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Abstract

In this work, we consider a scheme for the computation of integrals of Gaussian functions with products of wavelets, which is applicable to wavelet bases given only implicitly in terms of refinement relations. The integrals under consideration arise in wavelet discretizations of operator equations involving separable approximations of Coulomb potentials. Motivated by this application, we study in particular the case of large exponents in the Gaussian terms. The numerical tests demonstrate the practical efficiency of the method.

1 Introduction

Let $\{\psi_\nu\}_{\nu\in\nabla}$, with ∇ a suitable index set, be a basis of compactly supported wavelets for $L_2(\mathbb{R})$. In what follows, we consider algorithms for evaluating integrals of the form

$$\int_{\mathbb{R}} e^{-\alpha x^2}\,\psi_{\nu_1}\,\psi_{\mu_1}\,dx \tag{1}$$

$$\int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\,(\psi_{\nu_1}\otimes\psi_{\nu_2})\,(\psi_{\mu_1}\otimes\psi_{\mu_2})\,dx\,, \tag{2}$$

where $\nu_1,\mu_1,\nu_2,\mu_2\in\nabla$, with a possibly large parameter $\alpha>0$. Integrals of the type (1), (2) arise in particular in wavelet discretizations of Schrödinger-type operators involving approximations of Coulomb potentials by sums of separable functions, for instance,

$$\frac{1}{|x|}\approx\sum_k \omega_k e^{-\alpha_k|x|^2}\,,\qquad \frac{1}{|x-y|}\approx\sum_k \omega_k e^{-\alpha_k|x-y|^2}\,,\qquad x,y\in\mathbb{R}^3\,, \tag{3}$$

where the largest ω_k and α_k tend to infinity for increasing accuracy of the approximations in (3).

In this work, we consider an integration scheme based on a representation of the integrals (1) and (2) in terms of Fourier transforms. With the Fourier transform of f defined by $(\mathcal{F}f)(\xi):=(\sqrt{2\pi})^{-\frac{1}{2}}\int f(x)e^{-ix\xi}\,dx$, as a straightforward consequence of the Plancherel and convolution theorems one obtains the identities

$$\int_{\mathbb{R}} e^{-\alpha x^2}\,\psi_\nu(x)\,\psi_\mu(x)\,dx=(2\alpha)^{-\frac{1}{2}}\int_{\mathbb{R}} e^{-\xi^2/(4\alpha)}\mathcal{F}\big(\psi_\nu\,\psi_\mu\big)(\xi)\,d\xi \tag{4}$$

as well as

$$\int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\,\psi_{\nu_1}(x_1)\,\psi_{\nu_2}(x_2)\,\psi_{\mu_1}(x_1)\,\psi_{\mu_2}(x_2)\,dx=\sqrt{\frac{\pi}{\alpha}}\int_{\mathbb{R}} e^{-\xi^2/(4\alpha)}\overline{\mathcal{F}\big(\psi_{\nu_1}\,\psi_{\mu_1}\big)(\xi)}\,\mathcal{F}\big(\psi_{\nu_2}\,\psi_{\mu_2}\big)(\xi)\,d\xi\,. \tag{5}$$

As a consequence of the analyticity properties of the integrands on the right hand sides, the trapezoidal rule is suitable for approximating these one-dimensional integrals. We give a convergence analysis based on sinc theory [22] for this quadrature and propose a procedure for numerically evaluating the arising Fourier transforms of products of wavelets. The resulting quadrature scheme is in principle applicable to any compactly supported wavelet basis, although in the case of large exponents α it is more efficient for wavelets of higher regularity. An

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interesting feature of the method, particularly in comparison to existing other approaches that do not impose further structural restrictions on the wavelets, is that integrals corresponding to different wavelet indices can be evaluated essentially independently of each other, but many quantities required in the evaluation of the integrands can still be precomputed.

It should be noted that the proposed integration scheme and its error analysis can in principle be adapted to substantially more general coefficient functions than Gaussians, provided that they have suitable decay and smoothness and that their Fourier transforms are available, but as we are especially interested in the asymptotic dependence on the exponent α in the Gaussian terms, we restrict ourselves to this case. We shall, however, additionally consider slightly modified integrals: In the transcorrelated formulation [2] of the electronic Schrödinger equation (see also [1]), using a separable approximation similar to (3) of a modified potential term of the form $(x-y)/|x-y|\cdot(\mathrm{grad}_x - \mathrm{grad}_y)$, one needs to deal with integrals of the form

$$\int (x_1 - x_2) e^{-\alpha(x_1-x_2)^2} \big[(\partial_{x_1} - \partial_{x_2})(\psi_{\nu_1} \otimes \psi_{\nu_2})\big](\psi_{\mu_1} \otimes \psi_{\mu_2})\, dx\,. \tag{6}$$

We will treat this case alongside (1) and (2) in this work; for (6), one has the identity

$$\begin{aligned}\int_{\mathbb{R}^2} (x_1 - x_2) e^{-\alpha(x_1-x_2)^2} \big[(\partial_{x_1} - \partial_{x_2})\psi_{\nu_1}(x_1)\,\psi_{\nu_2}(x_2)\big]\psi_{\mu_1}(x_1)\,\psi_{\mu_2}(x_2)\, dx \\ = -\frac{i}{2}\sqrt{\frac{\pi}{\alpha^3}} \int_{\mathbb{R}} \xi e^{-\xi^2/(4\alpha)} \Big(\overline{\mathcal{F}\big(\psi'_{\nu_1}\,\psi_{\mu_1}\big)(\xi)}\,\mathcal{F}\big(\psi_{\nu_2}\,\psi_{\mu_2}\big)(\xi) \\ - \overline{\mathcal{F}\big(\psi_{\nu_1}\,\psi_{\mu_1}\big)(\xi)}\,\mathcal{F}\big(\psi'_{\nu_2}\,\psi_{\mu_2}\big)(\xi)\Big)\, d\xi\,.\end{aligned} \tag{7}$$

On the basis of this representation, one can proceed similarly as for (4) and (5).

Before turning to the description and analysis of the integration scheme that is the subject of this work, we discuss some preliminaries in the remainder of this section. In Subsection 1.1, we state some notational conventions and specify the types of quadrature error estimates that are relevant for the applications of interest. In Subsection 1.2, we briefly review a straightforward quadrature scheme that has been used previously in a similar form by other authors. As our considerations will show, this approach already allows a satisfactory treatement of the one-dimensional integrals (1). However, it becomes too expensive for practical purposes in the case of the two-dimensional integrals (2), which serves as a motivation for the developments in this work. Relations to known schemes are discussed in Subsection 1.3.

In Section 2, an error analysis of the trapezoidal rule applied to the Fourier representations (4), (5), and (7) is given. A recursion-based scheme for evaluation of the arising Fourier transforms of products of wavelets, which does not require further quadrature, will be the subject of Section 3. In Section 4, we describe a practical implementation and demonstrate the efficiency of the resulting scheme in numerical experiments.

