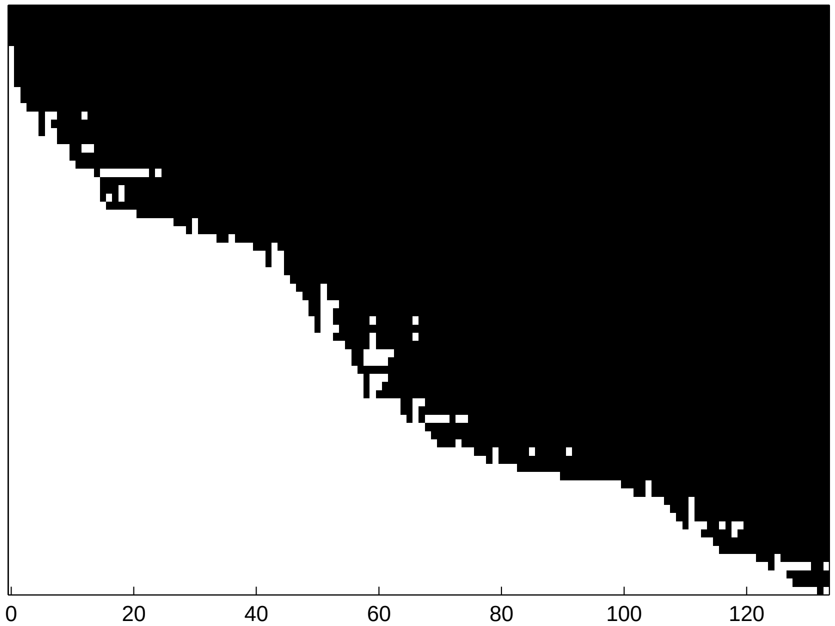

Figure 7.4. Problem ($\delta 3$): maximum rank on each subdivision element $\bar{\Lambda}_{3,n}$ (rows) in dependence on iteration number (columns). Here white corresponds to zero, black to one.

iteration, the multilinear ranks of all iterates on the subdivision elements remain bounded by the ranks of the true solution, that is, by $(1,1,1)$. The gradual increase in the number of active subdivision elements, each with multilinear ranks $(1,1,1)$, can be seen in Figure 7.4. Let (r_n) be the sequence of multilinear ranks on the subdivision elements of the current iterate, then each row corresponds to the evolution of the maximum multilinear rank $\max_k r_{n,k}$ on $\bar{\Lambda}_{3,n}$ for an n. Here the subdivision elements are ordered by first appearance in the iteration. Note that this behaviour of the ranks depends on an appropriate choice of the parameters: if either the recompression error tolerances are chosen too low, or if the approximation of the operator is too inaccurate, slightly larger multilinear ranks can occur during the course of the iteration.

Tables 7.1 and 7.2 show the evolution of multilinear ranks and and mode frame sizes (i.e., active wavelet coefficient counts for each mode frame) for a selected number of iterations. Each row in the tables corresponds to a subdivision element $\bar{\Lambda}_{3,n}$, with the corresponding level ranges given in the leftmost column. Iterations with a coarsening step at the end of an outer iteration are printed in italics.

7.1.2 Hydrogen

The electronic Schrödinger problem for hydrogen in atomic units reads

$$H_{\mathrm{H}} u := -\frac{1}{2}\Delta u - \frac{1}{|x|} u = \lambda u \,. \tag{H}$$

The ground state eigenvalue is $\lambda_0 = -\frac{1}{2}$, with eigenfunction

$$u_0(x) = \pi^{-\frac{1}{2}} e^{-|x|}\,, \quad x \in \mathbb{R}^3\,.$$

For the Coulomb potential on $\mathbb{R}^3$, we use a separable expansion of the form

$$\int_{\mathbb{R}^3} \frac{1}{|x|} \Psi_\mu \Psi_\nu \,\mathrm{d}x \approx \sum_k \omega_k \prod_{i=1}^{3} \int_{\mathbb{R}} e^{-\alpha_k x_i^2} \psi_{\mu_i} \psi_{\nu_i} \,\mathrm{d}x_i\,, \quad \mu,\nu \in \nabla^3 \tag{7.1}$$

as analyzed in Section 6.3, with coefficients based on the best approximations by exponential sums provided in [70].

The accuracy of this separable expansion is adjusted, on the basis of the estimate of Theorem 6.5, to be of the same order as the current target tolerance in the approximate application of the operator. The sets of coefficients ω_k and α_k in general differ completely for different errors. To avoid too frequent recomputation of integrals, it is therefore preferable to change this approximation only after several iteration steps. We use a fixed sequence of separable expansions with accuracy improving approximately as a power of two. The resulting total ranks of the approximation of H_{H} are shown in Figure 7.5.

For the approximate application by wavelet compression of each summand on the right hand side of (7.1), we use the construction of Theorem 6.20 and Remark 6.21. Matrix entries are computed by the Fourier transform-based method developed in Section 6.6. Note that the reference scheme based on triple products, as discussed in Subsection 6.6.1, could in principle yield a better overall convergence rate for these one-electron integrals, but in our present setting turns out to be quantitatively much more expensive than the Fourier transform-based scheme.

The convergence of residual and eigenvalue approximations shown in Figure 7.6 is less regular than in the previous example due to the adjustment of the operator approximations. The convergence of the first iterates on a one-dimensional section, after a coarsening step, is shown in Figure 7.7. Since the approximate potentials are smooth, the iterates show a more gradual increase in the gradient near the cusp than in the previous example (cf. Figure 7.2).

Figure 7.8 shows the total number of coefficients in the mode frames, in dependence of the current residual estimate, which is again used as a substitute for the error in H^1. As in the previous example,

Table 7.1. Problem ($\delta 3$): multilinear ranks of iterates on the first 20 appearing parts $\bar{\Lambda}_{3,n}$ of the subdivision. Iterations with coarsening are in italics.

total iteration number	5	6	*7*	8	9	10	11	12	*13*	14	15	16	17	18	*19*	20
outer iteration number	0	0	*0*	1	1	1	1	1	*1*	2	2	2	2	2	*2*	3
$[-2,-2] \times [-2,-2] \times [-2,-2]$	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[-1,-1] \times [-2,-2] \times [-2,-2]$	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[-2,-2] \times [-1,-1] \times [-2,-2]$	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[-2,-2] \times [-2,-2] \times [-1,-1]$	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[-2,-1] \times [-2,-1] \times [0,1]$	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[0,1] \times [-2,-1] \times [-2,-1]$	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[-2,-1] \times [0,1] \times [-2,-1]$	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[2,5] \times [-2,1] \times [-2,1]$	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[-2,1] \times [2,5] \times [-2,1]$	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[-2,1] \times [-2,1] \times [2,5]$	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[-2,-2] \times [-1,-1] \times [-1,-1]$	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[-1,-1] \times [-2,-2] \times [-1,-1]$	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[-1,-1] \times [-1,-1] \times [-2,-2]$	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[-1,-1] \times [-1,-1] \times [-1,-1]$		(1,1,1)			(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[-2,-1] \times [0,0] \times [0,0]$		(1,1,1)		(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[0,0] \times [-2,-1] \times [0,0]$		(1,1,1)			(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[0,0] \times [0,0] \times [-2,-1]$					(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[6,13] \times [-2,5] \times [-2,5]$							(1,1,1)	(1,1,1)			(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[-2,5] \times [6,13] \times [-2,5]$							(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)
$[-2,5] \times [-2,5] \times [6,13]$								(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)

Table 7.2. Problem ($\delta 3$): mode sizes of iterates corresponding to Table 7.1.

total iteration number	5	6	*7*	8	9	10	11	12	*13*	14	15	16	17	18	*19*	20
outer iteration number	0	0	*0*	1	1	1	1	1	*1*	2	2	2	2	2	*2*	3
$[-2,-2] \times [-2,-2] \times [-2,-2]$	(15,15,15)	(16,16,16)	*(13,13,13)*	(17,17,17)	(17,17,17)	(17,17,17)	(17,17,17)	(17,17,17)	*(14,13,14)*	(17,18,17)	(17,18,17)	(17,18,17)	(17,18,17)	(17,18,17)	*(15,15,15)*	(15,16,15)
$[-1,-1] \times [-2,-2] \times [-2,-2]$	(11,11,11)	(11,11,11)	*(7,11,11)*	(10,11,11)	(11,11,11)	(11,13,11)	(11,13,14)	(11,13,14)	*(11,12,12)*	(11,12,12)	(11,15,15)	(11,15,15)	(12,15,15)	(12,15,15)	*(9,13,13)*	(11,15,13)
$[-2,-2] \times [-1,-1] \times [-2,-2]$	(11,11,13)	(14,11,14)	*(10,8,10)*	(11,8,11)	(11,8,11)	(14,11,11)	(14,11,14)	(14,11,14)	*(12,9,12)*	(14,11,14)	(14,12,14)	(14,12,14)	(14,12,14)	(14,12,14)	*(13,9,13)*	(13,11,13)
$[-2,-2] \times [-2,-2] \times [-1,-1]$	(14,13,11)	(14,14,11)	*(10,10,9)*	(13,11,9)	(13,14,9)	(13,14,9)	(14,14,9)	(14,14,11)	*(12,12,9)*	(12,12,11)	(15,15,11)	(15,15,11)	(15,15,11)	(15,15,11)	*(13,13,9)*	(13,13,11)
$[-2,-1] \times [-2,-1] \times [0,1]$	(18,18,14)	(19,19,15)	*(15,15,14)*	(15,15,17)	(20,19,18)	(20,19,21)	(20,19,21)	(20,21,21)	*(19,19,15)*	(19,19,20)	(19,19,20)	(24,23,20)	(24,23,20)	(24,23,20)	*(20,20,17)*	(20,20,17)
$[0,1] \times [-2,-1] \times [-2,-1]$	(15,18,18)	(19,20,20)	*(14,15,15)*	(17,15,15)	(17,19,19)	(21,19,19)	(21,19,19)	(21,19,19)	*(16,19,19)*	(20,19,19)	(20,19,19)	(20,19,23)	(20,23,23)	(20,23,23)	*(17,19,20)*	(18,19,20)
$[-2,-1] \times [0,1] \times [-2,-1]$	(18,15,16)	(19,16,19)	*(15,14,15)*	(15,17,15)	(19,17,19)	(19,21,19)	(19,21,19)	(19,21,19)	*(19,16,19)*	(19,16,19)	(19,21,19)	(22,21,22)	(22,21,22)	(24,21,22)	*(20,17,20)*	(20,18,20)
$[2,5] \times [-2,1] \times [-2,1]$	(27,16,16)	(28,20,20)	*(21,14,14)*	(27,18,14)	(27,18,20)	(27,22,20)	(29,25,25)	(29,25,25)	*(26,18,18)*	(29,25,25)	(29,25,25)	(33,28,29)	(33,28,29)	(33,29,29)	*(29,25,25)*	(29,25,25)
$[-2,1] \times [2,5] \times [-2,1]$	(16,27,17)	(19,28,19)	*(13,22,13)*	(19,28,19)	(19,28,19)	(19,28,22)	(25,28,22)	(27,31,27)	*(18,27,18)*	(25,27,25)	(28,32,25)	(28,32,25)	(28,32,29)	(29,34,29)	*(25,28,25)*	(25,34,25)
$[-2,1] \times [-2,1] \times [2,5]$	(17,17,28)	(19,18,28)	*(13,14,22)*	(19,19,28)	(21,19,28)	(21,24,28)	(21,24,28)	(28,27,31)	*(18,18,26)*	(25,25,30)	(25,25,30)	(29,28,33)	(29,29,33)	(29,29,33)	*(25,25,28)*	(25,25,33)
$[-2,-2] \times [-1,-1] \times [-1,-1]$	(10,6,6)	(10,7,7)	*(7,5,5)*	(10,7,7)	(10,8,9)	(10,8,9)	(10,8,9)	(10,8,9)	*(9,7,7)*	(12,7,7)	(12,7,7)	(12,7,7)	(12,8,9)	(12,8,9)	*(10,7,7)*	(13,7,7)
$[-1,-1] \times [-2,-2] \times [-1,-1]$	(7,9,7)	(7,9,7)	*(5,7,5)*	(7,9,7)	(7,9,7)	(7,9,7)	(7,12,7)	(7,12,7)	*(7,9,7)*	(7,12,7)	(9,12,9)	(9,12,9)	(9,12,9)	(9,12,9)	*(7,10,7)*	(7,13,7)
$[-1,-1] \times [-1,-1] \times [-2,-2]$	(7,7,9)	(7,7,9)	*(5,5,7)*	(7,7,9)	(7,7,9)	(7,7,11)	(7,7,11)	(7,7,11)	*(7,7,9)*	(7,7,12)	(7,7,12)	(9,9,12)	(9,9,12)	(9,9,12)	*(7,7,10)*	(7,7,13)
$[-1,-1] \times [-1,-1] \times [-1,-1]$		(5,5,5)			(5,5,5)	(6,6,6)	(6,6,6)	(7,7,7)		(6,6,6)	(7,7,7)	(7,7,7)	(7,7,7)	(7,7,7)	*(5,5,5)*	(7,7,7)
$[-2,-1] \times [0,0] \times [0,0]$		(9,5,5)		(9,5,5)	(12,5,5)	(12,5,5)	(12,7,7)	(12,7,7)	*(4,4,4)*	(12,7,7)	(12,7,7)	(12,7,7)	(15,7,7)	(15,7,7)	*(9,6,5)*	(15,6,7)
$[0,0] \times [-2,-1] \times [0,0]$		(5,9,5)			(5,11,5)	(5,12,5)	(7,12,7)	(7,12,7)	*(3,4,3)*	(7,13,7)	(7,13,7)	(7,13,7)	(7,13,7)	(7,15,7)	*(6,9,6)*	(7,15,7)
$[0,0] \times [0,0] \times [-2,-1]$					(5,5,11)	(5,5,12)	(6,6,12)	(7,7,12)	*(4,4,3)*	(7,7,13)	(7,7,13)	(7,7,13)	(7,7,13)	(7,7,13)	*(6,6,9)*	(6,6,15)
$[6,13] \times [-2,5] \times [-2,5]$							(14,13,12)	(18,14,14)			(18,15,15)	(28,15,16)	(31,15,16)	(31,15,16)	*(19,14,14)*	(28,14,14)
$[-2,5] \times [6,13] \times [-2,5]$							(11,14,13)	(13,21,13)	*(8,10,9)*	(8,19,9)	(11,26,11)	(15,30,11)	(15,32,16)	(15,33,16)	*(10,21,9)*	(15,29,15)
$[-2,5] \times [-2,5] \times [6,13]$								(14,14,19)	*(4,5,8)*	(9,9,14)	(11,11,26)	(15,12,29)	(16,16,32)	(16,16,36)	*(10,10,20)*	(15,15,30)

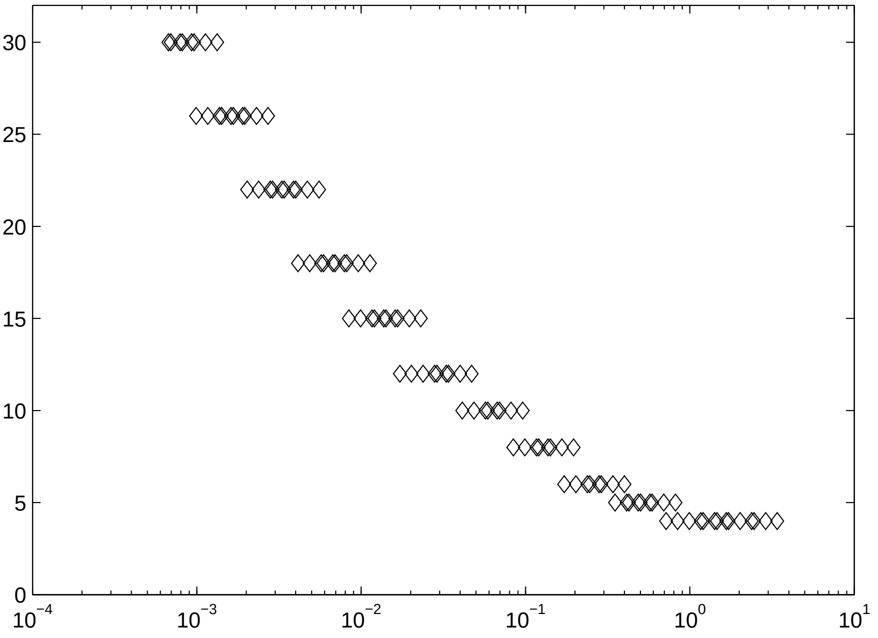

Figure 7.5. Problem (H): number of separable terms in the operator approximation, in dependence on the error tolerance η.

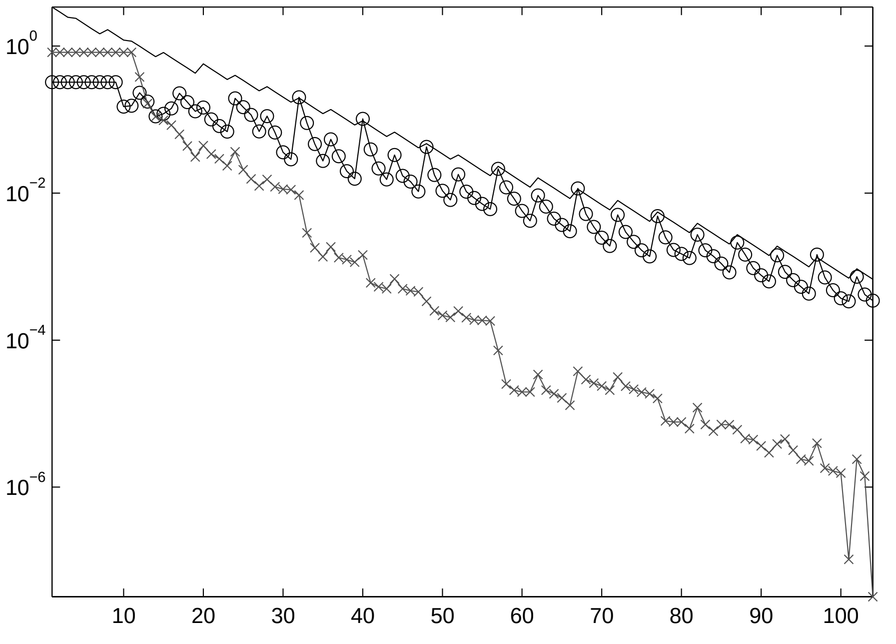

Figure 7.6. Problem (H): ∘ residual, × eigenvalue approximation for each iteration step; the line gives the current error tolerance η.

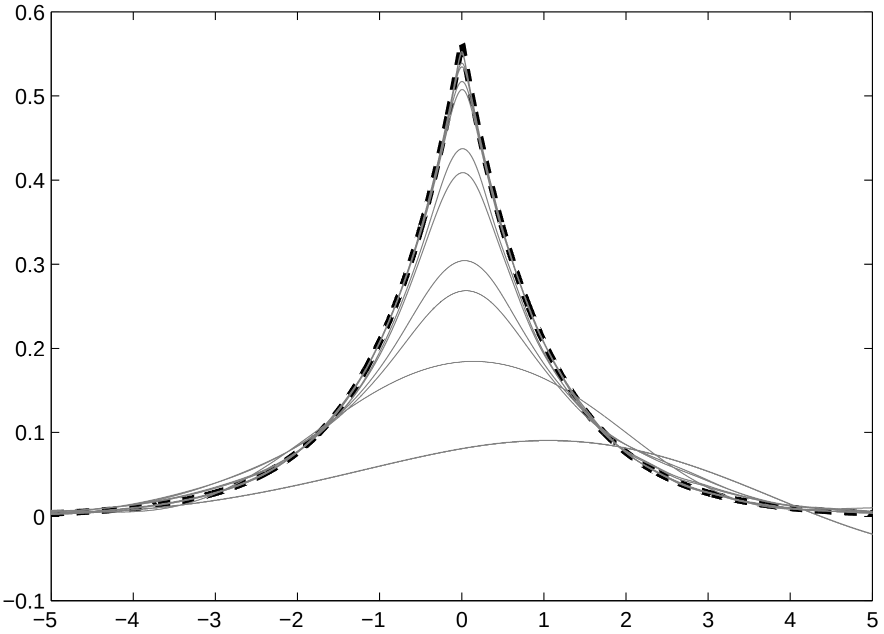

Figure 7.7. Problem (H): convergence of the first 15 iterates, including the starting value, on the section $(x_1, 0, 0)$.