1.1 Notation and Relevant Types of Error Estimates

Our precise assumptions and notations for wavelet bases are as follows: Let φ and ψ be the scaling function and mother wavelet, respectively, of a compactly supported wavelet basis of $L_2(\mathbb{R})$, where one case of particular interest are the orthonormal Daubechies wavelets [5]. Defining the uniform notation

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

with the index set $\nabla := \{\nu = (j_0, k, 0)\colon k \in \mathbb{Z}\} \cup \{\nu = (j,k,1)\colon j,k \in \mathbb{Z}, j \geq j_0\}$ with a $j_0 \in \mathbb{Z}$, we have that $\{\psi_\nu\}_{\nu\in\nabla}$ is a basis for $L_2(\mathbb{R})$ that comprises scaling functions on level j_0 and wavelets on all levels greater or equal to j_0. For $\nu = (j,k,s) \in \nabla$ we shall use the notations

$$|\nu| := j\,, \quad \mathrm{k}(\nu) := k\,, \quad \mathrm{s}(\nu) := s\,.$$

The schemes considered here use the wavelet basis only implicitly via the compactly supported coefficient sequences $(h_k)_{k\in\mathbb{Z}}$ and $(g_k)_{k\in\mathbb{Z}}$ in the refinement equations

$$\varphi = \sqrt{2}\sum_k h_k\,\varphi(2\cdot - k)\,, \qquad \psi = \sqrt{2}\sum_k g_k\,\varphi(2\cdot - k)\,. \tag{8}$$

In principle, these relations can be used to approximate point values of the wavelets via the cascade algorithm (see, e.g., [6]), 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 any point evaluations in what follows.

Our integration error estimates will be specifically adapted to the application to separable approximations of Coulomb potentials as in (3). The two approaches for obtaining such approximations that we have in mind here are on the one hand best approximations by exponential sums as analyzed, e.g., in [3] and computed numerically in [15], and on the other hand constructions based on sinc approximation as considered in [17; 16]. Although the asymptotic convergence properties are quite similar, the former yields quantitatively better approximations that are preferable in practice. The latter, however, has the advantage of providing estimates for the size of the corresponding coefficients: in particular, it can be shown that $\omega_k \lesssim \sqrt{\alpha_k}$. We shall assume such an estimate to hold in our error analysis. Taking this scaling into account, for the application in (3) we need to estimate quadrature errors for the scaled integrals

$$\sqrt{\alpha}\int_{\mathbb{R}} e^{-\alpha x^2}\,\psi_{\nu_1}\,\psi_{\mu_1}\,dx\,, \quad \sqrt{\alpha}\int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\,(\psi_{\nu_1}\otimes\psi_{\nu_2})\,(\psi_{\mu_1}\otimes\psi_{\mu_2})\,dx\,. \tag{9}$$

For applications to Schrödinger-type equations, the potentials approximated in (3) 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 available for this setting [1], one finds that an error $\varepsilon_0 > 0$ in the approximation (3), with respect to the norm $\|\cdot\|_{H^1\to H^{-1}}$, requires a separable expansion with $\max_k \alpha_k \sim \varepsilon_0^{-2}$.

Note that provided $\varphi \in H^{1+\varepsilon}(\mathbb{R})$ for some $\varepsilon > 0$, we have that $\{2^{-|\nu|}\psi_\nu\}_{\nu\in\nabla}$ is a Riesz basis of $H^1(\mathbb{R})$, 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 $H^1(\mathbb{R}^2)$; see, e.g., [14; 8]. As a consequence, one finds that in order to ensure a certain accuracy in the full separable representations (3) in operator norm $H^1 \to H^{-1}$, it suffices to control the quadrature error in the rescaled matrices

$$\begin{gathered} 2^{-|\nu_1|-|\mu_1|}\sqrt{\alpha}\int_{\mathbb{R}} e^{-\alpha x^2}\,\psi_{\nu_1}\,\psi_{\mu_1}\,dx\,, \\ (2^{2|\nu_1|}+2^{2|\nu_2|})^{-\frac12}(2^{2|\mu_1|}+2^{2|\mu_2|})^{-\frac12}\sqrt{\alpha}\int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\,(\psi_{\nu_1}\otimes\psi_{\nu_2})\,(\psi_{\mu_1}\otimes\psi_{\mu_2})\,dx\,. \end{gathered} \tag{10}$$

In other words, integrals corresponding to higher wavelet levels in general 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 (9) instead. We shall, however, make use of the practically relevant rescaling (10) in our numerical tests in Section 4.

1.2 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 a scheme is too expensive in the case of the two-dimensional integrals (2), it serves as a reference in our numerical tests in Section 4.

For the following discussion, we assume θ, $\tilde\theta$ to be compactly supported, biorthogonal scaling functions. Consequently, (1) and (2) can be approximated by expansions[1]

$$\sum_{k\in\mathbb{Z}}\int \sqrt{\alpha}\,e^{-\alpha x^2}\tilde\theta_{J_1,k}(x)\,dx\int_{\mathbb{R}}\theta_{J_1,k}\,\psi_\nu\,\psi_\mu\,dx\,, \tag{11}$$

$$\sum_{k\in\mathbb{Z}^2}\int \sqrt{\alpha}\,e^{-\alpha(x_1-x_2)^2}\tilde\theta_{J_2,k_1}\otimes\tilde\theta_{J_2,k_2}\,dx\int_{\mathbb{R}}\theta_{J_2,k_1}\,\psi_{\nu_1}\,\psi_{\mu_1}\,dx\int_{\mathbb{R}}\theta_{J_2,k_2}\,\psi_{\nu_2}\,\psi_{\mu_2}\,dx\,, \tag{12}$$

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 [4], and has been used similarly to our present setting in [9]. The advantage of such an expansion is that all arising coefficients can be evaluated only on the basis of the refinement relations (8); 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 (1), (2) by the expansions (11), (12), 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.

Proposition 1. *Let θ and $\tilde\theta$ have orders of polynomial reproduction $p-1$ and $\tilde p-1$, respectively, let $\varphi, \psi \in C^\tau(\mathbb{R})$ 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*

$$J_1 \geq \min\Big\{\tfrac1p\log_2\varepsilon^{-1} + \tfrac12\big(1+\tfrac1p\big)\log_2\alpha,\ \tfrac1q\log_2\varepsilon^{-1} + \max\{|\nu_1|,|\mu_1|\} + \tfrac{1}{2q}(|\nu_1|+|\mu_1|)\Big\}$$

[1] One could also consider wavelet expansions instead, but since the functions under consideration do not have isolated singularities, there is no gain compared to the expansion in scaling functions to be expected in our present setting.

and

$$\mathcal{K}^{(1)}_{J_1,\varepsilon} := \Big\{k \in \mathbb{Z}\colon\ |x| \le \alpha^{-\frac12}|\ln\varepsilon|^{\frac12}\ \ \textit{for all } x \in \operatorname{supp}\tilde\theta_{J_1,k}\Big\}\,,$$

we have

$$\Big|\int_{\mathbb{R}} e^{-\alpha x^2}\,\psi_{\nu_1}\,\psi_{\mu_1}\,dx - \sum_{k\in\mathcal{K}^{(1)}_{J_1,\varepsilon}} \int \sqrt{\alpha}e^{-\alpha x^2}\tilde\theta_{J_1,k_1}\,dx \int_{\mathbb{R}} \theta_{J_1,k_1}\,\psi_{\nu_1}\,\psi_{\mu_1}\,dx\Big| \le C_1\varepsilon\,,$$

and for $J_2 \in \mathbb{Z}$ such that

$$J_2 \ge \min\Big\{\tfrac1p\log_2\varepsilon^{-1} + \tfrac12\big(1+\tfrac1p\big)\log_2\alpha,\ \tfrac1q\log_2\varepsilon^{-1} + \max\{|\nu_1|,|\mu_1|,|\nu_2|,|\mu_2|\} + \tfrac{1}{2q}(|\nu_1|+|\mu_1|+|\nu_2|+|\mu_2|)\Big\} \quad (13)$$

and

$$\mathcal{K}^{(2)}_{J_2,\varepsilon} := \Big\{k \in \mathbb{Z}^2\colon\ |x_1-x_2| \le \alpha^{-\frac12}(\max\{\tfrac14,\ln\varepsilon^{-1}\})^{\frac12}\ \ \textit{for all } (x_1,x_2) \in \operatorname{supp}\tilde\theta_{J_2,k_1}\otimes\tilde\theta_{J_2,k_2}\Big\}\,,$$

we have

$$\Big|\int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\,(\psi_{\nu_1}\otimes\psi_{\nu_2})\,(\psi_{\mu_1}\otimes\psi_{\mu_2})\,dx - \sum_{k\in\mathcal{K}_{J_2,\varepsilon}} \int \sqrt{\alpha}e^{-\alpha(x_1-x_2)^2}\tilde\theta_{J_2,k_1}\otimes\tilde\theta_{J_2,k_2}\,dx \int_{\mathbb{R}} \theta_{J_2,k_1}\,\psi_{\nu_1}\,\psi_{\mu_1}\,dx \int_{\mathbb{R}} \theta_{J_2,k_2}\,\psi_{\nu_2}\,\psi_{\mu_2}\,dx\Big| \le C_2\varepsilon\,.$$

We next 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 $j_{\mathrm{sum}} = |\nu_1|+|\mu_1|+|\nu_2|+|\mu_2|$. The number of coefficients to be summed over for each integral can be estimated, up to a constant, by

$$\begin{aligned}2^{J-j_{\max}}\max\big\{1,2^{J-j_{\min}}\big(\alpha^{-1}\ln\varepsilon^{-1}\big)^{\frac12}\big\} &\lesssim \min\big\{\varepsilon^{-\frac1p}\alpha^{\frac12(1+p^{-1})}2^{-j_{\max}}\max\{1,\varepsilon^{-\frac1p}\alpha^{\frac{1}{2p}}2^{-j_{\min}}(\ln\varepsilon^{-1})^{\frac12}\}\,,\\ &\qquad \varepsilon^{-\frac1q}2^{\frac{1}{2q}j_{\mathrm{sum}}}\max\{1,\varepsilon^{-\frac1q}2^{\frac{1}{2q}j_{\mathrm{sum}}}2^{j_{\max}-j_{\min}}\alpha^{-\frac12}(\ln\varepsilon^{-1})^{\frac12}\}\big\}\,. \quad (14)\end{aligned}$$

The number of triple products that are required for this single integral is of order

$$\begin{aligned}\max\{1,||\mu_1|-|\nu_1||,||\mu_2|-|\nu_2||\}\ 2^{J-j_{\min}} &\lesssim \max\{1,||\mu_1|-|\nu_1||,||\mu_2|-|\nu_2||\}\\ &\quad\times\min\big\{\varepsilon^{-\frac1p}\alpha^{\frac12(1+p^{-1})}2^{-j_{\min}}\,,\ \varepsilon^{-\frac1q}2^{\frac{1}{2q}j_{\mathrm{sum}}}2^{j_{\max}-j_{\min}}\big\}\,. \quad (15)\end{aligned}$$

The total number of different triple products required for *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,

$$\mathcal{O}\big(\max\{1,||\mu_1|-|\nu_1||,||\mu_2|-|\nu_2||\}\ \min\{\varepsilon^{-\frac1p}\alpha^{\frac12(1+p^{-1})}\,,\varepsilon^{-\frac1q}2^{\frac{1}{2q}(|\nu_1|+|\mu_1|+|\nu_2|+|\mu_2|)}2^{\max\{|\nu_1|,|\mu_1|,|\nu_2|,|\mu_2|\}}\}\big)\,.$$

In the case of the expansion (11) for the one-dimensional integrals (1), 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

$$\mathcal{O}\big(\max\big\{1,\min\{\varepsilon^{-\frac1p}\alpha^{\frac12(1+p)},\varepsilon^{-\frac1q}2^{\max\{|\mu_1|,|\nu_1|\}}2^{\frac{1}{2q}(|\mu_1|+|\nu_1|)}\}\min\{2^{-\max\{|\mu_1|,|\nu_1|\}},\alpha^{-\frac12}|\ln\varepsilon|^{\frac12}\}\big\}\big)\,. \quad (16)$$

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

$$\mathcal{O}\big(\max\big\{1,\min\{\varepsilon^{-\frac1p}\alpha^{\frac{1}{2p}},\varepsilon^{-\frac1q}2^{\frac{1}{2q}(|\mu_1|+|\nu_1|)}2^{\max\{|\mu_1|,|\nu_1|\}}\alpha^{-\frac12}\}|\ln\varepsilon|^{\frac12}\big\}\big)\,. \quad (17)$$

Remark 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* (14), (16) *for $|\nu_1| = |\mu_1| = |\nu_2| = |\mu_2| = 0$. To this end, we make the typical assumptions $p > q$, $q \ge 2$, 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 (2), *in* (12) *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* (1), *$\mathcal{O}(\varepsilon^{-(p+1)^{-1}(1+q^{-1})})$ coefficients are required in* (11).

In summary, in the case of the one-dimensional integrals (1) it can be seen from (16) and (17) 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 (2), 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 (15), 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 one- and two-dimensional integrals is essentially the following: In the one-dimensional case, for large α the Gaussian coefficients are concentrated at a point, and therefore only triple products with basis functions having support close to this point are actually needed; 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.

We finally come to the numerical evaluation of the coefficients in the expansions (11), (12). 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 and ψ.