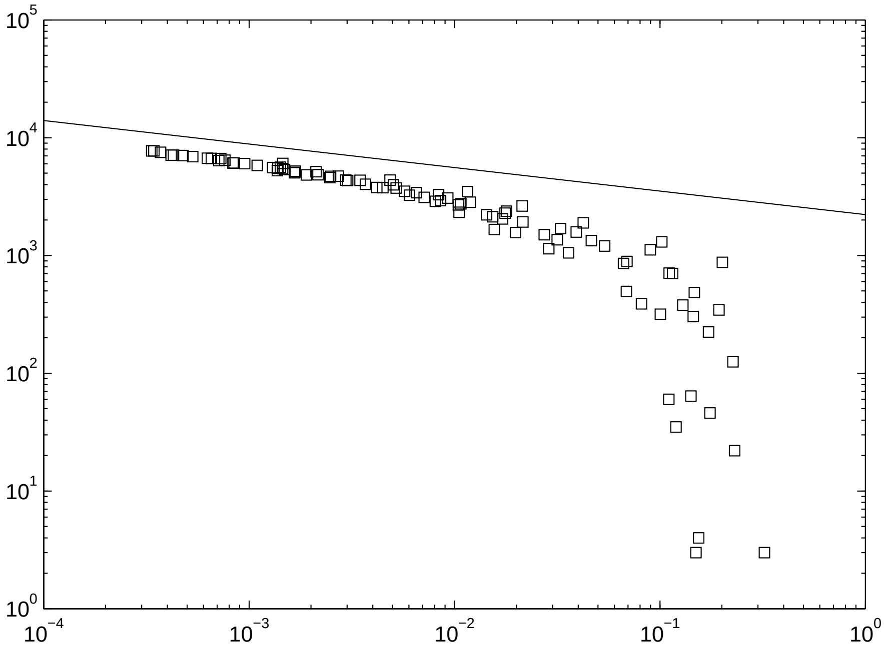

Figure 7.8. Problem (H): total number of nonzero coefficients in mode frames, in dependence on residual estimate. The line has slope $-\frac{1}{5}$.

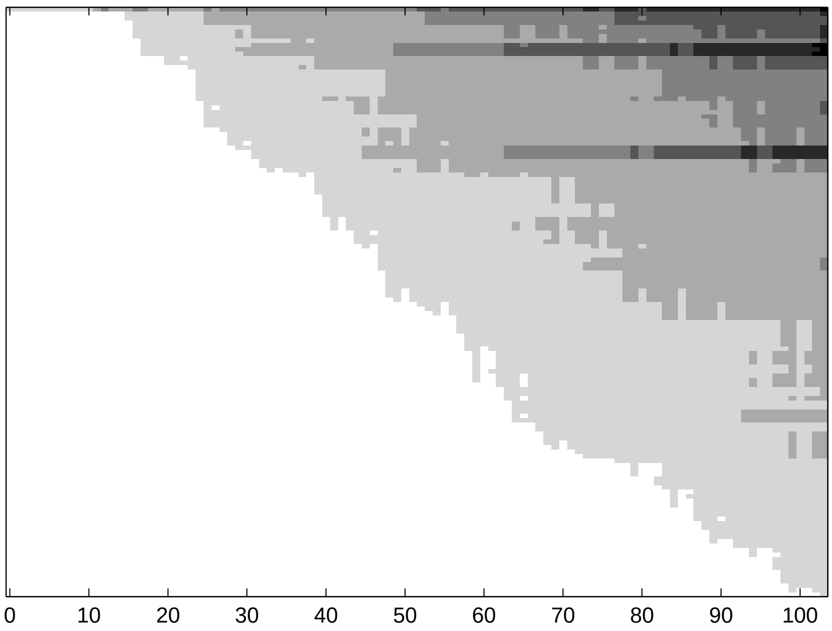

Figure 7.9. Problem (H): maximum ranks on subdivision elements (rows) in dependence on the iteration number (columns). Black corresponds to the maximum value 6.

the best possible rate for the wavelet basis is approached.

The evolution of the ranks on the subdivision elements during the iteration is visualized in Figure 7.9 in the same manner as in Figure 7.4 in the previous example. In the present case, u_0 does not have an expansion of finite rank, and a gradual increase of ranks during the iteration is observed. The maximum arising value of $\max_i r_{n,i}$ is 6. Tables 7.3 and 7.4 show, as in the previous example, the evolution of multilinear ranks and and mode sizes for a selected number of iteration numbers.

7.2 Six-Dimensional Problems

In the following problems, each tensor factor corresponds to a subset of ∇^2. Recall that the corresponding separation $\nabla^6 = \nabla^2 \times \nabla^2 \times \nabla^2$ is required for dealing with electron interaction, both concerning low-rank approximability of solutions and approximation of the interaction potential. In each case, we start from the index set consisting of the single element $(\bar\nu_0, \ldots, \bar\nu_0) \in \nabla^6$ with $\bar\nu_0 = (j_0, 0, 0)$.

7.2.1 Delta Potentials

We first consider a problem of the same form as ($\delta 3$) on $\mathbb{R}^6$,

$$H_{\delta 6} u := -\tfrac{1}{2}\Delta u - \sum_{i=1}^{6} \delta_{x_i} u = \lambda u\,. \qquad (\delta 6)$$

Table 7.3. Problem (H): multilinear ranks of iterates on the first 20 appearing parts $\bar{\Lambda}_{3,n}$ of the subdivision. Iterations with coarsening are in italics.

total iteration number	20	21	22	*23*	24	25	26	*27*	28	29	30	*31*	32	33	34	*35*
outer iteration number	5	5	5	*5*	6	6	6	*6*	7	7	7	*7*	8	8	8	*8*
$[-2,-2]\times[-2,-2]\times[-2,-2]$	(2,2,2)	(2,2,2)	(2,2,2)	*(2,2,2)*	(2,2,2)	(2,2,2)	(3,3,3)	*(2,2,2)*	(3,3,3)	(3,3,3)	(3,3,3)	*(3,3,3)*	(3,3,3)	(3,3,3)	(3,3,3)	*(3,3,3)*
$[-1,-1]\times[-2,-2]\times[-2,-2]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(2,2,2)	*(2,1,2)*	(2,1,2)	(2,2,2)	(2,2,2)	*(2,2,2)*	(2,2,2)	(2,2,2)	(2,2,2)	*(2,2,2)*
$[-2,-2]\times[-2,-2]\times[-1,-1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(2,1,2)	*(2,1,2)*	(2,2,2)	(2,2,2)	(2,2,2)	*(2,2,2)*	(2,2,2)	(2,2,2)	(2,2,2)	*(2,2,2)*
$[-2,-2]\times[-1,-1]\times[-2,-2]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(2,2,1)	*(2,2,2)*	(2,2,2)	(2,2,2)	(2,2,2)	*(2,2,2)*	(2,2,2)	(2,2,2)	(2,2,2)	*(2,2,2)*
$[-2,-2]\times[-1,-1]\times[-1,-1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,2,2)	(1,2,2)	(1,2,2)	*(1,2,2)*
$[-1,-1]\times[-2,-2]\times[-1,-1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(2,1,2)	*(1,1,1)*	(2,1,2)	(2,1,2)	(2,2,2)	*(2,1,2)*
$[-1,-1]\times[-1,-1]\times[-2,-2]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(2,2,1)	*(1,1,1)*	(2,2,1)	(2,2,1)	(2,2,2)	*(2,2,1)*
$[-1,-1]\times[-1,-1]\times[-1,-1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*
$[0,1]\times[-2,-1]\times[-2,-1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(2,1,2)	(2,2,2)	(2,2,2)	*(2,2,2)*
$[-2,-1]\times[0,1]\times[-2,-1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(2,2,2)	*(2,2,2)*	(2,2,2)	(2,2,2)	(2,2,2)	*(2,2,2)*
$[-2,-1]\times[-2,-1]\times[0,1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(2,1,2)*	(2,1,2)	(2,2,2)	(2,2,2)	*(2,2,2)*
$[-2,-1]\times[0,0]\times[0,0]$		(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*
$[0,0]\times[-2,-1]\times[0,0]$		(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*
$[0,0]\times[0,0]\times[-2,-1]$					(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*
$[-2,-1]\times[0,0]\times[1,1]$						(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*
$[-2,-1]\times[1,1]\times[0,0]$						(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*
$[0,0]\times[-2,-1]\times[1,1]$						(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*
$[1,1]\times[-2,-1]\times[0,0]$						(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*
$[0,0]\times[1,1]\times[-2,-1]$						(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*
$[1,1]\times[0,0]\times[-2,-1]$						(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*

Table 7.4. Problem (H): mode sizes of iterates corresponding to Table 7.3.

total iteration number	20	21	22	*23*	24	25	26	*27*	28	29	30	*31*	32	33	34	*35*
outer iteration number	5	5	5	*5*	6	6	6	*6*	7	7	7	*7*	8	8	8	*8*
$[-2,-2]\times[-2,-2]\times[-2,-2]$	(17,17,18)	(22,22,20)	(22,22,21)	*(17,17,17)*	(21,21,21)	(21,21,21)	(22,22,22)	*(18,18,18)*	(22,22,22)	(23,23,23)	(23,23,23)	*(18,18,18)*	(23,23,23)	(23,23,23)	(24,24,24)	*(21,20,21)*
$[-1,-1]\times[-2,-2]\times[-2,-2]$	(9,11,11)	(9,11,11)	(9,11,11)	*(8,11,11)*	(10,14,14)	(12,14,14)	(12,16,16)	*(11,15,15)*	(12,15,16)	(12,15,16)	(13,16,16)	*(11,15,16)*	(12,16,16)	(12,17,17)	(12,18,18)	*(11,17,17)*
$[-2,-2]\times[-2,-2]\times[-1,-1]$	(11,11,9)	(11,11,9)	(15,15,11)	*(11,11,8)*	(14,14,10)	(15,15,11)	(16,16,11)	*(15,15,10)*	(15,16,12)	(15,16,12)	(15,16,12)	*(15,16,10)*	(16,16,11)	(17,17,12)	(18,18,13)	*(17,17,11)*
$[-2,-2]\times[-1,-1]\times[-2,-2]$	(11,9,11)	(11,9,11)	(11,9,11)	*(11,8,11)*	(14,10,14)	(15,12,15)	(16,12,16)	*(15,12,15)*	(15,12,16)	(15,12,16)	(15,12,16)	*(15,11,16)*	(16,12,16)	(17,12,17)	(18,13,18)	*(17,11,17)*
$[-2,-2]\times[-1,-1]\times[-1,-1]$	(11,7,7)	(11,7,7)	(11,11,11)	*(10,7,7)*	(11,8,8)	(11,8,8)	(15,10,10)	*(12,9,9)*	(15,9,11)	(15,9,11)	(15,10,11)	*(14,9,9)*	(14,9,10)	(16,9,10)	(16,10,11)	*(15,9,9)*
$[-1,-1]\times[-2,-2]\times[-1,-1]$	(6,9,5)	(7,9,10)	(7,9,10)	*(7,9,7)*	(8,11,8)	(8,11,8)	(10,15,10)	*(9,12,9)*	(11,15,9)	(11,15,9)	(11,15,10)	*(9,14,9)*	(9,15,9)	(9,15,9)	(11,16,12)	*(9,15,9)*
$[-1,-1]\times[-1,-1]\times[-2,-2]$	(5,5,9)	(5,5,9)	(11,11,13)	*(7,7,10)*	(8,8,12)	(8,8,12)	(10,10,15)	*(9,9,12)*	(11,9,15)	(11,9,15)	(11,9,15)	*(9,9,14)*	(9,9,15)	(9,9,15)	(11,12,17)	*(9,9,15)*
$[-1,-1]\times[-1,-1]\times[-1,-1]$	(7,7,7)	(8,8,8)	(8,8,8)	*(5,5,5)*	(7,8,8)	(7,8,8)	(9,9,9)	*(7,7,7)*	(10,10,10)	(10,10,10)	(10,10,10)	*(9,9,9)*	(9,9,9)	(9,9,9)	(9,9,9)	*(9,9,9)*
$[0,1]\times[-2,-1]\times[-2,-1]$	(5,12,12)	(5,12,12)	(14,18,19)	*(7,14,14)*	(10,16,16)	(16,21,21)	(20,22,22)	*(14,21,21)*	(19,21,21)	(20,23,23)	(21,23,23)	*(16,22,22)*	(17,22,22)	(19,23,23)	(19,24,23)	*(18,23,23)*
$[-2,-1]\times[0,1]\times[-2,-1]$	(12,5,12)	(12,5,12)	(19,14,20)	*(14,6,14)*	(15,12,17)	(21,15,21)	(23,19,22)	*(21,15,21)*	(21,15,21)	(23,21,23)	(23,21,23)	*(23,16,23)*	(23,18,23)	(23,19,23)	(24,20,23)	*(23,18,23)*
$[-2,-1]\times[-2,-1]\times[0,1]$	(12,12,5)	(12,12,5)	(19,20,15)	*(15,14,7)*	(15,14,7)	(21,21,15)	(23,22,19)	*(21,21,15)*	(21,21,15)	(23,23,21)	(24,23,21)	*(22,22,16)*	(22,22,17)	(23,23,19)	(23,23,20)	*(23,23,18)*
$[-2,-1]\times[0,0]\times[0,0]$		(13,6,6)	(13,6,6)		(14,6,6)	(16,7,7)	(16,7,7)	*(15,7,7)*	(15,7,7)	(23,9,9)	(23,9,9)	*(16,7,7)*	(19,9,9)	(23,9,9)	(23,9,9)	*(19,8,8)*
$[0,0]\times[-2,-1]\times[0,0]$		(6,13,6)	(6,13,6)	*(4,5,4)*	(7,14,7)	(7,14,7)	(8,20,8)	*(7,14,7)*	(7,20,7)	(7,20,7)	(11,23,11)	*(7,16,7)*	(9,19,9)	(9,23,9)	(9,23,9)	*(8,19,8)*
$[0,0]\times[0,0]\times[-2,-1]$					(6,6,14)	(7,7,16)	(7,7,16)	*(7,7,15)*	(7,7,15)	(9,9,23)	(10,9,23)	*(7,7,16)*	(9,9,20)	(9,9,23)	(9,9,23)	*(9,8,19)*
$[-2,-1]\times[0,0]\times[1,1]$						(11,5,6)	(11,5,6)	*(7,5,5)*	(7,5,5)	(17,7,7)	(17,7,7)	*(11,5,7)*	(13,7,7)	(17,7,7)	(20,9,9)	*(16,7,7)*
$[-2,-1]\times[1,1]\times[0,0]$						(11,6,5)	(11,6,5)	*(7,5,5)*	(7,5,5)	(17,7,7)	(17,7,7)	*(12,5,5)*	(13,7,6)	(17,7,9)	(17,7,9)	*(16,7,7)*
$[0,0]\times[-2,-1]\times[1,1]$						(5,10,6)	(5,10,6)	*(5,7,5)*	(5,7,5)	(7,17,7)	(7,17,7)	*(5,12,5)*	(6,13,7)	(9,17,7)	(9,17,7)	*(7,16,7)*
$[1,1]\times[-2,-1]\times[0,0]$						(6,10,5)	(6,10,5)	*(5,7,5)*	(5,7,5)	(7,17,7)	(7,17,7)	*(5,12,5)*	(7,13,6)	(7,17,9)	(7,17,9)	*(7,15,7)*
$[0,0]\times[1,1]\times[-2,-1]$						(5,6,11)	(5,6,11)	*(5,5,7)*	(5,5,7)	(7,7,17)	(7,7,17)	*(5,6,12)*	(7,7,13)	(7,7,17)	(9,10,20)	*(7,7,16)*
$[1,1]\times[0,0]\times[-2,-1]$						(6,5,11)	(6,5,11)	*(5,5,7)*	(5,5,7)	(7,7,17)	(7,7,17)	*(5,5,12)*	(7,6,13)	(7,9,17)	(7,9,17)	*(7,7,15)*

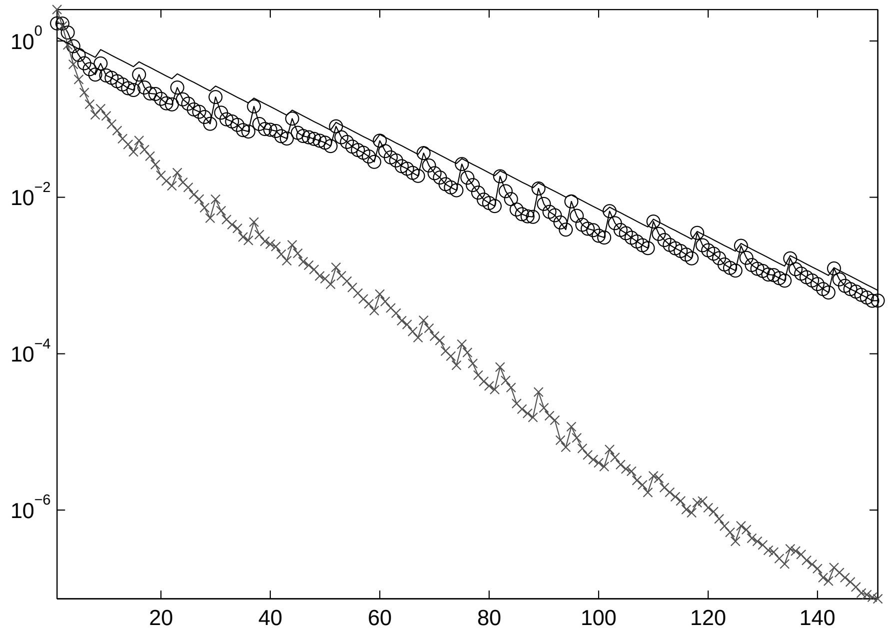

Figure 7.10. Problem ($\delta 6$): $\circ$ residual, $\times$ eigenvalue approximation for each iteration step; the line gives the current error tolerance η.

Again, this operator can be written as a sum of three separable terms, each acting on vectors on ∇^2. The lowest eigenvalue is given by $\lambda_0 = -3$, with corresponding eigenfunction

$$u_0(x) = \prod_{i=1}^{6} e^{-|x_i|}\,, \quad x \in \mathbb{R}^6\,.$$

Similarly to the three-dimensional example, on each part $\bar{\Lambda}_{6,n}$ of the subdivision of the wavelet index set, the coefficients $\mathbf{u}_0$ have multilinear rank $(1,1,1)$.

Note that since there is no electron interaction and no diagonal cusp here, this problem could also be treated by a six-dimensional version of the subdivision constructed in Section 5.2.3, with tensor factors that live on ∇. As in the three-dimensional case, we use $j_0 = -2$ in this example, and also perform the iteration with exactly the same parameters.

The resulting residual estimates and eigenvalue errors are shown in Figure 7.10. The results are very similar to the three-dimensional case, in particular concerning the multilinear ranks shown in Table 7.5, but as can be seen from Table 7.6, the mode sizes of the two-dimensional factors are considerably larger here. The increase of the total number of parameters in the mode frames in dependence on the current residual estimate, shown in Figure 7.11, again approaches the best rate that is possible for the wavelet basis over the course of the iteration. However, this happens later than in the three-dimensional case.

We may also compare the observed complexity of apply in the three- and six-dimensional cases to what may be expected. Here we monitor the total number of additions made to the mode frames of the output during each call of apply during the iteration, where we can hope to approach the underlying theoretical bound for the s^*-compressibility of the lower-dimensional components of the operator.

As Figure 7.12 shows, this is observed in both cases, with quantitatively larger values in the present example with two-dimensional mode frames. This difference is again related to the different numbers of degrees of freedom in the mode frames. Note that since the construction of apply in

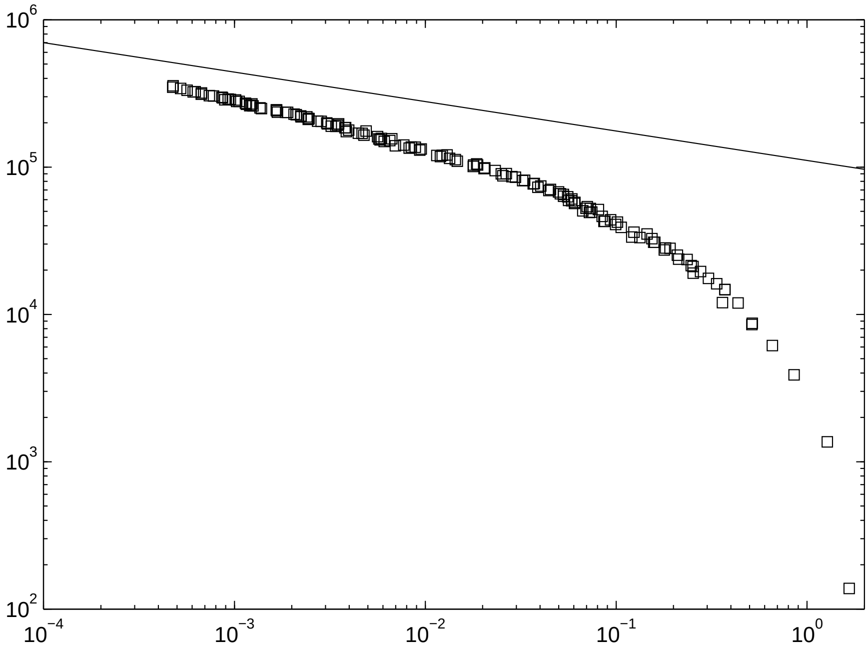

Figure 7.11. Problem ($\delta 6$): total number of nonzero coefficients in mode frames, in dependence on residual estimate. The black line has slope $-\frac{1}{5}$.

this case is based on the available estimates for the operator entries, we cannot obtain a better complexity, even though these estimates may not be sharp.