The arising integrals over triple products can be evaluated by computing $\int \theta_{0,k}\, \varphi_{0,l}\, \varphi \, dx$ from a constrained eigenvalue problem derived from the scaling relations (8), and recursively applying the scaling relations to reduce all further integrals to this case, cf. [4].

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

$$\int x^n \tilde{\theta}\, dx = 0\,, \quad 0 < n < p\,. \tag{18}$$

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 $s \le p$ we have

$$\left| \int_{\mathbb{R}} f\, \tilde{\theta}_{\tilde{J},k}\, dx - 2^{-\tilde{J}/2} f(2^{-\tilde{J}}k) \right| \lesssim 2^{-s\tilde{J}} |f|_{C^s}\,, \quad \tilde{J} \in \mathbb{Z}\,.$$

The property (18) is satisfied, for instance, by Coiflets [6] and by Deslaurier-Dubuc-Sweldens wavelets [7; 23]. For the error in the coefficients, using Taylor expansion, (18), and the same estimate as in (39), we thus obtain

$$\left| \int \sqrt{\alpha} e^{-\alpha(x_1-x_2)^2} \tilde{\theta}_{\tilde{J},k_1}(x_1)\, \tilde{\theta}_{\tilde{J},k_2}(x_2)\, dx - 2^{-\tilde{J}} \sqrt{\alpha} e^{-\alpha 2^{-2\tilde{J}}(k_1-k_2)^2} \right| \lesssim 2^{-p\tilde{J}} \alpha^{\frac{1}{2}(1+p)}\,,$$

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 (13), it may be necessary to choose $\tilde{J} > J_2$ and subsequently obtain the coefficients of the Gaussian term on level J_2 by downsampling.

In summary, we may conclude that for the one-dimensional integrals (1), the approach considered above yields a potentially quite efficient method. However, it becomes unacceptably expensive for the two-dimensional integrals as in (2) or (6). As we shall see, with the proposed scheme based on integration in Fourier domain, substantially better complexity can be obtained for the two-dimensional integrals; in particular, one obtains a comparably negligible memory overhead.

For the one-dimensional integrals, if a large p is used, the scheme discussed above will in general be asymptotically advantageous over the scheme proposed in this work. However, with the alternative scheme that we consider in the next section, individual integrals for different wavelet coefficients can be computed largely independently of each other. This is in contrast to the rather tightly coupled evaluation of triple products by recursions required by the approach considered above.

1.3 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 [24] and [19]. In this approach, the wavelets are treated as weight functions. It is, however, 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 (2).

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 [20] 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 [9], 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 (1), (2) in a computational scheme. The quadrature developed in [9] 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 (9), and subsequently an approach via Fourier transforms based on identities similar to (4) and (5) 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 (4) and (5) concerning the representation in terms of Fourier transforms of related integrals can also be found in [13] 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 somewhat different in that we consider potentials approximated by Gaussians, leading to one- or two-dimensional factors whose Fourier transforms are again of Gaussian type. The Fourier transforms of the compactly supported wavelets under consideration here in general do not have a closed-form representation, but the resulting combined integrands in Fourier domain are analytic functions.

For piecewise polynomial wavelets, the computation of integrals of the form (1), (2) has been considered in [26]. In the particular case of piecewise polynomial wavelets, the approach given there is potentially more efficient than the scheme considered here, and the method developed in this work is therefore of interest mainly in the case of wavelets that do not have this additional structure, such as Daubechies wavelets.

2 Convergence Analysis for the Trapezoidal Rule in Fourier Domain

When using compactly supported wavelets, the integrands in the transformed integrals

$$\frac{1}{\sqrt{2}}\int_{\mathbb{R}} e^{-\xi^2/(4\alpha)}\mathcal{F}\big(\psi_\nu\,\psi_\mu\big)(\xi)\,d\xi\,,\quad \sqrt{\pi}\int_{\mathbb{R}} e^{-\xi^2/(4\alpha)}\overline{\mathcal{F}\big(\psi_{\nu_1}\,\psi_{\mu_1}\big)(\xi)}\,\mathcal{F}\big(\psi_{\nu_2}\,\psi_{\mu_2}\big)(\xi)\,d\xi\,,$$

and

$$-i\frac{\sqrt{\pi}}{2\alpha}\int_{\mathbb{R}} \xi e^{-\xi^2/(4\alpha)}\Big(\overline{\mathcal{F}\big(\psi'_{\nu_1}\,\psi_{\mu_1}\big)(\xi)}\,\mathcal{F}\big(\psi_{\nu_2}\,\psi_{\mu_2}\big)(\xi) - \overline{\mathcal{F}\big(\psi_{\nu_1}\,\psi_{\mu_1}\big)(\xi)}\,\mathcal{F}\big(\psi'_{\nu_2}\,\psi_{\mu_2}\big)(\xi)\Big)\,d\xi$$

obtained by the identities (4), (5), (7), and rescaled as in (9), are restrictions to $\mathbb{R}$ of entire 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

$$\int_{\mathbb{R}} u(\xi)\,d\xi \approx h\sum_{k=-N}^{N} u(kh)\,,$$

where the error is estimated by

$$\Big|\int_{\mathbb{R}} u(\xi)\,d\xi - h\sum_{k\in\mathbb{Z}} u(kh)\Big| + \Big|h\sum_{|k|>N} u(kh)\Big|\,. \tag{19}$$

For given h, the behaviour of the second term in (19) 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 3 below 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 2. *Let $u(\xi) = (8\sqrt{\pi})^{-1}\alpha^{-(n+\frac{1}{2})}\xi^n e^{-(4\alpha)^{-1}\xi^2}\phi(\xi)$ with $\alpha>0$, $|\phi(\xi)|\le e^{\kappa|\Im\xi|}$, $\kappa>0$, and $n\in\{0,1\}$. For any $d>0$, if*

$$h = \frac{2\pi d}{\ln\delta^{-1} + n\ln(\alpha^{-1}d + 2(\pi\alpha)^{-1/2}) + (4\alpha)^{-1}d^2 + \kappa d} \tag{20}$$

for $\delta > 0$ with $\delta \le \frac{1}{2}(\alpha^{-1}d + 2(\pi\alpha)^{-1/2})^n e^{(4\alpha)^{-1}d^2+\kappa d}$, then

$$\left| \int_{\mathbb{R}} u(\xi)\, d\xi - h \sum_{k\in\mathbb{Z}} u(hk) \right| \le \delta\,.$$

Remark 2. *Note that if $n = 0$ and $\delta < 1$, then h as in (20) is maximal for the choice $d = 2(\alpha|\ln\delta|)^{\frac{1}{2}}$, and the condition on δ in Lemma 2 is ensured by $\delta \le 2^{-1/2}$. In the case $n = 1$, $\delta < 1$, with the same choice of d this condition holds for $\delta \le (\pi\alpha)^{-1/4}$.*

For the proof of Lemma 2, we take the following definition and theorem from [22].

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

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

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

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

Theorem 3 ([22], Theorem 3.2.1)**.** *Let u be analytic in $\mathcal{D}_d$ with $N_1(u, \mathcal{D}_d) < \infty$, then*

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

Proof of Lemma 2. Note first that for $\xi_1, \xi_2 \in \mathbb{R}$ such that $\xi_1 + i\xi_2 \in \mathcal{D}_d$,

$$\left|(\xi_1 + i\xi_2)^n e^{-(4\alpha)^{-1}(\xi_1+i\xi_2)^2}\right| \le (|\xi_1| + d)^n e^{-(4\alpha)^{-1}\xi_1^2} e^{(4\alpha)^{-1}d^2}\,,$$

for $n = 0, 1$, and as a consequence

$$\begin{aligned} N_1(u, \mathcal{D}_d) &\le 2(8\sqrt{\pi})^{-1}\alpha^{-\frac{1}{2}-n} e^{(4\alpha)^{-1}d^2} e^{\kappa d} \int_{\mathbb{R}} (|\xi| + d)^n e^{-(4\alpha)^{-1}\xi^2}\, d\xi \\ &= 2(8\sqrt{\pi})^{-1}\big(2\sqrt{\pi}(\alpha^{-1}d)^n + 4n\alpha^{-\frac{1}{2}}\big)\, e^{(4\alpha)^{-1}d^2} e^{\kappa d} \\ &= \tfrac{1}{2}\big(\alpha^{-1}d + 2(\pi\alpha)^{-\frac{1}{2}}\big)^n e^{(4\alpha)^{-1}d^2+\kappa d}\,, \qquad n = 0, 1\,. \end{aligned} \tag{21}$$

By Theorem 3, if $e^{-2\pi d/h} \le \frac{1}{2}$,

$$\left| \int_{\mathbb{R}} u(x)\, dx - h \sum_{k\in\mathbb{Z}} u(kh) \right| \le 2e^{-2\pi d/h} N_1(u, \mathcal{D}_d)\,, \tag{22}$$

and combining this with (21), we see that if h is chosen as in the assertion, the upper bound on the right hand side of (22) equals δ, provided that $\delta \le \frac{1}{2}(\alpha^{-1}d+2(\pi\alpha)^{-1/2})^n e^{(4\alpha)^{-1}d^2+\kappa d}$. This ensures both that $e^{-2\pi d/h} \le \frac{1}{2}$ and that the denominator in (20) is positive. □

We now return to the second error term in (19), 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 4. *Let $|u(\xi)| \le c|\xi|^n e^{-(4\alpha)^{-1}\xi^2}$ for $\xi \in \mathbb{R}$, $n \in \{0, 1\}$. Then for any $h > 0$ and $N \in \mathbb{N}$,*

$$h \sum_{|k|>N} |u(kh)| \le \begin{cases} 4c\,\alpha\,(Nh)^{-1}\, e^{-(4\alpha)^{-1}(Nh)^2}\,, & n = 0\,, \\ 8\sqrt{2}\,c\,\alpha^{3/2}\,(Nh)^{-1}\, e^{-(8\alpha)^{-1}(Nh)^2}\,, & n = 1\,. \end{cases}$$

Proof. In the case $n = 0$, proceeding similarly as in [11, Lemma 2.4], we obtain

$$h \sum_{|k|>N} |u(kh)| \le 2ch \sum_{k=N+1}^{\infty} e^{-(4\alpha)^{-1}(kh)^2} \le 2ch \int_N^{\infty} e^{-(4\alpha)^{-1}(xh)^2}\, dx$$

by monotonicity, and furthermore

$$\le 2ch \int_N^{\infty} \frac{2(4\alpha)^{-1}h^2 x}{2(4\alpha)^{-1}h^2 N} e^{-(4\alpha)^{-1}h^2x^2}\, dx = 4c\alpha(Nh)^{-1} e^{-(4\alpha)^{-1}(Nh)^2}\,.$$

For $n = 1$,

$$h \sum_{|k|>N} |u(kh)| \le 2ch \sum_{k=N+1}^{\infty} khe^{-(4\alpha)^{-1}(kh)^2} \le 2^{\frac{3}{2}} ch\alpha^{\frac{1}{2}} \sum_{k=N+1}^{\infty} e^{-(8\alpha)^{-1}(kh)^2}, \tag{23}$$

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 (23) can be estimated further by

$$2^{\frac{3}{2}} ch\alpha^{\frac{1}{2}} \int_N^{\infty} \frac{2(8\alpha)^{-1}h^2 x}{2(8\alpha)^{-1}h^2 N} e^{-(8\alpha)^{-1}(xh)^2} dx = 8\sqrt{2}\, c\, \alpha^{\frac{3}{2}} (Nh)^{-1} e^{-(8\alpha)^{-1}(Nh)^2}. \qquad \square$$

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 5. *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 $N \in \mathbb{N}$,*

$$h \sum_{|k|>N} |u(kh)| \le 2c\beta^{-1}(\kappa-1)^{-1}(1+\beta Nh)^{-(\kappa-1)}.$$

Proof. Similarly to Lemma 4, this follows with

$$h \sum_{|k|>N} |u(kh)| \le 2ch \sum_{k=N+1}^{\infty} (1+\beta kh)^{-\kappa} \le 2ch \int_N^{\infty} (1+\beta xh)^{-\kappa} dx. \qquad \square$$

For the specific integrands in which we are interested, a decay estimate as required for Lemma 5 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. *Let φ be a scaling function such that*

$$|\mathcal{F}\varphi(\xi)| \lesssim C(1+|\xi|)^{-\eta},$$

where $\eta > 1$, $C > 0$, then for the corresponding wavelet basis $\{\psi_\nu\}_{\nu\in\nabla}$ there exists $c_{\psi,\eta} > 0$ such that

$$\big|\mathcal{F}(\psi_\nu\psi_\mu)(\xi)\big| \le c_{\psi,\eta}\, 2^{\frac{1}{2}||\nu|-|\mu||} \big(1 + 2^{-\max\{|\nu|,|\mu|\}}|\xi|\big)^{-\eta}.$$

If additionally $\eta > 2$, there exists $\tilde{c}_{\psi,\eta} > 0$ with

$$\big|\mathcal{F}(\psi'_\nu\psi_\mu)(\xi)\big| \le \tilde{c}_{\psi,\eta}\, 2^{|\nu|} 2^{\frac{1}{2}||\nu|-|\mu||} \big(1 + 2^{-\max\{|\nu|,|\mu|\}}|\xi|\big)^{-(\eta-1)}.$$