7.2.2 Hooke's Law Atom

We next consider the explicitly solvable two-electron test problem (2.17), known as the Hooke's law atom or hookium,

$$H_{\mathrm{Hk}}u := -\frac{1}{2}\Delta u + \frac{1}{8}|x|^2 u + \frac{1}{|x_1 - x_2|}u = \lambda u\,. \tag{Hk}$$

Recall that the eigenpair corresponding to the lowest eigenvalue is given by

$$\lambda_0 = 2\,, \quad u_0 = c_0\left(1 + \tfrac{1}{2}|x_1 - x_2|\right)\exp\left(-\tfrac{1}{4}|x|^2\right), \tag{7.2}$$

where $c_0 = 2^{-1}(8\pi^{\frac{5}{2}} + 5\pi^3)^{-\frac{1}{2}}$. Without the Coulomb interaction potential, this problem would reduce to a tensor product harmonic oscillator with $\lambda_0 = \frac{3}{2}$ and $u_0 = \exp(-\frac{1}{4}|x|^2)$.

For the interaction potential on $\mathbb{R}^6$, with $\mu, \nu \in \nabla^6$, we use a separable expansion of the form

$$\int_{\mathbb{R}^6} \frac{1}{|x_1 - x_2|}\Psi_\mu\Psi_\nu\,\mathrm{d}x \approx \sum_k \omega_k \prod_{i=1}^{3}\int_{\mathbb{R}^2} e^{-\alpha_k(x_{1,i}-x_{2,i})^2}\,(\psi_{\mu_i}\,\psi_{\nu_i} \otimes \psi_{\mu_{i+3}}\,\psi_{\nu_{i+3}})(x_{1,i}, x_{2,i})\,\mathrm{d}(x_{1,i}, x_{2,i})\,, \tag{7.3}$$

for which an error estimate is given in Theorem 6.9. The accuracy of these approximations is increased in fixed steps as described for the one-electron potential in the case of hydrogen. The wavelet compression of the operators induced by the two-dimensional Gaussian factors on the right hand side is done according to Theorem 6.27, and integrals are evaluated by the Fourier-based method developed in Section 6.6.

Due to the unbounded harmonic oscillator potentials, H_{Hk} does not define a bounded operator $\mathrm{H}^1(\mathbb{R}^6) \to \mathrm{H}^{-1}(\mathbb{R}^6)$, and therefore the present example does not entirely fit the framework we have

Table 7.5. Problem ($\delta 6$): multilinear ranks of iterates on the first 20 appearing parts $\bar{\Lambda}_{6,n}$ of the subdivision. Iterations with coarsening are in italics.

total iteration number outer iteration number	5 0	6 0	7 0	*8* *0*	9 1	10 1	11 1	12 1	13 1	14 1	*15* *1*	16 2	17 2	18 2	19 2	20 2
$[-2,-2] \times [-2,-2] \times [-2,-2]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[-1,-1] \times [-2,-2] \times [-2,-2]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[-2,-2] \times [-1,-1] \times [-2,-2]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[-2,-2] \times [-2,-2] \times [-1,-1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[0,1] \times [-2,-1] \times [-2,-1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[-2,-1] \times [0,1] \times [-2,-1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[-2,-1] \times [-2,-1] \times [0,1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[-2,-2] \times [-1,-1] \times [-1,-1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[2,5] \times [-2,1] \times [-2,1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[-2,1] \times [2,5] \times [-2,1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[-2,1] \times [-2,1] \times [2,5]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[-1,-1] \times [-2,-2] \times [-1,-1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[-1,-1] \times [-1,-1] \times [-2,-2]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[-2,5] \times [6,13] \times [-2,5]$		(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[-1,-1] \times [-1,-1] \times [-1,-1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[-2,-1] \times [0,0] \times [0,0]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[0,0] \times [-2,-1] \times [0,0]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[0,0] \times [0,0] \times [-2,-1]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[-2,5] \times [-2,5] \times [6,13]$	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)
$[6,13] \times [-2,5] \times [-2,5]$		(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	*(1,1,1)*	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)

Table 7.6. Problem ($\delta 6$): mode sizes of iterates corresponding to Table 7.5.

total iteration number outer iteration number	5 0	6 0	7 0	*8* *0*	9 1	10 1	11 1	12 1	13 1	14 1	*15* *1*	16 2
$[-2,-2] \times [-2,-2] \times [-2,-2]$	(181,181,181)	(201,199,207)	(213,209,207)	*(131,125,127)*	(205,191,197)	(230,218,212)	(232,218,216)	(234,230,232)	(248,246,240)	(254,254,250)	*(156,158,162)*	(220,219,220)
$[-1,-1] \times [-2,-2] \times [-2,-2]$	(212,131,128)	(248,142,135)	(248,142,135)	*(182,120,118)*	(258,120,118)	(258,120,118)	(292,120,118)	(304,170,170)	(319,170,170)	(343,170,170)	*(261,144,144)*	(283,144,144)
$[-2,-2] \times [-1,-1] \times [-2,-2]$	(110,212,106)	(140,252,135)	(140,252,135)	*(116,178,116)*	(116,250,116)	(164,250,116)	(164,292,166)	(164,307,166)	(164,317,166)	(164,333,166)	*(148,252,144)*	(148,289,144)
$[-2,-2] \times [-2,-2] \times [-1,-1]$	(110,131,212)	(140,131,250)	(158,131,265)	*(110,120,188)*	(110,120,260)	(110,120,260)	(164,164,286)	(164,164,301)	(164,164,311)	(164,164,325)	*(144,146,246)*	(144,146,292)
$[0,1] \times [-2,-1] \times [-2,-1]$	(457,189,190)	(558,246,231)	(645,286,282)	*(431,215,208)*	(594,215,208)	(707,303,300)	(707,303,300)	(789,333,345)	(789,333,345)	(789,394,392)	*(568,301,301)*	(727,301,301)
$[-2,-1] \times [0,1] \times [-2,-1]$	(192,465,195)	(237,574,227)	(272,655,280)	*(209,435,204)*	(209,607,204)	(301,717,302)	(301,717,304)	(347,717,304)	(347,821,378)	(380,821,378)	*(303,578,300)*	(303,741,300)
$[-2,-1] \times [-2,-1] \times [0,1]$	(190,191,467)	(239,254,578)	(280,280,652)	*(209,215,436)*	(209,215,597)	(300,303,720)	(300,303,720)	(347,339,789)	(347,339,789)	(388,393,789)	*(307,301,578)*	(307,301,741)
$[-2,-2] \times [-1,-1] \times [-1,-1]$	(63,137,134)	(85,178,148)	(87,178,176)	*(67,101,102)*	(81,182,181)	(81,182,181)	(121,234,247)	(121,234,247)	(121,234,247)	(121,234,247)	*(112,159,159)*	(112,248,250)
$[2,5] \times [-2,1] \times [-2,1]$	(476,165,167)	(683,231,231)	(869,306,297)	*(468,191,190)*	(723,191,190)	(944,350,345)	(962,350,345)	(1118,412,411)	(1194,412,411)	(1302,501,503)	*(811,350,355)*	(1054,350,355)
$[-2,1] \times [2,5] \times [-2,1]$	(163,476,167)	(231,687,233)	(298,873,293)	*(189,464,189)*	(189,713,189)	(336,948,345)	(355,1004,345)	(418,1120,424)	(418,1208,424)	(495,1302,503)	*(353,809,357)*	(353,1059,357)
$[-2,1] \times [-2,1] \times [2,5]$	(161,165,480)	(231,231,695)	(298,306,872)	*(191,193,464)*	(191,193,717)	(332,348,958)	(332,348,1012)	(418,420,1122)	(418,474,1216)	(499,505,1308)	*(359,354,812)*	(359,354,1058)
$[-1,-1] \times [-2,-2] \times [-1,-1]$	(135,63,141)	(180,104,143)	(180,104,205)	*(103,63,102)*	(179,112,181)	(179,112,181)	(236,112,246)	(236,112,246)	(236,112,246)	(236,112,246)	*(161,110,157)*	(246,110,250)
$[-1,-1] \times [-1,-1] \times [-2,-2]$	(139,141,61)	(139,141,102)	(172,174,102)	*(101,103,65)*	(185,182,114)	(185,182,114)	(185,182,114)	(185,260,114)	(264,260,114)	(264,260,116)	*(159,158,108)*	(246,250,108)
$[-2,5] \times [6,13] \times [-2,5]$		(65,152,65)	(91,252,93)	*(53,98,51)*	(53,176,51)	(79,306,81)	(79,340,81)	(79,340,81)	(191,468,191)	(191,570,191)	*(79,234,81)*	(79,374,81)
$[-1,-1] \times [-1,-1] \times [-1,-1]$	(52,60,60)	(97,96,96)	(97,96,96)	*(62,60,60)*	(62,109,108)	(165,127,125)	(165,153,171)	(165,184,171)	(185,186,180)	(185,186,180)	*(97,97,97)*	(165,167,171)
$[-2,-1] \times [0,0] \times [0,0]$	(38,63,63)	(58,100,112)	(103,124,140)	*(30,63,55)*	(105,138,138)	(105,160,158)	(139,177,160)	(139,177,160)	(175,201,214)	(175,201,214)	*(97,112,112)*	(177,207,207)
$[0,0] \times [-2,-1] \times [0,0]$	(64,41,64)	(106,61,106)	(142,100,140)	*(52,32,53)*	(136,105,134)	(158,119,158)	(158,119,158)	(158,119,158)	(197,181,201)	(197,181,201)	*(106,97,110)*	(205,182,203)
$[0,0] \times [0,0] \times [-2,-1]$	(64,64,41)	(108,106,61)	(140,142,100)	*(52,50,32)*	(136,136,105)	(136,136,105)	(162,174,145)	(162,174,145)	(162,174,145)	(247,249,229)	*(98,100,87)*	(201,201,175)
$[-2,5] \times [-2,5] \times [6,13]$	(41,43,88)	(65,67,154)	(91,91,252)	*(51,53,98)*	(51,53,174)	(81,81,292)	(81,81,344)	(81,81,344)	(187,193,490)	(187,193,584)	*(81,81,238)*	(81,81,378)
$[6,13] \times [-2,5] \times [-2,5]$		(144,65,65)	(192,104,108)		(102,61,65)	(256,142,141)	(328,142,141)	(406,142,141)	(482,142,149)	(572,142,149)	*(252,133,133)*	(382,133,133)

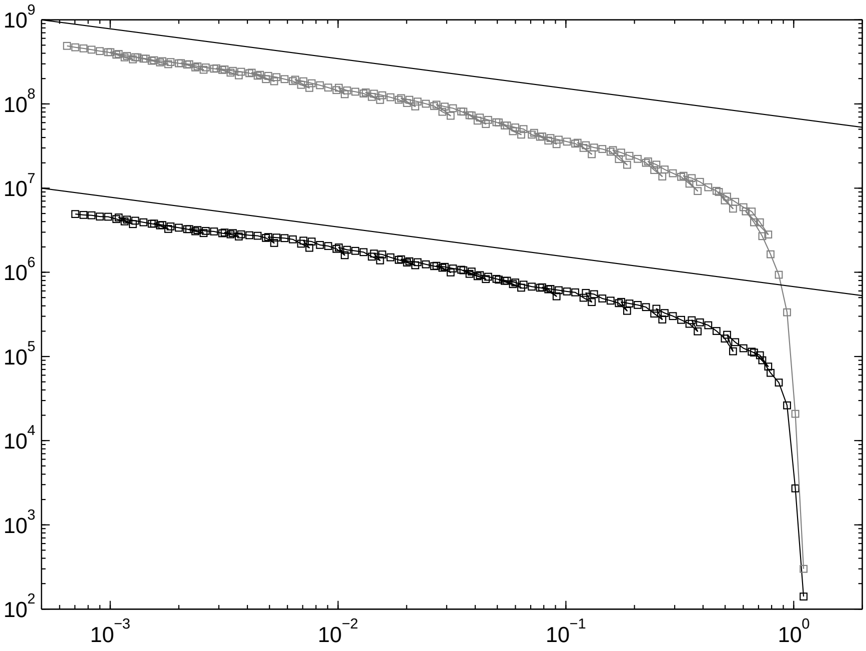

Figure 7.12. Problems ($\delta 3$) and ($\delta 6$): total number of additions to output mode frames in apply, in dependence on current error tolerance η; comparison of ($\delta 3$) (black) and ($\delta 6$) (gray). The black lines have slope $-\frac{1}{2.82}$.

developed so far. To obtain a bounded operator on all of $\mathbb{R}^6$, one could instead work on a subspace $\tilde{\mathcal{H}} \subset \mathrm{H}^1(\mathbb{R}^6)$ with weighted inner product

$$\langle v, w \rangle_{\tilde{\mathcal{H}}} = \int_{\mathbb{R}^6} \mathrm{D}v \cdot \mathrm{D}w + (1 + |x|^2) v\, w \,\mathrm{d}x \,.$$

Unfortunately, the diagonal rescaling with respect to this modified inner product again leads to a rank increase.

Our main interest in the test problem (Hk) is to study the complexity of the produced approximations in comparison to the theoretical results of Section 4.3. We therefore treat also Problem (Hk) in a manner that fits our algorithmic framework. Note that for any ball $B_R(0) \subset \mathbb{R}^6$, H_{Hk} defines a bounded operator $\mathrm{H}^1(B_R(0)) \to \mathrm{H}^{-1}(B_R(0))$, with norm dependent on R. Thus problem (Hk) can be treated in the same way as the other examples, but with increasing support of the iterates the convergence properties of the iteration deteriorate, and the admissible iteration step size decreases. Unlike in the other examples, where for a suitable choice of parameters, the scheme in principle converges to any accuracy, in the present case we thus need to choose parameters that are suitable up to a required target accuracy.

The resulting growth in operator norm over the course of the iteration can be seen in the results shown in Figure 7.13: in later iterations, with a correspondingly larger support of iterates, the coarsening step leads to a larger relative increase in the residual. In this example, the convergence of eigenvalues does not follow a clear pattern and depends strongly on the approximation of the interaction potential.

In Theorem 4.34, we have obtained an estimate for the number of nonzero coefficients in the mode frames that are required for a given H^1–error ε: for wavelets of sufficiently high order, and up to additional logarithmic terms, we expect the number of coefficients in the mode frames to grow essentially as $\varepsilon^{-\frac{2}{3}}$. Since the sufficiently precise evaluation of the actual eigenfunction error in H^1 would be prohibitively expensive, we again consider the number of coefficients in dependence

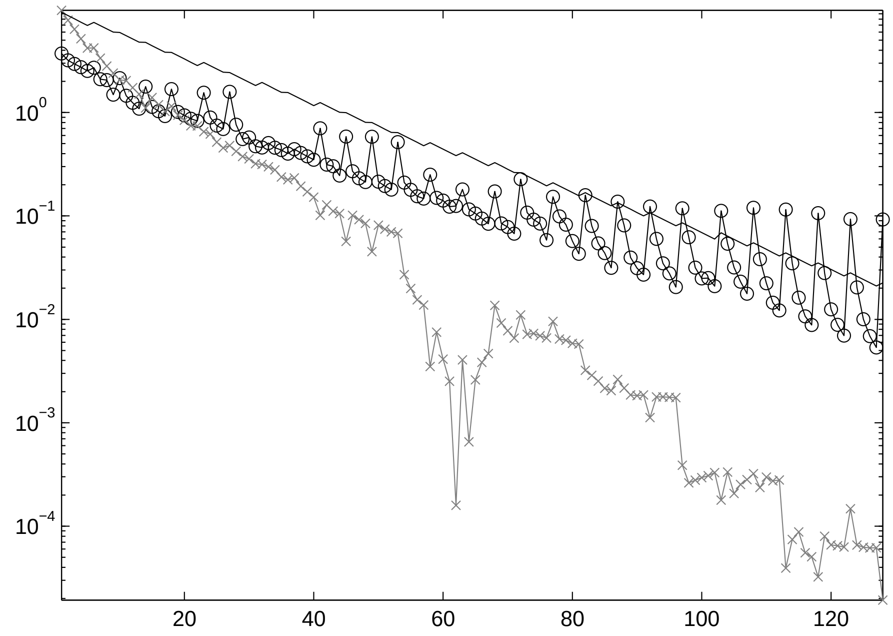

Figure 7.13. Problem (Hk): ○ residual, × eigenvalue approximation for each iteration step; the line gives the current error tolerance η.

on the current residual estimate. As shown in Figure 7.14, the expected asymptotic behaviour can be observed numerically for small values of the residual.

A second factor influencing the complexity of iterates, however, is the compressibility of lower-dimensional operator components. For the two-dimensional factors in the separable expansion of the interaction potential, Theorem 6.27 only yields $s^* < 1$. We therefore also need to expect a stronger growth in the number of active indices between coarsening steps. This discrepancy between the number of active coefficients produced by the operator application and those remaining after the coarsening steps can be seen clearly in Figure 7.15 and Tables 7.7 and 7.8, which show the evolution of multilinear ranks and mode sizes during the iteration.

In Figure 7.16, we compare one-dimensional sections of three iterates of outer iteration steps before and after the corresponding coarsening operation to the true solution. Note that the iterates before coarsening are clearly closer to the solution. As can be seen from Figure 7.13, however, there is only a small difference in the eigenvalue errors obtained with the respective operator approximation tolerances for the iterates before and after coarsening.

7.2.3 Helium

We finally consider the two-electron atomic system of helium as in (2.14),

$$H_{\mathrm{He}} u := -\frac{1}{2}\Delta u - 2\left(\frac{1}{|x_1|} + \frac{1}{|x_2|}\right)u + \frac{1}{|x_1 - x_2|}u = \lambda u\,. \tag{He}$$

As discussed in Section 2.3, there is no known closed-form solution for the ground state eigenpair (λ_0, u_0), but highly accurate approximations to $\lambda_0 \approx -2.903724$, as given in (2.15), are known. The ingredients for approximating the operators arising in this problem have already appeared in the previous examples: The interaction potential is treated as in the case of hookium, and the nuclear potentials are, up to the tensorization with three-dimensional identity operators, handled in the same way as in the example of hydrogen.

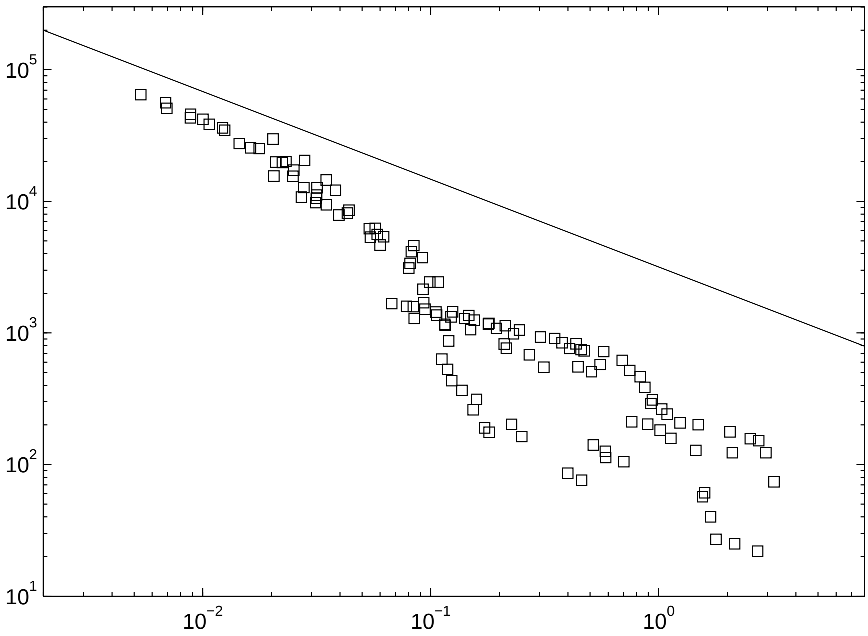

Figure 7.14. Problem (Hk): total number of nonzero coefficients in mode frames, in dependence on residual estimate. The line has slope $-\frac{2}{3}$.

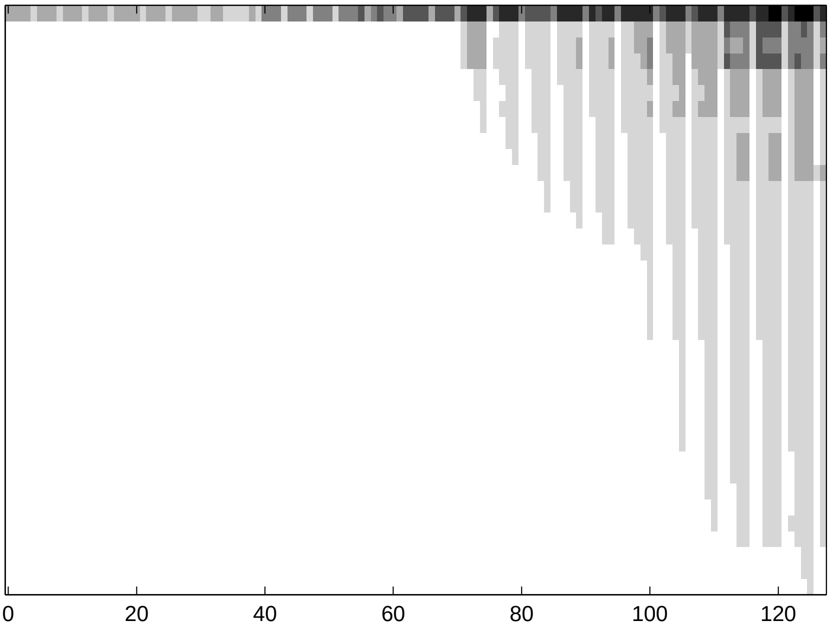

Figure 7.15. Problem (Hk): maximum ranks on subdivision elements (rows) in dependence on the iteration number (columns). Black corresponds to the maximum value 6.