Proof. Note first that $|\mathcal{F}\psi_\nu(\xi)| = 2^{-|\nu|/2}|\mathcal{F}\psi(2^{-|\nu|}\xi)| \lesssim 2^{-|\nu|/2}(1+2^{-|\nu|}|\xi|)^{-\eta}$. It thus remains to estimate

$$\big|\mathcal{F}(\psi_\nu\psi_\mu)(\xi)\big| = \frac{\big|(\mathcal{F}\psi_\nu * \mathcal{F}\psi_\mu)(\xi)\big|}{\sqrt{2\pi}} \lesssim 2^{-\frac{1}{2}(|\nu|+|\mu|)} \int_{\mathbb{R}} (1+2^{-|\nu|}|\xi-\tau|)^{-\eta}(1+2^{-|\mu|}|\tau|)^{-\eta}\, d\tau,$$

which can be done by the argument in [12, Proposition 2.2.7]: On the one hand,

$$\int_{\{|\xi-\tau|\ge\frac{1}{2}|\xi|\}} (1+2^{-|\nu|}|\xi-\tau|)^{-\eta}(1+2^{-|\mu|}|\tau|)^{-\eta}\, d\tau \le (1+2^{-|\nu|-1}|\xi|)^{-\eta} \int_{\mathbb{R}} (1+2^{-|\mu|}|\tau|)^{-\eta}\, d\tau,$$

on the other hand, since $|\xi-\tau| \le \frac{1}{2}|\xi|$ implies $|\tau| \ge \frac{1}{2}|\xi|$,

$$\int_{\{|\xi-\tau|\le\frac{1}{2}|\xi|\}} (1+2^{-|\nu|}|\xi-\tau|)^{-\eta}(1+2^{-|\mu|}|\tau|)^{-\eta}\, d\tau \le (1+2^{-|\mu|-1}|\xi|)^{-\eta} \int_{\mathbb{R}} (1+2^{-|\nu|}|\tau|)^{-\eta}\, d\tau.$$

In summary, this yields the first part of the assertion; the second part follows in the same way with $|\mathcal{F}(\psi'_\nu)(\xi)| = 2^{|\nu|/2}|\mathcal{F}(\psi')(2^{-|\nu|}\xi)| \lesssim 2^{|\nu|/2}(1+2^{-|\nu|}|\xi|)^{-(\eta-1)}$. $\square$

Corollary 7. *Let $\{\psi_\nu\}_{\nu\in\nabla}$ be a Daubechies wavelet basis with N vanishing moments, then we have*

$$\big|\mathcal{F}(\psi_\nu\psi_\mu)(\xi)\big| \le C_N 2^{\frac{1}{2}||\nu|-|\mu||} \big(1 + 2^{-\max\{|\nu|,|\mu|\}}|\xi|\big)^{-\eta(N)},$$

where

$$\eta(N) := -N + \frac{\ln 3}{2\ln 2}(N-1) - \frac{1}{4\ln 2}\ln N.$$

Proof. From [6, eq. (7.1.19), (7.1.23)], we obtain $|\mathcal{F}\varphi(\xi)| \lesssim (1+|\xi|)^{-N+(2\ln 2)^{-1}\ln(N^{-1/2}3^{N-1})}$, and the claim follows with Proposition 6. □

Remark 3. *More generally, for any wavelet family such that $\psi \in H^k(\mathbb{R})$, $k \in \mathbb{N}$, one finds by integration by parts*

$$|\mathcal{F}\varphi(\xi)| \lesssim \min\{1, |\xi|^{-k}\} \lesssim (1+|\xi|)^{-k}\,. \tag{24}$$

For Daubechies wavelets, however, Proposition 7 yields substantially faster decay for given N than (24) *combined with Sobolev regularity estimates as provided, e.g., in [21].*

For putting the above results together for the particular integrals of interest, we introduce the following additional notation: for $\nu, \mu \in \nabla$, let

$$l_{\mu\nu} := \sup\{|x| :\ x \in \operatorname{supp}\psi_\nu\psi_\mu\}$$

and for $\nu, \mu \in \nabla^2$,

$$L_{\mu\nu} := \sup\{|x-y| :\ x \in \operatorname{supp}\psi_{\nu_1}\psi_{\mu_1},\, y \in \operatorname{supp}\psi_{\nu_2}\psi_{\mu_2}\}\,.$$

We estimate quadrature errors for the integrals (1) and (2) in Theorem 8. An analogous result for (6) is provided by Theorem 9. 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 (3).

Theorem 8 below explicitly gives an appropriate choice of the integration step size h. For the required number of integration points N, we obtain two separate estimates, the first one related to α, the second one to the smoothness of the wavelets; the choice of N is determined by the minimum of these two values.

Remark 4. *Before we come to the results, a comment on the role of the quantities $l_{\mu\nu}$ and $L_{\mu\nu}$ that appear in the estimates is in order.*

Note first that in the case of the one-dimensional integrals, if for all $x \in \operatorname{supp}\psi_\mu\psi_\nu$ we have $\sqrt{\alpha}\,e^{-\alpha x^2} \le C\varepsilon$ with a suitable fixed $C > 0$, then the value of the integral is bounded by the error tolerance, and hence no computation is required; 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 $\sqrt{\alpha}\,e^{-\alpha(x_1-x_2)^2} \le C\varepsilon$.

Taking the support size of the wavelets for a given level and the estimate $\ln\alpha \lesssim \ln\varepsilon^{-1}$ into account, for the indices for which an approximation of the integral needs to be computed we find the conditions

$$l_{\mu\nu} \lesssim \alpha^{-\frac{1}{2}}|\ln\varepsilon|^{\frac{1}{2}} + 2^{-\max\{|\nu|,|\mu|\}}\,,$$
$$L_{\mu\nu} \lesssim \alpha^{-\frac{1}{2}}|\ln\varepsilon|^{\frac{1}{2}} + 2^{-\min\{\max\{|\nu_1|,|\mu_1|\},\max\{|\nu_2|,|\mu_2|\}\}}\,.$$

This needs to be taken into account in interpreting the result of the following theorem.

Theorem 8. *Let $\alpha > 0$ and let $\{\psi_\nu\}_{\nu\in\nabla}$ be a wavelet basis with scaling function φ satisfying $|\mathcal{F}\varphi(\xi)| \lesssim (1+|\xi|)^{-\eta}$ for $\eta > 1$, and with the normalization $\|\psi_\nu\|_{L_2} = 1$. Let $\varepsilon > 0$ with $\varepsilon \le \sqrt{\alpha}$, 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 $\tilde\eta_1 := \eta - 1$,*

$$N \ge \min\Big\{\pi^{-1}\big(\big|\ln(8\sqrt{\alpha})^{-1}\varepsilon\big| + \sqrt{\alpha}\,l_{\nu\mu}\big|\ln(8\sqrt{\alpha})^{-1}\varepsilon\big|^{\frac{1}{2}}\big)\,,$$
$$C_{\psi,\eta}\big(\alpha^{-\frac{1}{2}}\big|\ln(8\sqrt{\alpha})^{-1}\varepsilon\big|^{\frac{1}{2}} + l_{\nu\mu}\big)2^{(2\tilde\eta_1)^{-1}||\nu|-|\mu||}2^{(1+\tilde\eta_1^{-1})\max\{|\nu|,|\mu|\}}\,\varepsilon^{-\tilde\eta_1^{-1}}\Big\}, \tag{25}$$

where $C_{\psi,\eta} > 0$, then we have the estimate

$$\Big|\sqrt{\alpha}\int_{\mathbb{R}} e^{-\alpha x^2}\psi_\nu\psi_\mu\,dx - \frac{h}{\sqrt{2}}\sum_{k=-N}^{N} e^{-(4\alpha)^{-1}(kh)^2}\mathcal{F}(\psi_\nu\psi_\mu)(kh)\Big| \le \varepsilon\,.$$