Table 7.7. Problem (Hk): multilinear ranks of iterates on the first 20 appearing parts $\bar{\Lambda}_{6,n}$ of the subdivision. Iterations with coarsening are in italics.

total iteration number	*107*	108	109	110	111	*112*	113	114	115	116	*117*	118	119
outer iteration number	*22*	23	23	23	23	*23*	24	24	24	24	*24*	25	25
[0, 0] × [0, 0] × [0, 0]	*(3,3,3)*	(4,4,4)	(5,5,5)	(5,5,5)	(5,5,5)	*(3,3,3)*	(5,4,4)	(5,5,5)	(5,5,5)	(5,5,5)	*(4,4,3)*	(5,5,5)	(5,5,5)
[1, 1] × [0, 0] × [0, 0]	*(1,1,1)*	(2,2,2)	(2,2,2)	(2,2,2)	(2,2,2)	*(1,1,1)*	(4,4,4)	(3,3,3)	(3,3,3)	(3,3,3)	*(1,1,1)*	(4,3,4)	(4,3,4)
[0, 0] × [1, 1] × [0, 0]	*(1,1,1)*	(2,2,2)	(2,2,2)	(2,2,2)	(2,2,2)	*(1,1,1)*	(2,3,2)	(2,2,2)	(2,2,2)	(2,3,2)	*(1,1,1)*	(3,4,3)	(3,3,3)
[0, 0] × [0, 0] × [1, 1]		(2,2,2)	(2,2,2)	(2,2,2)	(2,2,2)	*(1,1,1)*	(4,4,4)	(3,3,3)	(3,3,3)	(3,3,3)	*(1,1,1)*	(3,4,4)	(3,4,4)
[0, 0] × [1, 1] × [1, 1]		(1,1,1)	(1,2,2)	(1,2,2)	(1,2,2)		(1,1,1)	(1,2,2)	(1,2,2)	(1,2,2)		(1,1,1)	(1,2,2)
[1, 1] × [1, 1] × [0, 0]		(1,1,1)	(1,1,1)	(2,2,1)	(2,2,1)		(1,1,1)	(2,2,1)	(2,2,1)	(2,2,1)		(1,1,1)	(2,2,1)
[1, 1] × [0, 0] × [1, 1]		(1,1,1)	(2,1,2)	(2,1,2)	(2,1,2)		(1,1,1)	(2,1,2)	(2,1,2)	(2,1,2)		(1,1,1)	(2,1,2)
[1, 1] × [1, 1] × [1, 1]		(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)
[0, 1] × [2, 3] × [0, 1]		(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)	(2,2,2)	(2,2,2)		(1,1,1)	(1,1,1)
[2, 3] × [0, 1] × [0, 1]		(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)	(2,1,2)	(2,2,2)		(1,1,1)	(1,1,1)
[0, 1] × [0, 1] × [2, 3]		(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)	(2,2,2)	(2,2,2)		(1,1,1)	(1,1,1)
[0, 1] × [2, 2] × [2, 2]		(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)
[2, 2] × [0, 1] × [2, 2]		(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)
[2, 2] × [2, 2] × [0, 1]		(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)
[2, 2] × [2, 2] × [2, 2]			(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)
[0, 1] × [2, 2] × [3, 3]			(1,1,1)	(1,1,1)	(1,1,1)			(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)
[0, 1] × [3, 3] × [2, 2]			(1,1,1)	(1,1,1)	(1,1,1)			(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)
[2, 2] × [0, 1] × [3, 3]			(1,1,1)	(1,1,1)	(1,1,1)			(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)
[3, 3] × [0, 1] × [2, 2]			(1,1,1)	(1,1,1)	(1,1,1)			(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)
[2, 2] × [3, 3] × [0, 1]			(1,1,1)	(1,1,1)	(1,1,1)			(1,1,1)	(1,1,1)	(1,1,1)		(1,1,1)	(1,1,1)

Table 7.8. Problem (Hk): mode sizes of iterates corresponding to Table 7.7.

total iteration number	*107*	108	109	110	111	*112*	113	114	115	116	*117*	118	119
outer iteration number	*22*	23	23	23	23	*23*	24	24	24	24	*24*	25	25
[0, 0] × [0, 0] × [0, 0]	*(246,247,246)*	(742,754,754)	(924,923,925)	(1013,987,988)	(1048,1026,1028)	*(277,277,277)*	(814,814,814)	(978,970,974)	(1048,1077,1052)	(1103,1114,1104)	*(307,307,307)*	(847,847,847)	(991,994,993)
[1, 1] × [0, 0] × [0, 0]	*(37,14,14)*	(598,251,251)	(844,325,328)	(1137,332,334)	(1327,334,340)	*(54,28,28)*	(802,295,295)	(985,352,353)	(1359,391,389)	(1494,391,389)	*(78,35,35)*	(920,351,351)	(1213,383,382)
[0, 0] × [1, 1] × [0, 0]	*(14,37,14)*	(255,679,251)	(332,902,329)	(332,1077,330)	(332,1278,330)	*(28,54,28)*	(289,664,285)	(345,905,343)	(366,1369,365)	(370,1476,367)	*(35,79,35)*	(351,918,351)	(390,1237,388)
[0, 0] × [0, 0] × [1, 1]		(256,256,737)	(332,332,916)	(346,347,1106)	(349,349,1298)	*(28,28,56)*	(297,295,802)	(353,353,999)	(370,369,1355)	(370,369,1407)	*(35,35,77)*	(351,351,918)	(383,382,1161)
[0, 0] × [1, 1] × [1, 1]		(199,229,229)	(227,336,336)	(227,336,336)	(271,346,348)		(230,255,257)	(232,273,269)	(274,463,465)	(274,472,465)		(264,323,323)	(266,433,418)
[1, 1] × [1, 1] × [0, 0]		(230,229,198)	(327,325,230)	(339,337,230)	(343,337,230)		(257,255,230)	(373,371,232)	(377,375,243)	(438,510,269)		(326,323,266)	(416,435,266)
[1, 1] × [0, 0] × [1, 1]		(230,198,229)	(343,230,342)	(349,230,346)	(349,231,346)		(257,230,257)	(371,232,381)	(371,244,383)	(382,275,402)		(325,264,323)	(422,266,425)
[1, 1] × [1, 1] × [1, 1]		(175,178,178)	(210,208,212)	(210,208,212)	(210,208,212)		(184,184,184)	(184,184,184)	(249,311,311)	(259,323,318)		(243,243,243)	(243,243,243)
[0, 1] × [2, 3] × [0, 1]		(255,325,255)	(323,720,323)	(372,1380,370)	(374,1951,374)		(309,440,308)	(358,971,362)	(453,1852,458)	(457,2034,458)		(385,709,385)	(457,1320,457)
[2, 3] × [0, 1] × [0, 1]		(325,255,255)	(719,324,324)	(1160,366,366)	(1912,370,372)		(440,308,308)	(899,382,384)	(1897,460,460)	(2004,464,460)		(709,383,384)	(1323,457,457)
[0, 1] × [0, 1] × [2, 3]		(255,255,325)	(323,323,719)	(354,354,1302)	(365,363,1901)		(309,308,440)	(358,362,943)	(454,458,1850)	(456,458,2001)		(385,385,709)	(457,457,1371)
[0, 1] × [2, 2] × [2, 2]		(205,122,122)	(251,235,234)	(251,235,234)	(251,235,234)		(240,175,175)	(255,282,278)	(255,403,409)	(305,409,416)		(297,261,259)	(299,345,343)
[2, 2] × [0, 1] × [2, 2]		(124,206,122)	(235,253,234)	(235,253,234)	(235,253,234)		(175,239,175)	(276,255,278)	(276,255,278)	(407,255,396)		(259,297,259)	(341,297,339)
[2, 2] × [2, 2] × [0, 1]		(124,122,206)	(235,235,253)	(235,235,253)	(430,428,253)		(175,175,239)	(276,278,255)	(276,278,255)	(276,278,255)		(259,261,297)	(345,347,301)
[2, 2] × [2, 2] × [2, 2]			(169,169,169)	(169,169,169)	(169,169,169)		(113,113,113)	(206,208,208)	(206,208,208)	(206,208,208)		(191,191,191)	(243,243,243)
[0, 1] × [2, 2] × [3, 3]			(148,80,137)	(148,80,137)	(249,184,453)			(188,117,214)	(188,117,214)	(270,227,544)		(146,80,129)	(204,144,331)
[0, 1] × [3, 3] × [2, 2]			(148,136,78)	(148,136,78)	(249,453,182)			(188,214,117)	(251,493,199)	(251,493,199)		(146,129,79)	(204,331,144)
[2, 2] × [0, 1] × [3, 3]			(78,148,137)	(78,148,137)	(184,249,454)			(119,192,214)	(119,192,214)	(220,264,545)		(79,146,129)	(142,204,334)
[3, 3] × [0, 1] × [2, 2]			(134,148,78)	(324,218,146)	(324,218,146)			(214,192,117)	(214,192,117)	(546,266,220)		(129,146,79)	(334,204,144)
[2, 2] × [3, 3] × [0, 1]			(78,136,148)	(78,136,148)	(182,454,249)			(119,214,192)	(119,214,192)	(222,550,266)		(79,129,146)	(142,334,204)

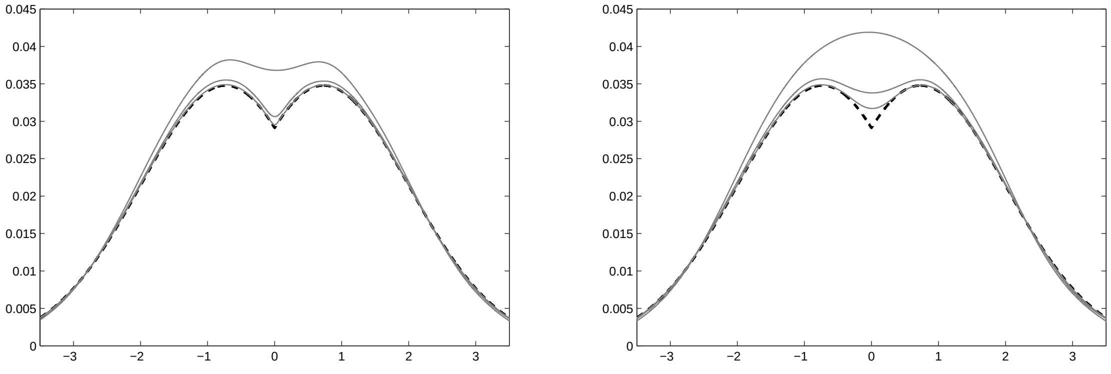

Figure 7.16. Problem (Hk): convergence of iterates at the end of outer iterations 15, 20, and 25 (total iteration numbers 71, 96, and 122) to the exact solution on the section $(x_1, 0, 0, 0, 0, 0)$. Left: before coarsening step, right: after coarsening step.

Note that in contrast to the previous example of hookium, $H_{\mathrm{He}} \colon \mathrm{H}^1(\mathbb{R}^6) \to \mathrm{H}^{-1}(\mathbb{R}^6)$ satisfies the assumptions of our convergence analysis. In particular, the diagonal rescaling provides similarly effective preconditioning as in the case of hydrogen, and the iteration step size can be chosen substantially larger than for hookium.

The numerical treatment of (He), in particular the approximate application of the Hamiltonian, is more expensive than in the other examples due to a combination of several difficulties: the operator ranks required for a given target tolerance are more than three times as large as for hydrogen; the approximation of the nuclear cusps, which are more pronounced than in the case of hydrogen, already requires a substantial number of wavelet coefficients; and the approximate application of the interaction potential to the iterates accordingly becomes more expensive than in the case of hookium.

Our results therefore do not cover a range of error tolerances as low as in the simpler test cases. The obtained residual approximations and eigenvalue errors are shown in Figure 7.17. The convergence pattern shows some variations, in particular after steps with a switch to more accurate potential approximations. In the later iterations, however, the eigenvalue error remains below 4×10^{-3}.

For the helium ground state we do not have a tensor approximability result as the one for hookium in Theorem 4.34. The observed growth of the total number of entries in the mode frames as shown in Figure 7.18, however, is consistent with the same asymptotic rate that we have obtained for hookium. The evolution of multilinear ranks and mode frame sizes over the course of the iteration is shown in Figure 7.19 and Tables 7.9 and 7.10; again we observe a gradual increase in the ranks of iterates, where the maximum arising multilinear rank on a subdivision element is $(9, 9, 9)$.

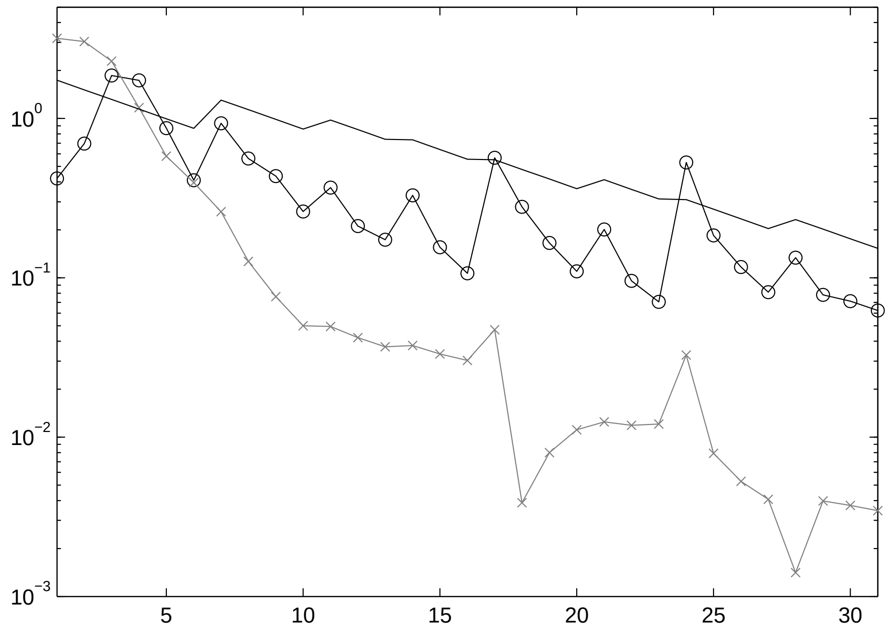

Figure 7.17. Problem (He): ○ residual, × eigenvalue approximation for each iteration step; the line gives the current error tolerance η.

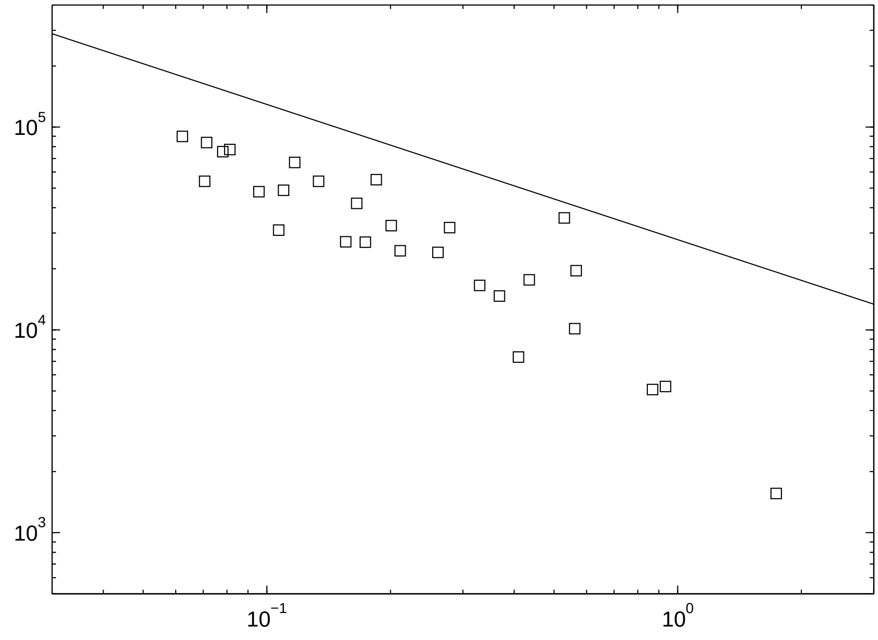

Figure 7.18. Problem (He): total number of nonzero coefficients in mode frames, in dependence on residual estimate. The line has slope $-\frac{2}{3}$.

Table 7.9. Problem (He): multilinear ranks of iterates on the first 20 appearing parts $\bar{\Lambda}_{6,n}$ of the subdivision. Iterations with coarsening are in italics.

total iteration number	*20*	21	22	*23*	24	25	26	*27*	28	29	30	*31*
outer iteration number	*4*	5	5	*5*	6	6	6	*6*	7	7	7	*7*
$[-2,-2]\times[-2,-2]\times[-2,-2]$	*(4,4,4)*	(4,4,4)	(4,4,4)	*(4,4,4)*	(4,4,4)	(4,4,4)	(4,4,4)	*(4,4,4)*	(4,4,4)	(4,4,4)	(5,5,5)	*(5,5,5)*
$[-1,-1]\times[-2,-2]\times[-2,-2]$	*(4,4,4)*	(4,4,4)	(4,4,4)	*(4,4,4)*	(5,4,4)	(5,4,4)	(5,4,4)	*(6,4,4)*	(6,4,4)	(6,4,4)	(6,5,5)	*(6,6,6)*
$[-2,-2]\times[-1,-1]\times[-2,-2]$	*(4,4,4)*	(4,4,4)	(4,4,4)	*(4,4,4)*	(4,5,4)	(4,5,4)	(4,5,4)	*(4,6,4)*	(4,6,4)	(4,6,4)	(5,6,5)	*(6,6,6)*
$[-2,-2]\times[-2,-2]\times[-1,-1]$	*(4,4,4)*	(4,4,4)	(4,4,4)	*(4,4,4)*	(4,4,5)	(4,4,5)	(4,4,5)	*(4,4,6)*	(4,4,6)	(4,4,6)	(5,5,6)	*(6,6,6)*
$[-2,-2]\times[-1,-1]\times[-1,-1]$	*(4,5,5)*	(4,5,5)	(4,6,6)	*(4,6,6)*	(4,6,6)	(4,6,6)	(4,6,6)	*(4,6,6)*	(4,6,6)	(4,6,6)	(5,7,7)	*(5,6,6)*
$[-1,-1]\times[-2,-2]\times[-1,-1]$	*(5,4,5)*	(5,4,5)	(6,4,6)	*(6,4,6)*	(6,4,6)	(6,4,6)	(6,4,6)	*(6,4,6)*	(6,4,6)	(6,4,6)	(7,5,7)	*(7,5,6)*
$[-1,-1]\times[-1,-1]\times[-2,-2]$	*(5,5,4)*	(5,5,4)	(6,6,4)	*(6,6,4)*	(6,6,4)	(6,6,4)	(6,6,4)	*(6,6,4)*	(6,6,4)	(6,6,4)	(7,7,5)	*(6,6,5)*
$[-1,-1]\times[-1,-1]\times[-1,-1]$	*(5,5,5)*	(5,5,5)	(5,5,5)	*(5,5,5)*	(5,5,5)	(6,6,6)	(6,6,6)	*(6,6,6)*	(6,6,6)	(7,6,6)	(8,7,8)	*(7,7,7)*
$[0,1]\times[-2,-1]\times[-2,-1]$	*(6,5,5)*	(6,5,5)	(6,5,5)	*(6,6,6)*	(6,6,6)	(6,6,6)	(9,6,6)	*(8,7,7)*	(8,7,7)	(9,7,7)	(9,9,9)	*(9,9,9)*
$[-2,-1]\times[0,1]\times[-2,-1]$	*(5,6,5)*	(5,6,5)	(5,6,5)	*(6,6,6)*	(6,6,6)	(6,6,6)	(6,9,6)	*(7,9,7)*	(7,9,7)	(7,9,7)	(9,9,9)	*(9,9,9)*
$[-2,-1]\times[-2,-1]\times[0,1]$	*(5,5,6)*	(5,5,6)	(5,5,6)	*(6,6,6)*	(6,6,6)	(6,6,6)	(6,6,8)	*(7,7,8)*	(7,7,8)	(7,7,9)	(9,9,9)	*(9,9,9)*
$[-2,-1]\times[0,0]\times[0,0]$	*(4,6,6)*	(4,6,6)	(4,6,6)	*(4,6,6)*	(4,6,7)	(5,7,7)	(6,7,7)	*(6,8,8)*	(6,8,8)	(6,9,9)	(6,9,9)	*(7,9,9)*
$[0,0]\times[-2,-1]\times[0,0]$	*(6,4,6)*	(6,4,6)	(6,4,6)	*(6,4,6)*	(6,4,6)	(7,5,7)	(7,6,7)	*(8,6,8)*	(8,6,7)	(9,6,9)	(9,6,9)	*(9,7,9)*
$[0,0]\times[0,0]\times[-2,-1]$	*(5,6,4)*	(5,4,4)	(6,6,4)	*(6,6,4)*	(6,6,4)	(7,7,5)	(7,7,6)	*(8,8,6)*	(8,8,6)	(9,9,6)	(9,9,6)	*(9,9,7)*
$[0,0]\times[0,0]\times[0,0]$	*(4,4,4)*	(4,4,4)	(4,4,4)	*(5,5,5)*	(6,6,6)	(6,6,6)	(7,7,7)	*(7,7,7)*	(7,7,7)	(8,8,8)	(8,9,9)	*(8,8,8)*
$[-2,-1]\times[0,0]\times[1,1]$	*(2,3,3)*	(2,3,3)	(3,3,3)	*(3,4,4)*	(4,4,4)	(4,5,5)	(4,5,5)	*(4,5,5)*	(4,5,5)	(4,5,5)	(5,5,5)	*(5,6,6)*
$[-2,-1]\times[1,1]\times[0,0]$	*(2,3,3)*	(2,3,3)	(3,3,3)	*(3,4,4)*	(4,4,4)	(4,5,5)	(4,5,5)	*(4,5,5)*	(4,5,5)	(4,5,5)	(5,5,5)	*(5,6,6)*
$[0,0]\times[-2,-1]\times[1,1]$	*(3,2,3)*	(3,2,3)	(3,3,3)	*(4,3,4)*	(4,4,4)	(5,4,5)	(5,4,5)	*(5,4,5)*	(5,4,5)	(5,4,5)	(5,5,5)	*(6,5,6)*
$[1,1]\times[-2,-1]\times[0,0]$	*(3,2,3)*	(3,2,3)	(3,3,3)	*(4,3,4)*	(4,4,4)	(5,4,5)	(5,4,5)	*(5,4,5)*	(5,4,5)	(5,4,5)	(5,5,5)	*(6,5,6)*
$[0,0]\times[1,1]\times[-2,-1]$	*(3,3,2)*	(3,3,2)	(3,3,3)	*(4,4,3)*	(4,4,4)	(5,5,4)	(5,5,4)	*(5,5,4)*	(5,5,4)	(5,5,4)	(5,5,5)	*(6,6,5)*

Table 7.10. Problem (He): mode sizes of iterates corresponding to Table 7.9.

total iteration number	*20*	21	22	*23*	24	25	26	*27*	28	29	30	*31*
outer iteration number	*4*	5	5	*5*	6	6	6	*6*	7	7	7	*7*
$[-2,-2]\times[-2,-2]\times[-2,-2]$	*(245,244,245)*	(359,362,359)	(416,362,430)	*(265,264,264)*	(361,358,358)	(389,387,391)	(392,390,394)	*(281,281,281)*	(394,394,393)	(431,429,429)	(460,452,447)	*(306,306,306)*
$[-1,-1]\times[-2,-2]\times[-2,-2]$	*(339,234,234)*	(451,291,291)	(514,292,292)	*(349,244,244)*	(451,298,298)	(512,328,324)	(559,340,339)	*(398,280,280)*	(534,336,339)	(578,359,359)	(598,376,375)	*(428,308,308)*
$[-2,-2]\times[-1,-1]\times[-2,-2]$	*(233,339,234)*	(291,450,291)	(291,492,291)	*(243,347,243)*	(296,447,296)	(326,512,325)	(340,558,340)	*(280,398,280)*	(337,535,335)	(354,581,355)	(375,599,377)	*(308,428,307)*
$[-2,-2]\times[-2,-2]\times[-1,-1]$	*(234,234,339)*	(291,291,444)	(291,291,502)	*(244,244,346)*	(297,296,442)	(329,329,509)	(340,342,558)	*(280,280,398)*	(338,337,534)	(354,354,583)	(377,377,596)	*(307,307,430)*
$[-2,-2]\times[-1,-1]\times[-1,-1]$	*(215,312,310)*	(281,417,415)	(281,417,415)	*(220,330,330)*	(290,424,424)	(310,463,468)	(324,511,508)	*(251,370,371)*	(331,507,503)	(343,540,542)	(349,565,562)	*(276,401,402)*
$[-1,-1]\times[-2,-2]\times[-1,-1]$	*(310,215,310)*	(417,283,416)	(417,283,416)	*(330,221,330)*	(424,289,422)	(465,309,465)	(510,324,507)	*(370,251,371)*	(499,334,499)	(529,341,540)	(562,350,562)	*(399,276,402)*
$[-1,-1]\times[-1,-1]\times[-2,-2]$	*(312,312,215)*	(419,420,281)	(419,420,281)	*(328,330,221)*	(424,422,290)	(463,464,309)	(507,507,324)	*(371,371,251)*	(499,499,332)	(523,536,339)	(563,562,352)	*(401,401,276)*
$[-1,-1]\times[-1,-1]\times[-1,-1]$	*(297,297,296)*	(404,403,399)	(404,403,399)	*(307,307,306)*	(414,414,413)	(447,447,447)	(485,488,482)	*(359,359,361)*	(493,492,486)	(517,519,521)	(538,534,532)	*(383,383,383)*
$[0,1]\times[-2,-1]\times[-2,-1]$	*(767,530,529)*	(1005,560,554)	(1200,622,619)	*(839,536,536)*	(1058,603,602)	(1215,692,690)	(1360,749,745)	*(1045,629,628)*	(1321,716,716)	(1442,782,775)	(1480,797,791)	*(1170,690,689)*
$[-2,-1]\times[0,1]\times[-2,-1]$	*(530,767,529)*	(562,1010,555)	(621,1200,618)	*(536,838,536)*	(605,1061,603)	(692,1217,691)	(749,1362,747)	*(631,1043,631)*	(719,1326,719)	(773,1447,765)	(798,1482,797)	*(692,1169,690)*
$[-2,-1]\times[-2,-1]\times[0,1]$	*(530,529,767)*	(563,560,1016)	(624,621,1200)	*(536,536,841)*	(600,600,1065)	(693,692,1225)	(749,750,1356)	*(629,629,1044)*	(719,719,1334)	(773,769,1457)	(799,797,1491)	*(693,693,1170)*
$[-2,-1]\times[0,0]\times[0,0]$	*(416,374,374)*	(554,474,474)	(554,474,474)	*(425,387,388)*	(552,484,482)	(589,524,524)	(610,570,571)	*(534,450,450)*	(659,598,600)	(659,613,615)	(678,623,625)	*(561,488,488)*
$[0,0]\times[-2,-1]\times[0,0]$	*(375,416,376)*	(470,555,469)	(470,555,471)	*(386,426,389)*	(483,548,485)	(523,589,525)	(571,612,569)	*(449,534,449)*	(596,659,600)	(612,659,611)	(651,699,638)	*(490,560,488)*
$[0,0]\times[0,0]\times[-2,-1]$	*(376,375,418)*	(472,471,559)	(472,471,559)	*(388,385,433)*	(481,480,542)	(524,524,595)	(568,569,612)	*(449,450,533)*	(600,563,660)	(626,623,672)	(635,625,672)	*(490,490,559)*
$[0,0]\times[0,0]\times[0,0]$	*(306,306,307)*	(480,477,478)	(481,478,479)	*(330,331,331)*	(461,460,460)	(478,474,469)	(510,522,521)	*(405,404,404)*	(565,558,563)	(565,558,563)	(568,564,572)	*(435,434,433)*
$[-2,-1]\times[0,0]\times[1,1]$	*(299,268,273)*	(331,346,432)	(479,398,505)	*(317,290,314)*	(353,326,471)	(474,428,509)	(474,433,527)	*(413,378,436)*	(413,414,540)	(576,489,651)	(576,489,651)	*(455,408,481)*
$[-2,-1]\times[1,1]\times[0,0]$	*(299,270,268)*	(330,434,345)	(480,502,397)	*(317,310,289)*	(353,473,324)	(474,517,430)	(474,529,435)	*(410,438,379)*	(412,534,412)	(576,622,463)	(576,625,463)	*(455,487,410)*
$[0,0]\times[-2,-1]\times[1,1]$	*(268,298,272)*	(348,330,436)	(408,485,514)	*(289,317,315)*	(377,351,475)	(402,463,514)	(446,494,530)	*(380,412,434)*	(414,412,539)	(463,577,598)	(463,577,601)	*(408,455,487)*
$[1,1]\times[-2,-1]\times[0,0]$	*(271,298,268)*	(436,331,349)	(506,481,396)	*(311,318,290)*	(475,349,375)	(521,463,408)	(540,501,447)	*(437,411,378)*	(537,412,415)	(598,575,462)	(601,575,462)	*(487,455,413)*
$[0,0]\times[1,1]\times[-2,-1]$	*(268,272,299)*	(350,438,330)	(405,519,477)	*(286,310,317)*	(377,477,394)	(403,522,461)	(436,531,471)	*(378,440,404)*	(417,547,519)	(463,592,526)	(466,595,540)	*(408,491,459)*

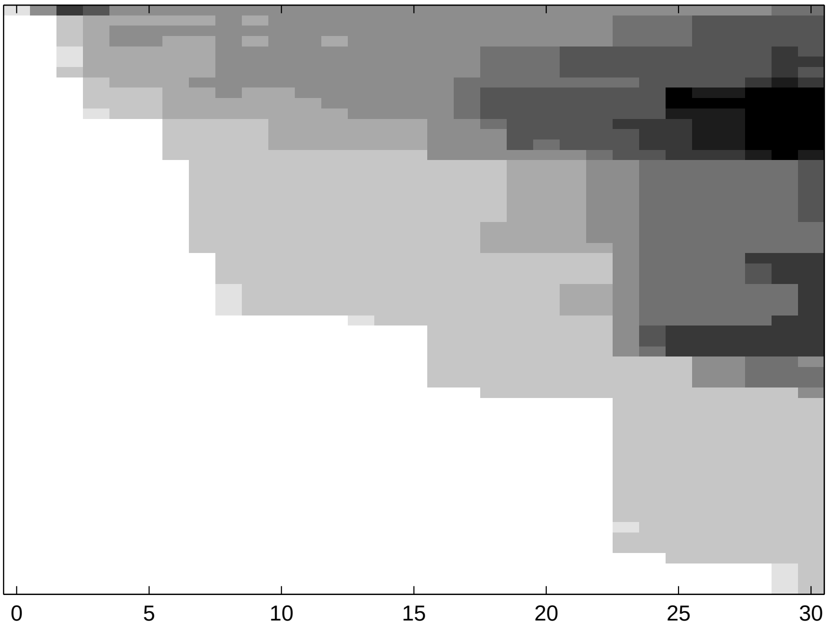

Figure 7.19. Problem (He): maximum ranks on subdivision elements (rows) in dependence on the iteration number (columns). Black corresponds to the maximum value 9.

8 Conclusion and Outlook

We have considered adaptive methods that exploit both low-rank structure of solutions, and their near-sparsity in a wavelet basis. We have studied in particular the approximation of two-electron wave functions, and the approximation of the operators arising in the corresponding eigenvalue problems.

For solutions of model problems, we have obtained approximation complexity estimates. These show that in certain cases of solutions with limited Besov regularity, the nonlinear parametrization of wavelet coefficients yields an improvement, compared with a direct wavelet approximation, in the achievable convergence rate in terms of the total number of parameters.

For the hookium model problem with electron interaction cusp, the results of Section 4.3 show that we can expect almost three times the approximation rate that would be possible with a direct wavelet approximation. The analytical estimate is confirmed by the numerical experiments, and similar numerical observations are made in the case of helium, where no corresponding analytical approximability result is available.

In examples with unlimited Besov regularity, such as hydrogen, we have seen that essentially, the best rate possible in the one-dimensional case for H^1–approximation by the wavelet basis is recovered. This can be achieved with standard adaptive wavelet methods based on anisotropic tensor product wavelets as well. For tensor decompositions of wavelet coefficients, however, the constants in the estimates can be expected to be more favorable in higher dimensions. Consider, for instance, the coefficients on an arbitrary fixed wavelet level in an approximation of a *separable* function in d dimensions with an isolated singularity at zero. If the wavelets have support size 10, we will then typically need at least the order of 10 basis functions in each coordinate direction. In a linearly parametrized wavelet expansion, this leads to 10^d degrees of freedom for this fixed wavelet level alone. In the present approach with a multiplicative parametrization, only $10d$ coefficients are required. Even in cases in which the same convergence rate is achieved by both constructions, for functions in higher dimensions with suitable structure, the total approximation complexity may thus be substantially more favorable for nonlinearly parametrized wavelet coefficients.

In this work, we have proven the convergence of adaptive low-rank schemes for the computation of such approximations. The total complexity of these methods remains to be investigated in further detail. The numerical experiments support the conjecture that one can expect a computational complexity that is optimal in a similar sense as in the case of adaptive wavelet methods.

In this regard, however, for two-electron problems there remains an issue with the approximation of the electron interaction Coulomb potential. For the resulting lower-dimensional factor matrices, our construction of compressed matrices yields s^*–compressibility with some $s^* < 1$ depending on the order of the wavelet basis. However, to make full use of approximability of solutions, we would need $s^* = \frac{3}{2}$. There is no clear indication in our numerical results that an asymptotically better construction of compressed matrices is possible. In order to circumvent the limitation by the s^*-compressibility of the interaction potential, it may therefore be necessary to make stronger use of structural a priori knowledge on the wavelet coefficients of interaction cusps.

For an improvement in the efficiency of the schemes in general, it may be useful to replace the Daubechies-type wavelets used here by orthonormal spline multiwavelets, which can yield substantially better compressibility of certain operators (e.g., of the Laplacian). By an appropriate modification of the given construction, however, we cannot expect to obtain $s^* \geq 1$ for the lower-dimensional components in the approximate interaction potential in this manner either, which can be seen from an inspection of the proof of Theorem 6.27. Apart from this, there are other possible benefits in using such spline basis functions, in particular simpler and potentially more efficient computation of integrals. This can improve the s^*-computability (cf. Definition 3.29) of operators, since the the methods for general wavelets considered in Sections 6.5 and 6.6 have the shortcoming that the number of operations required for the evaluation of each single matrix entry does not remain uniformly bounded.

Another direction for further developments are modifications to the basic algorithms that improve the quantitative behaviour. Algorithms 5.5 and 5.6 in their basic form have the advantage of a relatively transparent basic concept. A first modification, which yields a promising improvement in the numerical experiments of Chapter 7, are additional iterations on fixed index sets. Second, one may use improved approximations for Rayleigh quotients. We have not yet incorporated these options in our convergence analysis here. Moreover, the construction of eigenvalue solvers for nonsymmetric problems, which would allow the treatment of the explicitly correlated formulation of Section 2.2, would be of interest as well.

The tensor representation is used here essentially as a black box that provides the required operations, but one could also consider a combination of the developed wavelet concepts with different iterative schemes that are more directly adapted to the underlying tensor representations (as investigated, e.g., in [82]).

A particularly important point is the application of the iterative methods we have considered to problems in dimensions higher than six. This necessitates the use of alternatives to the Tucker format, which has been sufficient for our purposes in this work. Such alternatives are, for instance, the $\mathcal{H}$-Tucker format or the Tensor Train format. Different variants of tensor preconditioning that are intermediate between a direct application of rescaling operations and the levelwise subdivision considered here may be of interest in higher dimensions as well. The basic iterative schemes given in Chapter 5 can thus in principle be extended to higher-dimensional problems with a suitable tensor structure.

Concerning the application to the Schrödinger equation we have considered, the question arises whether there are practically feasible ways of improving the approximation of electron interaction cusps beyond the constraints that one obtains for tensor product bases. There are known methods, e.g., those of Hylleraas type discussed briefly in Section 2.3, that enable a better approximation of electron interaction cusps by suitable coordinate changes. The methods of this type known to date are, however, restricted to special systems with a limited number of electrons.

The basic concepts we have considered here are in principle applicable to systems with more than two electrons, but there are a number of additional difficulties – besides the higher dimensionality – that need to be addressed. This concerns, in particular, the partial antisymmetry conditions that need to be enforced for three or more electrons, and the handling of bivariate tensor factors corresponding to electron pairs. As noted in [154], the efficient application of operators in a direct wavelet discretization with antisymmetry constraints is not straightforward, and this is even less clear for wavelet coefficients represented in a tensor format. The corresponding operations on sums of separable functions, under antisymmetry constraints and combined with a fixed set of electron pair functions, have been considered in [113]. This raises the question whether similar results are possible for tensor formats imposing additional structure, such as the Tucker and $\mathcal{H}$-Tucker format.

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A Supplementary Proofs

A.1 Anisotropic Besov Regularity for Hooke's Law Atom

We follow the lines of [51, Lemma 2.1]; since the modification to the argument that we need only involves some detail changes, we adopt the notation from [51] and refer to specific equations in [51] that are changed. Recall that the proof in [51] applies to u_0 as in (4.5) without essential changes, but using the superexponential decay of u_0 towards infinity instead of the boundedness of the domain.

Proof of Theorem 4.14. We use $x, y \in \mathbb{R}^3$ as coordinates for $\mathbb{R}^6$. For the explicitly correlated eigenfunction w_0 as in (4.6), we make use of asymptotic smoothness property

$$\left|\partial_x^\alpha \partial_y^\beta w_0(x,y)\right| \le c_{\alpha,\beta} |x-y|^{3-|\alpha|-|\beta|} .$$

In particular, $\partial_{x_1}^3 w_0$ is uniformly bounded.

We assume $j_1 \ge j_2$ without restriction of generality. As in equation (2.8) in [51], we have

$$\sum_{i\in\Delta_0} 2^{-(3+1/2)j_1} 2^{-j_1} 2^{-3j_1} 2^{3j_2/2} \left\|\partial_{x_1}^3 w_0\right\|_{\infty,\Box_{j_1,a_1}\times\Box_i} \lesssim 2^{-15j_1/2+3j_2/2}$$

with $\mathcal{O}(1)$ summands on the left hand side. Equation (2.9) in [51] becomes, here with $p > 6$,

$$\begin{aligned}
&\sum_{i\in\Delta\setminus\Delta_0} 2^{-(p+3/2)j_1-3j_1+3j_2/2} \|\partial_{x_1}^p w_0\|_{\infty,\Box_{j_1,a_1}\times\Box_i} \\
&\qquad\qquad \lesssim 2^{-(p+3/2)j_1+3j_2/2} \sum_{i\in\Delta\setminus\Delta_0} 2^{-3j_1} \sup_{(x,y)\in\Box_{j_1,a_1}\times\Box_i} |x-y|^{3-p} \\
&\qquad\qquad \lesssim 2^{-(p+3/2)j_1+3j_2/2} \int_{2^{-j_1}}^{2^{-j_2+2}} r^{2+3-p}\, dr \lesssim 2^{-15j_1/2+3j_2/2} .
\end{aligned}$$

Equation (2.10) is replaced by

$$\begin{aligned}
\sum_{j_1\ge j_2\ge 0} 2^{qj_1} \sum_{a_1,a_2} |\langle \Psi_{j_1,j_2,a_1,a_2}, w_0\rangle|^q &\lesssim \sum_{j_1\ge j_2\ge 0} 2^{qj_1} 2^{3j_1} (2^{-15j_1/2+3j_2/2})^q \\
&= \sum_{j_1\ge 0} 2^{-(13q/2-3)j_1} \sum_{j_2\le j_1} 2^{3qj_2/2} \sim \sum_{j_1\ge 0} 2^{-(5q-3)j_1} ,
\end{aligned}$$

which requires $q > 3/5$. We replace (2.11) by

$$\begin{aligned}
&\sum_{a_1,a_2} |\langle \Psi_{j_1,j_2,a_1,a_2}, w_0\rangle|^q \\
&\quad\lesssim 2^{-(p+3/2)q(j_1+j_2)} \left\|\partial_{x_1}^p \partial_{y_1}^p w_0\right\|_{\infty,\Box_{j_1,a_1}\times\Box_{j_2,a_2}} \\
&\quad\lesssim \sum_{a_1,a_2} 2^{-(pq+3q/2-3)j_1} 2^{-(pq+3q/2-3)j_2} 2^{-3(j_1+j_2)} \sup_{(x,y)\in\Box_{j_1,a_1}\times\Box_{j_2,a_2}} |x-y|^{(3-2p)q} \\
&\quad\lesssim 2^{-(pq+3q/2-3)(j_1+j_2)} \int_{2^{-j_2}}^{\infty} r^{2+(3-2p)q}\, dr
\end{aligned}$$

where $2 + 3q - 2pq < -1$ follows with $p > \alpha + 1$ and $\alpha = 3/q - 3/2$, hence

$$\lesssim 2^{-(pq+3q/2-3)(j_1+j_2)} 2^{-(3+(3-2p)q)j_2} = 2^{-(pq+3q/2-3)j_1} 2^{(pq-9q/2)j_2} ,$$

and finally

$$\sum_{j_1 \geq j_2 \geq 0} 2^{qj_1} 2^{-(pq+3q/2-3)j_1} 2^{(pq-9q/2)j_2} \sim \sum_{j_1 \geq 0} 2^{-(pq+q/2-3)j_1} 2^{(pq-9q/2)j_1} = \sum_{j_1 \geq 0} 2^{-(5q-3)j_1} .$$

Thus w_0 is in the space $\tilde{\mathrm{B}}^\alpha_q(\mathbb{R}^3; 2)$ with $\alpha = 3/q - 3/2$ if $q > 3/5$, that is, if $\alpha < 7/2$. Analogously to the argument for u_0 in [51], it can be seen that this result is sharp. □

A.2 Norm Estimates for Gaussian-Type Functions

Proof of Lemma 4.28. The first part (4.27) is clear, and (4.28) follows from

$$|u|^2_{\mathrm{H}^s(\mathbb{R})} = \frac{1}{2\gamma} \int_{\mathbb{R}} |\xi|^{2s} e^{-\frac{\xi}{2\gamma}} \,\mathrm{d}\xi = (2\gamma)^{s-\frac{1}{2}} \int_{\mathbb{R}} |\xi|^{2s} e^{-\xi^2} \,\mathrm{d}\xi \,.$$

Let $s > 0$ and p as in (4.29), and let $\{\psi_\nu\}_{\nu\in\nabla}$ be an orthonormal, compactly supported wavelet basis on $\mathbb{R}$ with $m \geq s + 2$ vanishing moments. In what follows, we choose the lowest wavelet level $j_0 = 0$. We additionally assume that $\{\psi_\nu\}_{\nu\in\nabla}$ satisfies a norm equivalence for $\mathrm{B}^s_{p,p}$, that is,

$$\|u\|_{\mathrm{B}^s_{p,p}(\mathbb{R})} \sim \Bigl(\sum_{\nu\in\nabla} 2^{p|\nu|} |c_\nu|^p\Bigr)^{\frac{1}{p}} , \quad c_\nu := \langle u, \psi_\nu \rangle \,. \tag{A.1}$$

By Theorem 3.9 and our assumptions on s, (A.1) is ensured by $\psi_\nu \in \mathrm{H}^s(\mathbb{R})$.