(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 $\tilde\eta_2 := 2\eta - 1$,*

$$N \ge \min\Big\{\pi^{-1}\big(\big|\ln(8\sqrt{\alpha})^{-1}\varepsilon\big| + \sqrt{\alpha}\,L_{\nu\mu}\big|\ln(8\sqrt{\alpha})^{-1}\varepsilon\big|^{\frac{1}{2}}\big)\,,$$
$$\tilde C_{\psi,\eta}\big(\alpha^{-\frac{1}{2}}\big|\ln(8\sqrt{\alpha})^{-1}\varepsilon\big|^{\frac{1}{2}} + L_{\nu\mu}\big)2^{(2\tilde\eta_1)^{-1}(||\nu_1|-|\mu_1||+||\nu_2|-|\mu_2||)}$$
$$\times\, 2^{(1+\tilde\eta_1^{-1})\min\{\max\{|\nu_1|,|\mu_1|\},\max\{|\nu_2|,|\mu_2|\}\}}\,\varepsilon^{-\tilde\eta_1^{-1}}\,,$$
$$\tilde C_{\psi,\eta}\big(\alpha^{-\frac{1}{2}}\big|\ln(8\sqrt{\alpha})^{-1}\varepsilon\big|^{\frac{1}{2}} + L_{\nu\mu}\big)2^{(2\tilde\eta_2)^{-1}(||\nu_1|-|\mu_1||+||\nu_2|-|\mu_2||)}$$
$$\times\, 2^{\frac{1}{2}(1+\tilde\eta_2^{-1})(\max\{|\nu_1|,|\mu_1|\}+\max\{|\nu_2|,|\mu_2|\})}\,\varepsilon^{-\tilde\eta_2^{-1}}\Big\}, \tag{26}$$

where $\tilde{C}_{\psi,\eta} > 0$, then we have the estimate

$$\Big|\sqrt{\alpha}\int_{\mathbb{R}^2} e^{-\alpha(x-y)^2}\psi_{\nu_1}(x)\,\psi_{\nu_2}(y)\,\psi_{\mu_1}(x)\,\psi_{\mu_2}(y)\,d(x,y) \\ - h\sqrt{\pi}\sum_{k=-N}^{N} e^{-(4\alpha)^{-1}(kh)^2}\overline{\mathcal{F}(\psi_{\nu_1}\psi_{\mu_1})(kh)}\mathcal{F}(\psi_{\nu_2}\psi_{\mu_2})(kh)\Big| \le \varepsilon\,.$$

From the first bounds on N in the conditions (25), (26), it can be seen that for fixed α, we obtain exponential convergence with respect to N. However, in the applications of interest, the maximum required value of α is related to the error in operator norm ε in exponential sum approximations (3); in the specific example considered in Subsection 1.1, we have $\sqrt{\alpha} \sim \varepsilon^{-1}$. Assuming that we also aim for a quadrature error of order ε, for the largest values of α required in combination with a certain ε, we thus obtain a better estimate based on the second, η-dependent bounds on N in (25), (26). These yield algebraic convergence with respect to N, with rate depending on the smoothness of the wavelet basis. It should be noted, however, that in the case of the two-dimensional integrals, the resulting complexity of the computation of one integral, which is essentially $\mathcal{O}(\varepsilon^{-1/(2\eta-1)})$, improves almost twice as fast with increasing η as the result obtained for the reference scheme in Subsection 1.2. As can also be seen from the estimate, however, for certain combinations of large wavelet levels the constant in this latter estimate may deteriorate, and the quantitative behaviour is dominated by a term of order $\mathcal{O}(\varepsilon^{-1/(\eta-1)})$. Before coming to the proof, we make this more precise in the following remark.

Remark 5. *Taking Remark 4 and $\ln\alpha \lesssim |\ln\varepsilon|$ into account, Theorem 8 – recall the definitions of $\tilde{\eta}_1, \tilde{\eta}_2$ there – leads to a number of integration points N for the one-dimensional integral of point (i) that is of order*

$$N \lesssim \min\Big\{|\ln\varepsilon| + \alpha^{\frac{1}{2}}\,2^{-\max\{|\nu|,|\mu|\}}|\ln\varepsilon|^{\frac{1}{2}}\,, \\ \big(1+\alpha^{-\frac{1}{2}}2^{\max\{|\nu|,|\mu|\}}|\ln\varepsilon|\big)2^{(2\tilde{\eta}_1)^{-1}||\nu|-|\mu||\tilde{\eta}_1^{-1}\max\{|\nu|,|\mu|\}}\,\varepsilon^{-\tilde{\eta}_1^{-1}}\Big\}\,.$$

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

$$N \lesssim \min\Big\{|\ln\varepsilon| + \alpha^{\frac{1}{2}}\,2^{-\min\{m_1,m_2\}}|\ln\varepsilon|^{\frac{1}{2}}\,, \\ \big(1+\alpha^{-\frac{1}{2}}2^{\min\{m_1,m_2\}}|\ln\varepsilon|\big)2^{\tilde{\eta}_1^{-1}(\min\{m_1,m_2\}+\frac{1}{2}(d_1+d_2))}\,\varepsilon^{-\tilde{\eta}_1^{-1}}\,, \\ \big(2^{\frac{1}{2}|m_1-m_2|}+\alpha^{-\frac{1}{2}}2^{\frac{1}{2}(m_1+m_2)}|\ln\varepsilon|\big)2^{(2\tilde{\eta}_2)^{-1}(m_1+m_2+d_1+d_2)}\,\varepsilon^{-\tilde{\eta}_2^{-1}}\Big\}\,.$$

This shows in particular that 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.