Let $S_\nu := \operatorname{supp} \psi_\nu$. We partition ∇ into the sets

$$\begin{gathered} A := \{\nu \colon \mathrm{s}(\nu) = 0 \,,\ 0 \in S_\nu\} \,,\ \hat{A} := \{\nu \colon \mathrm{s}(\nu) = 0 \,,\ 0 \notin S_\nu\} \,, \\ B_j := \{\nu \colon |\nu| = j,\, \mathrm{s}(\nu) \neq 0,\, 0 \in S_\nu\} \,,\ \hat{B}_j := \{\nu \colon |\nu| = j,\, \mathrm{s}(\nu) \neq 0,\, 0 \notin S_\nu\} \,, \quad j \geq 0 \,. \end{gathered}$$

Since S_ν is closed, the supports of basis functions corresponding to elements of $\hat{A}$, $\hat{B}_j$ have positive distance from zero. By Hölder's inequality,

$$|c_\nu| \leq \|\psi_\nu\|_{\mathrm{L}_1} \sup_{x\in S_\nu} e^{-\gamma x^2} ,$$

and hence we obtain

$$\sum_{\nu\in A} |c_\nu|^p \lesssim 1 \,, \quad \sum_{\nu\in\hat{A}} |c_\nu|^p \lesssim \sum_{k\in\mathbb{Z}\setminus\{0\}} e^{-p\gamma k^2} \leq \int_{\mathbb{R}} e^{-p\gamma x^2} \,\mathrm{d}x \lesssim \gamma^{-\frac{1}{2}} \,.$$

Note that since we are mainly interested in the asymptotic dependence on γ, we treat terms that depend only on s or p as constants. Combining the vanishing moment properties of the wavelets for $n \leq m$ with Hölder's inequality and using Lemma 6.23, we obtain

$$\begin{aligned} |c_\nu| &\leq \|\psi_\nu\|_{\mathrm{L}_1} \inf_{g\in\Pi_{n-1}} \|u - g\|_{\mathrm{L}_\infty(S_\nu)} \lesssim (2^{\frac{1}{2}|\nu|} 2^{-|\nu|}) 2^{-n|\nu|} \|\mathrm{D}^n u\|_{\mathrm{L}_\infty(S_\nu)} \\ &\lesssim 2^{-(n+\frac{1}{2})|\nu|} \gamma^{\frac{n}{2}} \sup_{x\in S_\nu} |e^{-(\gamma/2)x^2}| \,. \end{aligned} \tag{A.2}$$

As a consequence, using (A.2) for $n_1, n_2 \in \mathbb{N}$ we obtain $\sum_{\nu\in B_j}|c_\nu|^p \lesssim 2^{-(n_1+\frac{1}{2})pj}\gamma^{\frac{pn_1}{2}}$ and

$$\sum_{\nu\in\hat{B}_j}|c_\nu|^p \lesssim \gamma^{\frac{pn_2}{2}} 2^{-(n_2+\frac{1}{2})pj} \sum_{k\in\mathbb{Z}\setminus\{0\}} e^{-p2^{-2j-1}\gamma k^2} \lesssim \gamma^{\frac{pn_2}{2}-\frac{1}{2}} 2^{-(n_2+\frac{1}{2})pj} 2^j \,.$$

Consequently, assuming that $n_1 > 1/2$ and $n_2 > 1/p + 1/2$, or equivalently, $n_2 > s$, we have

$$\begin{aligned}\sum_{\nu\in\nabla} 2^{p|\nu|}|c_\nu|^p &\lesssim 1 + \gamma^{-\frac{1}{2}} + \gamma^{\frac{pn_1}{2}} \sum_{j\geq 0} 2^{-p(n_1-\frac{1}{2})j} + \gamma^{\frac{pn_2}{2}-\frac{1}{2}} \sum_{j\geq 0} 2^{-(n_2p-1-\frac{p}{2})j} \\ &\lesssim 1 + \gamma^{-\frac{1}{2}} + \gamma^{\frac{pn_1}{2}}(n_1-\tfrac{1}{2})^{-1} + \gamma^{\frac{pn_2}{2}-\frac{1}{2}}(n_2-\tfrac{1}{p}-\tfrac{1}{2})^{-1}\,,\end{aligned}$$

where $(n_2-1/p-1/2)^{-1} < (n_2-s)^{-1}$. We choose $n_1 = 1$ and $n_2 = \lfloor s+\frac{1}{2}\rfloor+1$, so that $n_2 - s \in (\frac{1}{2}, \frac{3}{2}]$, to obtain

$$\|u\|_{\mathrm{B}^s_{p,p}} \lesssim 1 + \gamma^{-\frac{1}{2}s+\frac{1}{4}} + \gamma^{\frac{1}{2}} + \gamma^{\frac{1}{2}(n_2-s)+\frac{1}{4}}\,.$$

With $\tau := (n_2 - s)/2 - 1/4$ we arrive at (4.29).

With κ and c_n^* as in the hypothesis, (4.30) follows from

$$\int_{\mathbb{R}} |\mathrm{D}^n(\kappa u)|^2 \,\mathrm{d}x \lesssim \sum_{m=0}^{n} \int_{\mathbb{R}} |\mathrm{D}^m\kappa|^2 |\mathrm{D}^{n-m}u|^2 \,\mathrm{d}x \leq \sum_{m=0}^{n} \|\mathrm{D}^m\kappa\|_\infty^2 \int_{\operatorname{supp}\kappa} |\mathrm{D}^{n-m}u|^2 \,\mathrm{d}x$$

and (4.28). Furthermore, let $\hat{c}_\nu := \langle \kappa u, \psi_\nu\rangle$, then (A.2) is replaced by

$$|\hat{c}_\nu| \lesssim 2^{-(n+\frac{1}{2})|\nu|} c_n^* \Bigl(\sup_{x\in S_\nu} e^{-\gamma x^2} + \gamma^{\frac{n}{2}} \sup_{x\in S_\nu} e^{-(\gamma/2)x^2} \Bigr)\,,$$

which leads to the estimates

$$\sum_{\nu\in A\cup\hat{A}} |\hat{c}_\nu|^p \lesssim 1 + |\operatorname{supp}\kappa|\,, \qquad \sum_{\nu\in B_j} |\hat{c}_\nu|^p \lesssim 2^{-(n_1+\frac{1}{2})pj} |c_n^*|^p (1 + \gamma^{\frac{pn_1}{2}})\,,$$

as well as

$$\sum_{\nu\in\hat{B}_j} |\hat{c}_\nu|^p \lesssim 2^{-(n_2+\frac{1}{2})pj} 2^j |c_n^*|^p \bigl(|\operatorname{supp}\kappa| + \gamma^{\frac{pn_2}{2}-\frac{1}{2}} \bigr)\,.$$

Proceeding as in the case of (4.29), we thus obtain (4.31). □

Proof of Lemma 4.33. A direct calculation yields (4.43). By a rotation of coordinates, we find

$$\begin{aligned}|u|^2_{\mathrm{H}^s(\mathbb{R}^2)} &= \int_{\mathbb{R}^2} \bigl(|\xi_1|^2 + |\xi_2|^2\bigr)^s |\hat{u}|^2 \,\mathrm{d}\xi = \frac{1}{2\pi} \int_{\mathbb{R}^2} \bigl(|\xi_1|^2 + |\xi_2|^2\bigr)^s \left| \int_{\mathbb{R}^2} e^{-2\beta x_1^2 - \gamma|x|^2} e^{-ix\cdot\xi} \,\mathrm{d}x \right|^2 \mathrm{d}\xi \\ &= \frac{1}{4\gamma(\gamma+2\beta)} \int_{\mathbb{R}^2} \bigl(|\xi_1|^2 + |\xi_2|^2\bigr)^s e^{-\frac{\xi_1^2}{2(\gamma+2\beta)}} e^{-\frac{\xi_2^2}{2\gamma}} \,\mathrm{d}\xi\,.\end{aligned}$$

Since $\bigl(|\xi_1|^2 + |\xi_2|^2\bigr)^s \leq 2^{(s-1)_+}\bigl(|\xi_1|^{2s} + |\xi_2|^{2s}\bigr)$ and

$$\int_{\mathbb{R}^2} |\xi_1|^{2s} e^{-|\xi|^2} \,\mathrm{d}\xi = \sqrt{\pi}\,\Gamma(s+\tfrac{1}{2})\,,$$

we obtain (4.44). Note that for integer s, essentially the same result as (4.44) can also be obtained on the basis of the pointwise estimate of Lemma 6.23.

For the proof of (4.45), let $s > 0$ and $p = (s+\frac{1}{2})^{-1}$. We proceed similarly to the proof of Lemma 4.28. Let $\{\Psi_\nu\}_{\nu\in\nabla^2}$ be an orthonormal, compactly supported tensor product wavelet basis on $\mathbb{R}^2$

that satisfies a norm equivalence for $\tilde{\mathrm{B}}^s_p(\mathbb{R};2)$ and such that the corresponding univariate wavelet has $m \geq 2s+3$ vanishing moments. For what follows, we use a basis with scaling functions on level $j_0 = 0$. Recall that for $j \in \mathbb{N}_0^2$, ∇^2_j denotes the set of all $\nu \in \nabla^2$ with $|\nu| = j$. Due to the symmetries in u, the norm equivalence simplifies to

$$\|u\|_{\tilde{\mathrm{B}}^s_p(\mathbb{R};2)} \sim \Bigl(\sum_{j_1 \geq j_2 \geq 0} 2^{pj_1} \sum_{\nu \in \nabla^2_{(j_1,j_2)}} |c_\nu|^p \Bigr)^{\frac{1}{p}} , \quad c_\nu := \langle u, \Psi_\nu \rangle \,.$$

Let $S_\nu := \operatorname{supp} \Psi_\nu$. We partition ∇^2 into the sets

$$A_j := \{ \nu \in \nabla^2_j \colon\; 0 \in S_\nu \} , \quad \hat{A}_j := \{ \nu \in \nabla^2_j \colon\; 0 \notin S_\nu \} , \quad j \in \mathbb{N}_0^2 \,.$$

Note that since S_ν is closed, the supports of basis functions corresponding to elements of $\hat{A}_j$ have positive distance to zero.

Analogously to the proof of Lemma 4.28, by Hölder's inequality we obtain

$$\sum_{\nu \in A_{(0,0)}} |c_\nu|^p \lesssim 1 \,, \qquad \sum_{\nu \in \hat{A}_{(0,0)}} |c_\nu|^p \lesssim \gamma^{-\frac{1}{2}} (\gamma + 2\beta)^{-\frac{1}{2}} \,. \tag{A.3}$$

To estimate the contributions of the remaining levels, we use the vanishing moment property of the wavelets. Let $j_1 > 0$ and $j_2 \geq 0$ with $j_1 \geq j_2$. For $k \in \mathbb{Z}$, let $\Omega_{j_1,k} := \mathbb{R} \times [2^{-j_1}k, 2^{-j_1}(k+1)]$. Using vanishing moments with $n \leq m$ in the first coordinate direction, for any $\nu \in \nabla^2_{(j_1,j_2)}$ we obtain

$$|c_\nu|^p = \Bigl| \sum_{k_2} \int_{S_\nu \cap \Omega_{j_1,k_2}} u \Psi_\nu \,\mathrm{d}x \Bigr|^p \lesssim \sum_{k_2} 2^{-(n+1)p} \|\mathrm{D}^n_{x_1} u\|^p_{\mathrm{L}_\infty(S_\nu \cap \Omega_{j_1,k_2})} \,,$$

where the latter estimate holds because, as a consequence of $s \geq \frac{1}{2}$, we have $p \leq 1$. Note furthermore that

$$|\mathrm{D}^n_{x_1} u(x)| = \Bigl| \sum_{k=0}^{n} \binom{n}{k} e^{-\gamma x_2^2} (\mathrm{D}^k_{x_1} e^{-\gamma x_1^2}) (\mathrm{D}^{n-k}_{x_1} e^{-\gamma (x_1 - x_2)^2}) \Bigr|$$

which, by Lemma 6.23, can be estimated by

$$\lesssim (\gamma + \beta)^{\frac{n}{2}} e^{-(\beta/2)(x_1 - x_2)^2 - (\gamma/2)|x|^2} \,.$$

For each $j_1 > 0$ and $n_1, n_2 \leq m$ to be determined, proceeding analogously to the proof of Lemma 4.28 we thus conclude

$$\sum_{j_2=0}^{j_1} \sum_{\nu \in A_{(j_1,j_2)}} |c_\nu|^p \lesssim j_1 2^{-(n_1+1)pj_1} (\gamma + 2\beta)^{\frac{pn_1}{2}} \tag{A.4}$$

as well as

$$\sum_{j_2=0}^{j_1} \sum_{\nu \in \hat{A}_{(j_1,j_2)}} |c_\nu|^p \lesssim j_1 \gamma^{-\frac{1}{2}} (\gamma + \beta)^{\frac{pn_2}{2} - \frac{1}{2}} 2^{-(n_2+1)pj_1} 2^{2j_1} \,. \tag{A.5}$$

Putting (A.3), (A.4), and (A.5) together yields

$$\|u\|^p_{\tilde{\mathrm{B}}^s_p} \lesssim 1 + \gamma^{-\frac{1}{2}} (\gamma + \beta)^{-\frac{1}{2}} + (\gamma + \beta)^{\frac{pn_1}{2}} \sum_{j > 0} j 2^{-n_1 p j_1} + \gamma^{-\frac{1}{2}} (\gamma + \beta)^{\frac{pn_2}{2} - \frac{1}{2}} \sum_{j > 0} j 2^{-(pn_2 - 2)j} \,.$$

We set $n_1 = 1$, $n_2 = \lfloor 2s + \frac{3}{2} \rfloor + 1$, where in view of $\frac{2}{p} = 2s+1$, the latter choice ensures $n_2 - \frac{2}{p} \in (\frac{1}{2}, \frac{3}{2}]$.

We thus arrive at

$$\|u\|_{\tilde{\mathrm{B}}^s_p} \lesssim 1+\gamma^{-\frac{1}{p}}+(\gamma+\beta)^{\frac{1}{2}}+\gamma^{-\frac{1}{2p}}(\gamma+\beta)^{\frac{n_2}{2}-\frac{1}{2p}} = 1+\gamma^{-(s+\frac{1}{2})}+(\gamma+\beta)^{\frac{1}{2}}+\gamma^{-(\frac{s}{2}+\frac{1}{4})}(\gamma+\beta)^{\frac{1}{2}(n_2-\frac{2}{p})+\frac{s}{2}+\frac{1}{4}},$$

and with $\tau_2 := \frac{1}{4} + \frac{1}{2}(n_2 - \frac{2}{p})$, this yields the assertion. $\square$

A.3 Complexity of the Level Subdivision

Proof of Proposition 5.6. We proceed by induction over ℓ and d; let $n_{d,\ell} := \#\mathcal{J}^{(d)}_{\ell,\{1,\dots,d\}}$. For any $d \geq 2$, we have $n_{d,0} = 1$.

For the case $d = 2$, we obtain $n_{2,\ell+1} = 2n_{2,\ell} + 2$ for $\ell \geq 0$, and hence $n_{2,\ell} = 3 \cdot 2^\ell - 2$. It is clear from (5.33) that $\mathcal{J}^{(2)}_{\ell,\{1,2\}}$ is a partition of $\{0, \dots, 2^\ell - 1\}^2$.

Let now $d > 2$ be fixed, and suppose, for $n_{k,i}$ with $k \in \{2, \dots, d-1\}$ and $i \in \mathbb{N}_0$, that $n_{k,i}$ is of the form

$$n_{k,i} = 2^i \sum_{p=0}^{k-2} \alpha^k_p \, i^p \,, \quad \alpha^k_p \in \mathbb{R}\,, \tag{A.6}$$

which we have already shown for $k = 2$. From (5.34), we find

$$n_{d,\ell+1} = 2n_{d,\ell} + \sum_{k=2}^{d-1} \binom{d}{k} n_{k,\ell} + d\,. \tag{A.7}$$

Then since $n_{d,\ell}$ solves the inhomogeneous constant-coefficient linear recurrence (A.7), the representation (A.6) holds for $k = d$ as well (see e.g. [141]).

Suppose furthermore that $\mathcal{J}^{(k)}_{\ell,\{1,\dots,k\}}$ is a partition of $\{0, \dots, 2^\ell - 1\}^k$ for any $k \in \{2, \dots, d-1\}$ and each ℓ, then it is clear from the definition (5.36) that $\mathcal{J}^{(d)}_{\ell,D}$ is a partition of $\{0, \dots, 2^\ell - 1\}^d$ for any $D \subset \{1, \dots, d\}$ with $\#D = k$ and each ℓ. We now take ℓ fixed and assume further that $\mathcal{J}^{(d)}_{i,\{1,\dots,d\}}$ is a partition of $\{0, \dots, 2^i - 1\}^d$ for each $0 \leq i \leq \ell$. Then by (5.34), $\mathcal{J}^{(d)}_{\ell+1,\{1,\dots,d\}}$ is a union of 2^d sets, each of which is a partition of $\chi^{(d)}(D) + \{0, \dots, 2^\ell - 1\}^d$ for a distinct $D \subset \{1, \dots, d\}$, and therefore forms a partition of $\{0, \dots, 2^{\ell+1} - 1\}^d$.

Let $\mathcal{J}$ be a set of subsets of $\mathbb{Z}^2$, then we say that $\mathcal{J}$ has property (M) if

> For each $S \in \mathcal{J}$ there exists $\bar{d} \in \{1, \dots, d\}$ such that for all $j \in S$, we have $\max j = j_{\bar{d}}$. (M)

We now show by induction that for any d and ℓ, (M) holds for $\mathcal{J}^{(d)}_{\ell,\{1,\dots,d\}}$. We begin by showing (M) for $d = 2$ by induction over ℓ. For $\ell = 0$, the statement is clear. Assuming that (M) holds true for $d = 2$ and $\ell \in \mathbb{N}_0$, it also holds for $2^\ell b^{(2)}_{\{1,2\}} + \mathcal{J}^{(2)}_{\ell,\{1,2\}}$. That (M) holds for the singletons $2^\ell b^{(2)}_{\{1\}} + \mathcal{J}^{(2)}_{\ell,\{1\}} = (2^\ell, 0) + \mathcal{J}^{(2)}_{\ell,\{\}}$ and $2^\ell b^{(2)}_{\{2\}} + \mathcal{J}^{(2)}_{\ell,\{2\}} = (0, 2^\ell) + \mathcal{J}^{(2)}_{\ell,\{\}}$ is clear from the definition of $\mathcal{J}^{(2)}_{\ell,\{\}}$ in (5.32) as well, and thus by (5.33), (M) holds for $\mathcal{J}^{(2)}_{\ell+1,\{1,2\}}$.

For $d > 2$, (M) clearly holds for $\mathcal{J}^{(d)}_{0,\{1,\dots,d\}} = \mathcal{J}^{(d)}_{0,\{\}}$. For the induction step, we assume (M) to hold for $\mathcal{J}^{(i)}_{\ell,\{1,\dots,i\}}$ for some $\ell \in \mathbb{N}_0$ and for all $2 \leq i \leq d$, and show that it holds for $\mathcal{J}^{(d)}_{\ell+1,\{1,\dots,d\}}$. Let $k \in \{1, \dots, d\}$ and $D \subset \{1, \dots, d\}$ with $\#D = k$. If $k = 1$ or $k = d$, we see that (M) holds for $2^\ell b^{(d)}_D + \mathcal{J}^{(d)}_{\ell,D}$ immediately from the definitions as in the case $d = 2$. In the case $1 < k < d$, let $S \in 2^\ell b^{(d)}_D + \mathcal{J}^{(d)}_{\ell,D}$ and $j \in S$. Then by (5.36), we have $j_m < 2^\ell$ for all $m \in \{1, \dots, d\} \setminus D$ and $j_m \geq 2^\ell$ for all $m \in D$. Since (M) holds for $\mathcal{J}^{(k)}_{\ell,\{1,\dots,k\}}$ by hypothesis, it thus also holds for $2^\ell b^{(d)}_D + \mathcal{J}^{(d)}_{\ell,D}$. This completes the induction, and (M) thus holds for all d and ℓ. $\square$

A.4 Analysis of the Reference Triple Product Integration Scheme

Proof of Proposition 6.36. We prove the proposition for the two-dimensional case; the proof in the case of the the one-dimensional integrals follows the same lines. By the direct estimate for $\{\theta_{J,k}\}_k$,

$$\Big\|\sqrt{\alpha}e^{-\alpha(x_1-x_2)^2} - \sum_{k\in\mathbb{Z}^2} \langle \sqrt{\alpha}e^{-\alpha(\tilde{x}_1-\tilde{x}_2)^2}, \tilde{\theta}_{J,k_1}\otimes\tilde{\theta}_{J,k_2}\rangle \theta_{J,k_1}\otimes\theta_{J,k_2}\Big\|_\infty \\ \le 2^{-pJ}\sqrt{\alpha} \max_{\substack{i_1,i_2\ge 0\\ i_1+i_2=p}} \|\partial^{i_1}_{x_1}\partial^{i_2}_{x_2} e^{-\alpha(x_1-x_2)^2}\|_\infty\,.$$

Furthermore, by Lemma 6.23, we have

$$\|\partial^{i_1}_{x_1}\partial^{i_2}_{x_2} e^{-\alpha(x_1-x_2)^2}\|_\infty \lesssim \alpha^{p/2}\|e^{-(\alpha/2)(x_1-x_2)^2}\|_\infty\,, \quad i_1+i_2=p\,. \tag{A.8}$$

We use the direct estimate for $\{\tilde{\theta}_{J,k}\}_k$ to obtain

$$\Big\|\psi_{\nu_1}\,\psi_{\mu_1}\otimes\psi_{\nu_2}\,\psi_{\mu_2} - \sum_{k\in\mathbb{Z}^2}\langle\psi_{\nu_1}\,\psi_{\mu_1}\otimes\psi_{\nu_2}\,\psi_{\mu_2}, \theta_{J,k_1}\otimes\theta_{J,k_2}\rangle\tilde{\theta}_{J,k_1}\otimes\tilde{\theta}_{J,k_2}\Big\|_\infty \\ \le 2^{-qJ}\max_{\substack{i_1,i_2\ge 0\\ i_1+i_2=q}} \|\partial^{i_1}_{x_1}\partial^{i_2}_{x_2}(\psi_{\nu_1}\,\psi_{\mu_1}\otimes\psi_{\nu_2}\,\psi_{\mu_2})\|_\infty\,,$$

where $\|\partial^{i_1}_{x_1}\partial^{i_2}_{x_2}(\psi_{\nu_1}\,\psi_{\mu_1}\otimes\psi_{\nu_2}\,\psi_{\mu_2})\|_\infty \lesssim 2^{\frac{1}{2}(|\nu_1|+|\mu_1|+|\nu_2|+|\mu_2|)}2^{q\max\{|\nu_1|,|\mu_1|,|\nu_2|,|\mu_2|\}}$. As a consequence, the error in the expansion (6.109) can be estimated by

$$c\min\{2^{-pJ}\alpha^{\frac{1}{2}(p+1)}, 2^{-qJ}2^{\frac{1}{2}(|\nu_1|+|\mu_1|+|\nu_2|+|\mu_2|)}2^{q\max\{|\nu_1|,|\mu_1|,|\nu_2|,|\mu_2|\}}\}$$

with some $c>0$. For this expression to be bounded by $\varepsilon>0$, we need to choose

$$J\ge\min\Big\{\tfrac{1}{p}\log_2 c\varepsilon^{-1}+\tfrac{1}{2}\big(1+\tfrac{1}{p}\big)\log_2\alpha, \\ \tfrac{1}{q}\log_2 c\varepsilon^{-1}+\max\{|\nu_1|,|\mu_1|,|\nu_2|,|\mu_2|\}+\tfrac{1}{2q}(|\nu_1|+|\mu_1|+|\nu_2|+|\mu_2|)\Big\}\,. \tag{A.9}$$

Let

$$\mathcal{K}^{(2)}_{J,\varepsilon} := \Big\{k\in\mathbb{Z}^2\colon\ |x_1-x_2|\le\alpha^{-\frac{1}{2}}(\max\{\tfrac{1}{4},\ln\varepsilon^{-1}\})^{\frac{1}{2}}\ \text{ for all } (x_1,x_2)\in\operatorname{supp}\tilde{\theta}_{J,k_1}\otimes\tilde{\theta}_{J,k_2}\Big\}\,,$$

and assume that ε is sufficiently small such that $\ln\varepsilon^{-1}>\frac{1}{4}$. By the estimate

$$\int_y^\infty \sqrt{\alpha}\,e^{-\alpha x^2}\,\mathrm{d}x\le e^{-\alpha y^2}\ \text{ for } y\ge\frac{1}{2}\alpha^{-\frac{1}{2}}$$

we thus obtain

$$\bigg|\int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\,(\psi_{\nu_1}\otimes\psi_{\nu_2})\,(\psi_{\mu_1}\otimes\psi_{\mu_2})\,\mathrm{d}x \\ - \sum_{k\in\mathcal{K}^{(2)}_{J,\varepsilon}}\int\sqrt{\alpha}e^{-\alpha(x_1-x_2)^2}\tilde{\theta}_{J,k_1}\otimes\tilde{\theta}_{J,k_2}\,\mathrm{d}x\int_{\mathbb{R}}\theta_{J,k_1}\,\psi_{\nu_1}\,\psi_{\mu_1}\,\mathrm{d}x\int_{\mathbb{R}}\theta_{J,k_2}\,\psi_{\nu_2}\,\psi_{\mu_2}\,\mathrm{d}x\bigg|\lesssim\varepsilon$$

for J as in (A.9), with a constant independent of ε, assuming that $\ln\varepsilon^{-1}>\frac{1}{4}$. □

We now consider the number of coefficients required for a given error ε according to these estimates in the case of the two-dimensional integrals. To this end, for given $\nu_1,\mu_1,\nu_2,\mu_2\in\nabla$ we introduce the abbreviations $j_{\max} = \max\{|\nu_1|, |\mu_1|, |\nu_2|, |\mu_2|\}$, $j_{\min} = \min\{\max\{|\nu_1|, |\mu_1|\}, \max\{|\nu_2|, |\mu_2|\}\}$, and $j_{\text{sum}} = |\nu_1| + |\mu_1| + |\nu_2| + |\mu_2|$. The number of coefficients to be summed over for each integral can be estimated, up to a constant, by

$$\begin{aligned} 2^{J-j_{\max}} \max\bigl\{1, 2^{J-j_{\min}} \bigl(\alpha^{-1} \ln \varepsilon^{-1}\bigr)^{\frac{1}{2}}\bigr\} \\ \lesssim \min\bigl\{\varepsilon^{-\frac{1}{p}} \alpha^{\frac{1}{2}(1+p^{-1})} 2^{-j_{\max}} \max\{1, \varepsilon^{-\frac{1}{p}} \alpha^{\frac{1}{2p}} 2^{-j_{\min}} (\ln \varepsilon^{-1})^{\frac{1}{2}}\bigr\}\,, \\ \varepsilon^{-\frac{1}{q}} 2^{\frac{1}{2q} j_{\text{sum}}} \max\{1, \varepsilon^{-\frac{1}{q}} 2^{\frac{1}{2q} j_{\text{sum}}} 2^{j_{\max}-j_{\min}} \alpha^{-\frac{1}{2}} (\ln \varepsilon^{-1})^{\frac{1}{2}}\}\bigr\}\,. \end{aligned} \tag{A.10}$$

The number of triple products that are required for this single integral is of order

$$\begin{aligned} \max\{1, ||\mu_1| - |\nu_1||, ||\mu_2| - |\nu_2||\}\; 2^{J-j_{\min}} \lesssim \max\{1, ||\mu_1| - |\nu_1||, ||\mu_2| - |\nu_2||\} \\ \times \min\bigl\{\varepsilon^{-\frac{1}{p}} \alpha^{\frac{1}{2}(1+p^{-1})} 2^{-j_{\min}}\,,\ \varepsilon^{-\frac{1}{q}} 2^{\frac{1}{2q} j_{\text{sum}}} 2^{j_{\max}-j_{\min}}\bigr\}\,. \end{aligned} \tag{A.11}$$

The total number of different triple products required for the evaluation of *all* integrals of the same levels $|\nu_1|$, $|\nu_2|$, $|\mu_1|$, $|\mu_2|$, making use of shift invariance of these integrals, is of order $\max\{1, ||\mu_1| - |\nu_1||, ||\mu_2| - |\nu_2||\}\; 2^J$, that is,

$$\mathcal{O}\bigl(\max\{1, ||\mu_1|-|\nu_1||, ||\mu_2|-|\nu_2||\} \min\{\varepsilon^{-\frac{1}{p}} \alpha^{\frac{1}{2}(1+p^{-1})}\,, \varepsilon^{-\frac{1}{q}} 2^{\frac{1}{2q}(|\nu_1|+|\mu_1|+|\nu_2|+|\mu_2|)} 2^{\max\{|\nu_1|,|\mu_1|,|\nu_2|,|\mu_2|\}}\}\bigr)\,.$$

In the case of the expansion (6.108) for the one-dimensional integrals (6.93), the above line of arguments leads to a number of coefficients to be summed for each integral, and a number of corresponding triple products to be computed, that are both of order

$$\mathcal{O}\bigl(\max\bigl\{1, \min\{\varepsilon^{-\frac{1}{p}} \alpha^{\frac{1}{2}(1+p)}, \varepsilon^{-\frac{1}{q}} 2^{\max\{|\mu_1|,|\nu_1|\}} 2^{\frac{1}{2q}(|\mu_1|+|\nu_1|)}\} \min\{2^{-\max\{|\mu_1|,|\nu_1|\}}, \alpha^{-\frac{1}{2}} |\ln \varepsilon|^{\frac{1}{2}}\}\bigr\}\bigr)\,. \tag{A.12}$$

The total number of triple products for all one-dimensional integrals corresponding to indices of the same levels $|\nu_1|$, $|\mu_1|$ is of order

$$\mathcal{O}\bigl(\max\bigl\{1, \min\{\varepsilon^{-\frac{1}{p}} \alpha^{\frac{1}{2p}}, \varepsilon^{-\frac{1}{q}} 2^{\frac{1}{2q}(|\mu_1|+|\nu_1|)} 2^{\max\{|\mu_1|,|\nu_1|\}} \alpha^{-\frac{1}{2}}\} |\ln \varepsilon|^{\frac{1}{2}}\bigr\}\bigr)\,. \tag{A.13}$$

Remark A.1. *The total complexity in a framework of a discretization scheme thus depends on the interplay of exponential sum approximations and required wavelet indices. However, to give a specific example, let us consider the implications of the estimates* (A.10), (A.12) *for* $|\nu_1| = |\mu_1| = |\nu_2| = |\mu_2| = 0$. *To this end, we make the typical assumptions* $p > q$, $q \geq 2$, *and for simplicity neglect the logarithmic factors* $|\ln \varepsilon|$ *arising in the estimates.*

For both one- and two-dimensional integrals, the estimate is largest for $\alpha \sim \varepsilon^{-2q^{-1}(p-q)(p+1)^{-1}}$, *which is consistent with* $\max_k \alpha_k \lesssim \varepsilon^{-2}$ *for the underlying exponential sum approximations as discussed previously. We thus find that in this particular case, for the two-dimensional integrals* (6.94), *in* (6.109) *we need to sum over* $\mathcal{O}(\varepsilon^{-q^{-1}-(p+1)^{-1}(1+q^{-1})})$ *coefficients, whereas in the case of the one-dimensional integrals* (6.93), $\mathcal{O}(\varepsilon^{-(p+1)^{-1}(1+q^{-1})})$ *coefficients are required in* (6.108).

For the conclusions we can draw from the above complexity observations, see Subsection 6.6.1.

Bibliography

[1] Adams, R. A., and Fournier, J. J. F. *Sobolev Spaces*, second ed., vol. 140 of *Pure and Applied Mathematics Series.* Academic Press, 2003.

[2] Agmon, S. *Lectures on Exponential Decay of Solutions of Second-Order Elliptic Equations: Bounds on Eigenfunctions of N-Body Schrödinger Operators.* Mathematical Notes. Princeton University Press, 1982.

[3] Bachmayr, M. Hyperbolic wavelet discretization of the two-electron Schrödinger equation in an explicitly correlated formulation. *ESAIM: Mathematical Modelling and Numerical Analysis 46*, 06 (2012), 1337–1362.

[4] Balder, R., and Zenger, C. The solution of multidimensional real Helmholtz equations on sparse grids. *SIAM J. Sci. Comput. 17*, 3 (1996), 631–646.

[5] Ballani, J., and Grasedyck, L. A projection method to solve linear systems in tensor format. To appear in Num. Lin. Alg. Appl., 2012. DOI: 10.1002/nla.1818.

[6] Ballani, J., and Grasedyck, L. A projection method to solve linear systems in tensor format. SPP 1324 Preprint 46, 2010.

[7] Barinka, A. *Fast Evaluation Tools for Adaptive Wavelet Schemes.* PhD thesis, RWTH Aachen, March 2005.

[8] Barinka, A., Barsch, T., Charton, P., Cohen, A., Dahlke, S., Dahmen, W., and Urban, K. Adaptive wavelet schemes for elliptic problems – implementation and numerical experiments. *SIAM J. Sci. Comput. 23*, 3 (2001), 910–939.

[9] Bergh, J., and Löfström, J. *Interpolation Spaces: An Introduction.* Springer-Verlag, 1976.

[10] Bethe, H., and Salpeter, E. E. *Quantum Mechanics of One- and Two-Electron Atoms.* Springer-Verlag, Berlin, 1957.

[11] Beylkin, G. On the representation of operators in bases of compactly supported wavelets. *SIAM Journal on Numerical Analysis 29*, 6 (1992), 1716–1740.

[12] Beylkin, G., and Mohlenkamp, M. J. Numerical operator calculus in higher dimensions. *PNAS 99*, 16 (2002), 10246–10251.

[13] Beylkin, G., and Mohlenkamp, M. J. Algorithms for numerical analysis in high dimensions. *SIAM J. Sci. Comput. 26*, 6 (2005), 2133–2159.

[14] Beylkin, G., Mohlenkamp, M. J., and Perez, F. Approximating a wavefunction as an unconstrained sum of Slater determinants. *Journal of Mathematical Physics 49* (2008).

[15] Born, M., and Oppenheimer, R. J. Zur Quantentheorie der Molekeln. *Ann. d. Phys. 84* (1927), 457–484.

[16] Boys, S. F. The integral formulae for the variational solution of the molecular many-electron wave equations in terms of Gaussian functions with direct electronic correlation. *Proc. R. Soc. London, Ser. A 258* (1960), 402–411.

[17] Boys, S. F., and Handy, N. C. The determination of energies and wavefunctions with full electronic correlation. *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences 310*, 1500 (1969), 43–61.

[18] Braess, D. *Nonlinear Approximation Theory*. Springer-Verlag, 1986.

[19] Braess, D., and Hackbusch, W. On the efficient computation of high-dimensional integrals and the approximation by exponential sums. In *Multiscale, Nonlinear and Adaptive Approximation*, R. DeVore and A. Kunoth, Eds. Springer Berlin Heidelberg, 2009.

[20] Bungartz, H.-J. *Dünne Gitter und deren Anwendung bei der adaptiven Lösung der dreidimensionalen Poisson-Gleichung*. PhD thesis, Technische Universität München, 1992.

[21] Bungartz, H.-J., and Griebel, M. Sparse grids. *Acta Numerica 13* (2004), 147.

[22] Chatelin, F. *Spectral Approximation of Linear Operators*. Computer Science and Applied Mathematics. Academic Press, 1983.

[23] Cheney, W., and Light, W. *A Course in Approximation Theory*, vol. 101 of *Graduate Studies in Mathematics*. American Mathematical Society, 2000.

[24] Chinnamsetty, S. R., Espig, M., Flad, H.-J., and Hackbusch, W. Canonical tensor products as a generalization of Gaussian-type orbitals. *Zeitschrift für Physikalische Chemie 224* (2010), 681–694.

[25] Chinnamsetty, S. R., Espig, M., Khoromskij, B. N., Hackbusch, W., and Flad, H.-J. Tensor product approximation with optimal rank in quantum chemistry. *Journal of Chemical Physics 127*, 8 (2007), 084110.

[26] Chinnamsetty, S. R., Hackbusch, W., and Flad, H.-J. The tensor product approximation to single-electron systems. Tech. rep., MPI MIS Leipzig, 2009. Preprint 23/2009.

[27] Chinnamsetty, S. R., Luo, H., Hackbusch, W., Flad, H.-J., and Uschmajew, A. Bridging the gap between quantum Monte Carlo and F12-methods. *Chemical Physics 401* (2012), 36–44.

[28] Cioslowskia, J., and Pernal, K. The ground state of Harmonium. *Journal of Chemical Physics 113*, 19 (2000), 8434–8443.

[29] Cohen, A. *Numerical Analysis of Wavelet Methods*, vol. 32 of *Studies in Mathematics and Its Applications*. Elsevier, 2003.

[30] Cohen, A., Dahmen, W., and DeVore, R. Adaptive wavelet methods for elliptic operator equations: Convergence rates. *Mathematics of Computation 70*, 233 (2001), 27–75.

[31] Cohen, A., Dahmen, W., and DeVore, R. Adaptive wavelet methods II – beyond the elliptic case. *Foundations of Computational Mathematics 2*, 3 (2002), 203–245.

[32] Cohen, A., Dahmen, W., and DeVore, R. Adaptive wavelet schemes for nonlinear variational problems. *SIAM Journal on Numerical Analysis 41*, 5 (2004), 1785–1823.

[33] Dahmen, W. Wavelet and multiscale methods for operator equations. *Acta Numerica 6* (1997), 55–228.

[34] Dahmen, W. Wavelet methods for PDEs – some recent developments. *Journal of Computational and Applied Mathematics 128* (2001), 133–185.

[35] Dahmen, W., and Micchelli, C. A. Using the refinement equation for evaluating integrals of wavelets. *SIAM Journal on Numerical Analysis 30*, 2 (1993), 507–537.

[36] Dahmen, W., Rohwedder, T., Schneider, R., and Zeiser, A. Adaptive eigenvalue computation: complexity estimates. *Numerische Mathematik 110*, 3 (2008), 277–312.

[37] Daubechies, I. Orthonormal bases of compactly supported wavelets. *Communications on Pure and Applied Mathematics 41*, 7 (1988), 909–996.

[38] Daubechies, I. *Ten Lectures on Wavelets.* CBMS-NSF Regional Conference Series in Applied Mathematics. SIAM, Philadelphia, 1992.

[39] de Silva, V., and Lim, L.-H. Tensor rank and the ill-posedness of the best low-rank approximation problem. *SIAM Journal on Matrix Analysis and Applications 30*, 3 (2008), 1084–1127.

[40] Deslauriers, G., and Dubuc, S. Symmetric iterative interpolation processes. *Constructive Approximation 5*, 1 (1989), 49–68.

[41] DeVore, R. A. Nonlinear approximation. *Acta Numerica* (1998), 51–150.

[42] DeVore, R. A., Jawerth, B., and Popov, V. Compression of wavelet decompositions. *American Journal of Mathematics 114*, 4 (1992), 737–785.

[43] DeVore, R. A., Konyagin, S. V., and Temlyakov, V. N. Hyperbolic wavelet approximation. *Constructive Approximation 14* (1998), 1–26.

[44] Dijkema, T. J., Schwab, C., and Stevenson, R. An adaptive wavelet method for solving high-dimensional elliptic PDEs. *Constructive Approximation 30*, 3 (2009), 423–455.

[45] Donovan, G., Geronimo, J., and Hardin, D. Intertwining multiresolution analyses and the construction of piecewise-polynomial wavelets. *SIAM Journal on Mathematical Analysis 27*, 6 (1996), 1791–1815.

[46] Donovan, G., Geronimo, J., and Hardin, D. Orthogonal polynomials and the construction of piecewise polynomial smooth wavelets. *SIAM J. Math. Anal. 30*, 5 (1999), 1029–1056.

[47] Eckart, G., and Young, G. The approximation of one matrix by another of lower rank. *Psychometrika 1* (1936), 211–218.

[48] Flad, H.-J., Hackbusch, W., Khoromskij, B. N., and Schneider, R. *Matrix Methods: Theory, Algorithms and Applications.* World Scientific, 2010, ch. Concepts of Data-Sparse Tensor-Product Approximation in Many-Particle Modelling, pp. 313–347.

[49] Flad, H.-J., Hackbusch, W., Kolb, D., and Schneider, R. Wavelet approximation of correlated wave functions. I. Basics. *Journal of Chemical Physics 116*, 22 (2002), 9641–9657.

[50] Flad, H.-J., Hackbusch, W., and Schneider, R. Best N-term approximation in electronic structure calculations I. One-electron reduced density matrix. *ESAIM Mathematical Modelling and Numerical Analysis 40*, 1 (2006), 49.

[51] Flad, H.-J., Hackbusch, W., and Schneider, R. Best N-term approximation in electronic structure calculations. II. Jastrow factors. *ESAIM Mathematical Modelling and Numerical Analysis 41*, 2 (2007), 261.

[52] Flad, H.-J., and Schneider, R. s^*-compressibility of the discrete Hartree-Fock equation. *ESAIM: Mathematical Modelling and Numerical Analysis 46*, 05 (2012), 1055–1080.

[53] Fournais, S., Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T., and Østergaard Sørensen, T. Sharp regularity results for many-electron wave functions. *Communications in Mathematical Physics 255* (2005), 183–227.

[54] Fournais, S., Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T., and Østergaard Sørensen, T. Analytic structure of many-body Coulombic wave functions. *Communications in Mathematical Physics 289*, 1 (2009), 291–310.

[55] Frigo, M., and Johnson, S. G. The design and implementation of FFTW3. *Proceedings of the IEEE 93*, 2 (2005), 216–231. Special issue on "Program Generation, Optimization, and Platform Adaptation".

[56] Gantumur, T. An optimal adaptive wavelet method for nonsymmetric and indefinite elliptic problems. *Journal of Computational and Applied Mathematics 211*, 1 (2008), 90–102.

[57] Gantumur, T., Harbrecht, H., and Stevenson, R. An optimal adaptive wavelet method without coarsening of the iterands. *Mathematics of Computation 76*, 258 (2007), 615–629.

[58] Gantumur, T., and Stevenson, R. P. Computation of singular integral operators in wavelet coordinates. *Computing 76*, 1 (2006), 77–107.

[59] Gavrilyuk, I. P., Hackbusch, W., and Khoromskij, B. N. Data-sparse approximation to a class of operator-valued functions. *Mathematics of Computation 74*, 250 (2004), 681–708.

[60] Genovese, L., Deutsch, T., Neelov, A., Goedecker, S., and Beylkin, G. Efficient solution of Poisson's equation with free boundary conditions. *Journal of Chemical Physics 125*, 7 (2006), 074105.

[61] Gilbarg, D., and Trudinger, N. S. *Elliptic Partial Differential Equations of Second Order*. Classics in Mathematics. Springer Berlin Heidelberg, 1998.

[62] Grafakos, L. *Classical Fourier Analysis*, second ed. Graduate Texts in Mathematics. Springer, 2008.

[63] Grasedyck, L. Existence and computation of low Kronecker-rank approximations for large linear systems of tensor product structure. *Computing 72* (2004), 247–265.

[64] Grasedyck, L. Hierarchical singular value decomposition of tensors. *SIAM J. Matrix Anal. Appl. 31*, 4 (2010), 2029–2054.

[65] Griebel, M., and Hamaekers, J. A wavelet based sparse grid method for the electronic Schrödinger equation. In *Proceedings of the International Congress of Mathematicians* (Madrid, Spain, 2006), M. Sanz-Solé, J. Soria, J. Varona, and J. Verdera, Eds., vol. III, pp. 1473–1506.

[66] Griebel, M., and Hamaekers, J. Tensor product multiscale many-particle spaces with finite-order weights for the electronic Schrödinger equation. *Zeitschrift für Physikalische Chemie 224* (2010), 527–543.

[67] Griebel, M., and Harbrecht, H. Approximation of two-variate functions: Singular value decomposition versus regular sparse grids. INS preprint, Universität Bonn, 2011. No. 1109.

[68] Griebel, M., and Knapek, S. Optimized tensor-product approximation spaces. *Constructive Approximation 16*, 4 (2000), 525.

[69] Griebel, M., and Oswald, P. Tensor product type subspace splittings and multilevel iterative methods for anisotropic problems. *Advances in Computational Mathematics 4* (1995), 171–206.

[70] Hackbusch, W. Entwicklungen nach Exponentialsummen. Tech. Rep. 4, MPI Leipzig, 2005.

[71] Hackbusch, W. *Hierarchische Matrizen: Algorithmen und Analysis.* Springer, 2009.

[72] Hackbusch, W. *Tensor Spaces and Numerical Tensor Calculus*, vol. 42 of *Springer Series in Computational Mathematics.* Springer-Verlag Berlin Heidelberg, 2012.

[73] Hackbusch, W., and Khoromskij, B. N. Hierarchical Kronecker tensor-product approximation to a class of nonlocal operators in high dimensions. Preprint 48, MPI Leipzig, 2004.

[74] Hackbusch, W., Khoromskij, B. N., Sauter, S., and Tyrtyshnikov, E. Use of tensor formats in elliptic eigenvalue problems. *Numerical Linear Algebra with Applications 19*, 1 (2012), 133–151.

[75] Hackbusch, W., and Kühn, S. A new scheme for the tensor representation. *Journal of Fourier Analysis and Applications 15*, 5 (2009), 706–722.

[76] Hamaekers, J. *Tensor Product Multiscale Many–Particle Spaces with Finite–Order Weights for the Electronic Schödinger Equation.* PhD thesis, Universität Bonn, 2009.

[77] Hansen, M. *Nonlinear Approximation and Function Spaces of Domination Mixed Smoothness.* PhD thesis, Universität Jena, 2010.

[78] Harbrecht, H., Schneider, R., and Schwab, C. Multilevel frames for sparse tensor product spaces. *Numerische Mathematik 110*, 2 (2008), 199–220.

[79] Harrison, R. J., Fann, G. I., Yanai, T., Gan, Z., and Beylkin, G. Multiresolution quantum chemistry: Basic theory and initial applications. *Journal of Chemical Physics 121*, 23 (2004), 11587–11598.

[80] Hille, E. A class of reciprocal functions. *The Annals of Mathematics 27*, 4 (1926), 427–464.

[81] Hirschfelder, J. O. Removal of electron-electron poles from many-electron Hamiltonians. *Journal of Chemical Physics 39*, 11 (1963), 3145–3146.

[82] Holtz, S., Rohwedder, T., and Schneider, R. The alternating linear scheme for tensor optimization in the tensor train format. *SIAM Journal on Scientific Computing 34*, 2 (2012), A683–A713.

[83] Hörmander, L. *Linear Partial Differential Operators*, third ed., vol. 116 of *Grundlehren der mathematischen Wissenschaften.* Springer-Verlag, Berlin, 116.

[84] Hylleraas, E. Über den Grundzustand des Heliumatoms. *Z. Phys. 48* (1929), 469.

[85] Johnson, B. R., Modisette, J. P., Nordlander, P. J., and Kinsey, J. L. Quadrature integration for orthogonal wavelet systems. *The Journal of Chemical Physics 110*, 17 (1999), 8309–8317.

[86] Kato, T. Fundamental properties of Hamiltonian operators of Schrödinger type. *Trans. Amer. Math. Soc. 70* (1951), 195–211.

[87] Kato, T. On the existence of solutions of the Helium wave equation. *Trans. Amer. Math. Soc. 70* (1951), 212–218.

[88] Kato, T. On the eigenfunctions of many-particle systems in quantum mechanics. *Comm. Pure Appl. Math. X* (1957), 151–177.

[89] Kato, T. *Perturbation Theory for Linear Operators*, second ed., vol. 132 of *Grundlehren der mathematischen Wissenschaften.* Springer-Verlag, Berlin Heidelberg New York, 1976.

[90] Kestler, S., and Urban, K. Adaptive wavelet methods on unbounded domains. *Journal of Scientific Computing* (2012).

[91] Kestner, N. R., and Sinanoğlu, O. Study of electron correlation in Helium-like systems using an exactly soluble model. *Phys. Rev. 128*, 6 (1962), 2687–2692.

[92] Khoromskij, B. On tensor approximation of Green iterations for Kohn-Sham equations. *Computing and Visualization in Science 11*, 4 (2008), 259–271.

[93] Khoromskij, B. Tensor-structured preconditioners and approximate inverse of elliptic operators in $\mathbb{R}^d$. *Constructive Approximation 30*, 3 (2009), 599–620.

[94] Khoromskij, B., Khoromskaia, V., Chinnamsetty, S., and Flad, H.-J. Tensor decomposition in electronic structure calculations on 3D Cartesian grids. *Journal of Computational Physics 228*, 16 (2009), 5749—5762.

[95] Khoromskij, B. N., Khoromskaia, V., and Flad, H. J. Numerical solution of the Hartree-Fock equation in multilevel tensor-structured format. *SIAM J. Sci. Comp. 33*, 1 (2011), 45–65.

[96] Khoromskij, B. N., and Schwab, C. Tensor-structured Galerkin approximation of parametric and stochastic elliptic PDEs. *SIAM J. Sci. Comput. 33*, 1 (2011), 364–385.

[97] King, F. W., Quicker, D., and Langer, J. Compact wave functions for the Beryllium isoelectronic series, Li^- to Ne^{6+}: A standard Hylleraas approach. *The Journal of Chemical Physics 134*, 12 (2011), 124114.

[98] Klopper, W. R12 methods, Gaussian geminals. In *Modern Methods and Algorithms of Quantum Chemistry* (Jülich, 2000), J. Grotendorst, Ed., pp. 181–229.

[99] Klopper, W., and Kutzelnigg, W. Møller-Plesset calculations taking care of the correlation cusp. *Chemical Physics Letters 134*, 1 (1987), 17–22.

[100] Korobov, V. I. Nonrelativistic ionization energy for the helium ground state. *Phys. Rev. A 66*, 2 (2002), 024501.

[101] Kressner, D., and Tobler, C. Krylov subspace methods for linear systems with tensor product structure. *SIAM J. Matrix Anal. Appl. 31*, 4 (2010), 1688–1714.

[102] Kressner, D., and Tobler, C. Preconditioned low-rank methods for high-dimensional elliptic PDE eigenvalue problems. *Computational Methods in Applied Mathematics 11*, 3 (2011), 363–381.

[103] Kreusler, H.-C., and Yserentant, H. The mixed regularity of electronic wave functions in fractional order and weighted Sobolev spaces. *Numerische Mathematik 121*, 4 (2012), 781–802.

[104] Kutzelnigg, W. r_{12}-dependent terms in the wave function as closed sums of partial wave amplitudes for large ℓ. *Theor. Chim. Acta 68* (1985), 445–469.

[105] Kutzelnigg, W. Theory of the expansion of wave functions in a Gaussian basis. *International Journal of Quantum Chemistry 51*, 6 (1994), 447–463.

[106] Kutzelnigg, W., and Klopper, W. Wavefunctions with terms linear in the interelectronic coordinates to take care of the correlation cusp. I. General theory. *J. Chem. Phys. 94*, 3 (1991).

[107] Lathauwer, L. D., Moor, B. D., and Vandewalle, J. A multilinear singular value decomposition. *SIAM Journal on Matrix Analysis and Applications 21*, 4 (2000), 1253–1278.

[108] Light, W. A., and Cheney, E. W. *Approximation Theory in Tensor Product Spaces*, vol. 1169 of *Lecture Notes in Mathematics*. Springer-Verlag Berlin Heidelberg, 1985.

[109] Luo, H., Kolb, D., Flad, H.-J., Hackbusch, W., and Koprucki, T. Wavelet approximation of correlated wave functions. II. Hyperbolic wavelets and adaptive approximation schemes. *Journal of Chemical Physics 117*, 8 (2002), 3625–3638.

[110] Metselaar, A. *Handling Wavelet Expansions in Numerical Methods*. PhD thesis, University of Twente, 2002.

[111] Meyer, Y., and Coifman, R. *Wavelets: Calderon-Zygmund and multilinear operators*. Cambridge studies in advanced mathematics. Cambridge University Press, 1997.

[112] Mohlenkamp, M. J. A center-of-mass principle for the multiparticle Schrödinger equation. *Journal of Mathematical Physics 51*, 2 (2010), 022112.

[113] Mohlenkamp, M. J. Incorporating geminals into an unconstrained sum of Slater determinants. Tech. rep., 2010.

[114] Neelov, A., and Goedecker, S. An efficient numerical quadrature for the calculation of the potential energy of wavefunctions expressed in the Daubechies wavelet basis. *Journal of Computational Physics 217* (2006), 312–339.

[115] Nitsche, P.-A. *Sparse Tensor Product Approximation of Elliptic Problems*. PhD thesis, ETH Zürich, 2004.

[116] Nitsche, P.-A. Best N term approximation spaces for tensor product wavelet bases. *Constructive Approximation 24*, 1 (2006), 49.

[117] Nooijen, M., and Bartlett, R. J. Elimination of Coulombic infinities through transformation of the Hamiltonian. *Journal of Chemical Physics 109*, 19 (1998).

[118] Novak, E., and Wozniakowski, H. Approximation of infinitely differentiable multivariate functions is intractable. *Journal of Complexity 25* (2009), 398–404.

[119] Ojanen, H. Orthonormal compactly supported wavelets with optimal Sobolev regularity: Numerical results. *Applied and Computational Harmonic Analysis 10*, 1 (2001), 93.

[120] O'Neill, D. P., and Gill, P. M. W. Wave functions and two-electron probability distributions of the Hooke's-law atom and Helium. *Physical Review A 68*, 2 (2003), 022505.

[121] Oseledets, I. V. Tensor-train decomposition. *SIAM Journal on Scientific Computing 33*, 5 (2011), 2295–2317.

[122] Persson, B. J., and Taylor, P. R. Accurate quantum-chemical calculations: The use of Gaussian-type geminal functions in the treatment of electron correlation. *J. Chem. Phys. 105*, 14 (1996), 5915–5926.

[123] Prugovečki, E. *Quantum mechanics in Hilbert space*, vol. 41 of *Pure and Applied Mathematics*. Academic Press, 1971.

[124] Reed, M., and Simon, B. *Methods of Modern Mathematical Physics, I: Functional Analysis*. Academic Press, New York, 1972.

[125] Reed, M., and Simon, B. *Methods of Modern Mathematical Physics, II: Fourier Analysis, Self-Adjointness*. Academic Press, New York, 1975.

[126] Reed, M., and Simon, B. *Methods of Modern Mathematical Physics, IV: Analysis of Operators.* Academic Press, 1978.

[127] Rohwedder, T., Schneider, R., and Zeiser, A. Perturbed preconditioned inverse iteration for operator eigenvalue problems with applications to adaptive wavelet discretization. *Advances in Computational Mathematics 34*, 1 (2011), 43–66.

[128] Samson, C. C., Klopper, W., and Helgaker, T. Computation of two-electron Gaussian integrals for wave functions including the correlation factor $r_{12} \exp(-\gamma r_{12}^2)$. *Computer Physics Communications 149*, 1 (2002), 1–10.

[129] Schwab, C., and Stevenson, R. Adaptive wavelet algorithms for elliptic PDE's on product domains. *Mathematics of Computation 77* (2008), 71–92.

[130] Schwab, C., and Todor, R. A. Sparse finite elements for stochastic elliptic problems – higher order moments. *Computing 71*, 1 (2003), 43–63.

[131] Sickel, W., and Ullrich, T. Tensor products of Sobolev-Besov spaces and applications to approximation from the hyperbolic cross. *Journal of Approximation Theory 161*, 2 (2009), 748–786.

[132] Singer, K. The use of Gaussian (exponential quadratic) wave functions in molecular problems. I. general formulae for the evaluation of integrals. *Proc. R. Soc. London, Ser. A 258* (1960), 412–420.

[133] Smolyak, S. Quadrature and interpolation formulas for tensor products of certain classes of functions. *Dokl. Akad. Nauk SSSR 4* (1963), 240–243.

[134] Stenger, F. *Numerical Methods Based on Sinc and Analytic Functions*, vol. 20 of *Springer Series in Computational Mathematics.* Springer-Verlag, 1993.

[135] Stevenson, R. On the compressibility of operators in wavelet coordinates. *SIAM Journal on Mathematical Analysis 35*, 5 (2004), 1110–1132.

[136] Sweldens, W. The lifting scheme: A custom-design construction of biorthogonal wavelets. *Applied and Computational Harmonic Analysis 3*, 2 (1996), 186–200.

[137] Sweldens, W., and Piessens, R. Quadrature formulae and asymptotic error expansions for wavelet approximations of smooth functions. *SIAM Journal on Numerical Analysis 31*, 4 (1994), 2140–2164.

[138] Szalewicz, K., Jeziorski, B., Monkhorst, H. J., and Zabolitzky, J. G. Atomic and molecular correlation energies with explicitly correlated Gaussian geminals. I. Second-order perturbation treatment for He, Be, H_2, and LiH. *J. Chem. Phys. 78*, 3 (1983), 1420–1430.

[139] Ten-no, S. A feasible transcorrelated method for treating electronic cusps using a frozen Gaussian geminal. *Chemical Physics Letters 330* (2000), 169–174.

[140] Tobler, C. *Low-rank tensor methods for linear systems and eigenvalue problems.* PhD thesis, ETH Zürich, 2012.

[141] Townsend, M. *Discrete Mathematics: Applied Combinatorics and Graph Theory.* The Benjamin/Cummings Publishing Company, 1987.

[142] Triebel, H. *Interpolation Theory, Function Spaces, Differential Operators*, vol. 18 of *North Holland Mathematical Library.* North Holland, 1978.

[143] Triebel, H. *Theory of Function Spaces II*, vol. 84 of *Monographs in Mathematics*. Birkhäuser Verlag, 1992.

[144] Tucker, L. R. *Contributions to Mathematical Psychology*. Holt, Rinehart & Winston, New York, 1964, ch. The extension of factor analysis to three-dimensional matrices, pp. 109–127.

[145] Tucker, L. R. Some mathematical notes on three-mode factor analysis. *Psychometrika 31* (1966), 279–311.

[146] Uschmajew, A. Regularity of tensor product approximations to square integrable functions. *Constructive Approximation 34*, 3 (2011), 371–391.

[147] Vybiral, J. *Function spaces with dominating mixed smoothness*. PhD thesis, Universität Jena, 2005.

[148] Waldvogel, J. *Approximation and Computation*, vol. 42 of *Optimization and Its Applications*. Springer-Verlag, 2011, ch. Towards a general error theory of the trapezoidal rule.

[149] Weidmann, J. *Linear Operators in Hilbert spaces*, vol. 68 of *Graduate Texts in Mathematics*. Springer-Verlag, 1980.

[150] Yserentant, H. On the regularity of the electronic Schrödinger equation in Hilbert spaces of mixed derivatives. *Numerische Mathematik 98* (2004), 731–759.

[151] Yserentant, H. The hyperbolic cross space approximation of electronic wavefunctions. *Numerische Mathematik 105*, 4 (2007), 659–690.

[152] Yserentant, H. *Regularity and Approximability of Electronic Wave Functions*, vol. 2000 of *Lecture Notes in Mathematics*. Springer Berlin Heidelberg, 2010.

[153] Yserentant, H. The mixed regularity of electronic wave functions multiplied by explicit correlation factors. *ESAIM: Mathematical Modelling and Numerical Analysis 45*, 05 (2011), 803–824.

[154] Zeiser, A. *Direkte Diskretisierung der Schrödingergleichung auf dünnen Gittern*. PhD thesis, TU Berlin, 2010.

[155] Zeiser, A. Fast matrix-vector multiplication in the sparse-grid Galerkin method. *Journal of Scientific Computing 47*, 3 (2010), 328–346.

[156] Zeiser, A. On the optimality of the inexact inverse iteration coupled with adaptive finite element methods. Tech. rep., 2010. DFG SPP 1324 Preprint 57.

[157] Zeiser, A. Wavelet approximation in weighted Sobolev spaces of mixed order with applications to the electronic Schrödinger equation. *Constructive Approximation 35*, 3 (2012), 293–322.

[158] Zenger, C. Sparse grids. In *Parallel Algorithms for Partial differential Equations: Proceedings of the Sixth GAMM-Seminar* (Kiel, 1990), W. Hackbusch, Ed.

[159] Zweistra, H. J. A., Samson, C. C. M., and Klopper, W. Similarity-transformed Hamiltonians by means of Gaussian-damped interelectronic distances. *Collection of Czechoslovak Chemical Communications 68*, 2 (2003), 374–386.

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