Proof of Theorem 8. For part (i), note that by (4),

$$\sqrt{\alpha}\int_{\mathbb{R}} e^{-\alpha x^2}\psi_\nu\psi_\mu\,dx = \int_{\mathbb{R}} u_1(\xi)\,d\xi\,, \quad u_1(\xi) := 2^{-\frac{1}{2}}e^{-(4\alpha)^{-1}\xi^2}\mathcal{F}(\psi_\nu\psi_\mu)(\xi)\,.$$

Since $|\mathcal{F}(\psi_\nu\psi_\mu)(\xi_1+i\xi_2)| \le (2\pi)^{-\frac{1}{2}}e^{l_{\nu\mu}d}$ for $\xi_1,\xi_2 \in \mathbb{R}$ with $|\xi_2| \le d$, and by our assumption $\varepsilon \le \sqrt{\alpha}$ and Remark 2, we can apply Lemma 2 with $\delta = (8\sqrt{\alpha})^{-1}\varepsilon$, $\kappa = l_{\nu\mu}$, $n = 0$, and $d = 2(\alpha\ln\delta^{-1})^{1/2}$ to obtain

$$\Big|\int_{\mathbb{R}} u_1(\xi)\,d\xi - h\sum_{k\in\mathbb{Z}} u_1(kh)\Big| \le \frac{\varepsilon}{2}$$

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 4,

$$h\sum_{|k|>N}|u_1(kh)| \le 2\pi^{-\frac{1}{2}}\alpha\,(Nh)^{-1}e^{-(4\alpha)^{-1}(Nh)^2} \tag{27}$$

for $N \in \mathbb{N}$. On the other hand, by Proposition 6, $|u_1(\xi)| \lesssim 2^{\frac{1}{2}||\nu|-|\mu||}(1+2^{-\max\{|\nu|,|\mu|\}}|\xi|)^{-\eta}$ and hence

$$h\sum_{|k|>N}|u_1(kh)| \lesssim 2^{\frac{1}{2}||\nu|-|\mu||}2^{\max\{|\nu|,|\mu|\}}(1+2^{-\max\{|\nu|,|\mu|\}}Nh)^{-(\eta-1)} \tag{28}$$

with constants depending on η and the wavelet basis, which determine $C_{\psi,\eta}$ in (25). Using (25) in conjunction with (27), (28), we obtain

$$h\sum_{|k|>N}|u_1(kh)| \le \frac{\varepsilon}{2}\,,$$

completing the proof of part (i).

For part (ii), we obtain $|\overline{\mathcal{F}(\psi_{\nu_1}\psi_{\mu_1})(\xi_1+i\xi_2)}\mathcal{F}(\psi_{\nu_2}\psi_{\mu_2})(\xi_1+i\xi_2)| \le (2\pi)^{-1}e^{L_{\nu\mu}d}$ for $\xi_1,\xi_2\in\mathbb{R}$ with $|\xi_2|\le d$. Lemma 2 can therefore be applied exactly as before, but with $\kappa = L_{\nu\mu}$, to the integrand

$$u_2(\xi) := \sqrt{\pi}\, e^{-(4\alpha)^{-1}\xi^2}\overline{\mathcal{F}(\psi_{\nu_1}\psi_{\mu_1})(\xi)}\mathcal{F}(\psi_{\nu_2}\psi_{\mu_2})(\xi)\,. \tag{29}$$

The estimate (27) holds with u_1 replaced by u_2 as well, which yields the first condition on N in (26). Concerning an analogue of (28) 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. On the one hand, the right hand side can be estimated by

$$2^{\frac{1}{2}(||\nu_1|-|\mu_1||+||\nu_2|-|\mu_2||)}(1+2^{-\min\{\max\{|\nu_1|,|\mu_1|\},\max\{|\nu_2|,|\mu_2|\}\}}|\xi|)^{-\eta}\,, \tag{30}$$

corresponding to the second condition on N. On the other hand, we have

$$\begin{aligned}(1+2^{-\max\{|\nu_1|,|\mu_1|\}}|\xi|)^{-\eta}&(1+2^{-\max\{|\nu_2|,|\mu_2|\}}|\xi|)^{-\eta}\\ &\le (1+2^{-\max\{|\nu_1|,|\mu_1|\}}2^{-\max\{|\nu_2|,|\mu_2|\}}|\xi|^2)^{-\eta}\\ &\le 2^{\eta}(1+2^{-\frac{1}{2}(\max\{|\nu_1|,|\mu_1|\}+\max\{|\nu_2|,|\mu_2|\})}|\xi|)^{-2\eta}\,,\end{aligned}$$

leading to the third condition on N; in the latter case, Lemma 5 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 (30). The assertion thus follows by the assumption (26) on the choice of N. □

Remark 6. *Additionally, one could consider changes of variable that lead to faster decay of the integrand. An example of a standard substitution is $\xi = \tau\sinh t$ with a suitably chosen $\tau>0$, see, e.g., [25]. The resulting faster decay of the integrand, however, comes at the price of increased $N_1(\cdot,\mathcal{D}_d)$, which in our case 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 [17] in the construction of separable approximations, do not lead to an improvement in our context either: also in this case, 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) involving derivatives of wavelets, we obtain a result very similar to Theorem 8.

Theorem 9. *Let $\alpha>0$ and let $\{\psi_\nu\}_{\nu\in\nabla}$ be a wavelet basis with scaling function φ satisfying $|\mathcal{F}\varphi(\xi)|\lesssim(1+|\xi|)^{-\eta}$ for $\eta>2$, and with the normalization $\|\psi_\nu\|_{L^2}=1$. Let $\varepsilon>0$ with $\varepsilon\le\min\{1,b_\psi\}\min\{1,\sqrt{\alpha}\}$, and let $\nu,\mu\in\nabla^2$. If, with $b_\psi := \max\{\|\varphi'\|_{L^2},\|\psi'\|_{L^2}\}$ and $\delta := (8b_\psi\sqrt{\alpha})^{-1}\varepsilon$,*

$$h = \frac{2\pi\sqrt{\alpha}}{|\ln\delta|^{\frac{1}{2}}+L_{\nu\mu}\sqrt{\alpha}+(4|\ln\delta|)^{-\frac{1}{2}}\big(\ln 2\alpha^{-\frac{1}{2}}+\ln(|\ln\delta|^{\frac{1}{2}}+\pi^{-\frac{1}{2}})\big)}$$

and

$$\begin{aligned}N \ge h^{-1}\min\Big\{&\sqrt{8\alpha}\big|\ln(\sqrt{\alpha}\,\delta)\big|^{\frac{1}{2}}\,,\\ &\hat C_{\psi,\eta}2^{(2\tilde\eta_3)^{-1}(||\nu_1|-|\mu_1||+||\nu_2|-|\mu_2||)}2^{\frac{1}{2}(1+3\tilde\eta_3^{-1})(\max\{|\nu_1|,|\mu_1|\}+\max\{|\nu_2|,|\mu_2|\})}(\alpha\varepsilon)^{-\tilde\eta_3^{-1}}\Big\}\,,\end{aligned} \tag{31}$$

where $\tilde\eta_3 := 2\eta-3$ and $\hat C_{\psi,\eta}>0$, then we have

$$\begin{aligned}\Big|\sqrt{\alpha}\int_{\mathbb{R}^2}(x-y)e^{-\alpha(x-y)^2}&[(\partial_x-\partial_y)\psi_{\nu_1}(x)\,\psi_{\nu_2}(y)]\,\psi_{\mu_1}(x)\,\psi_{\mu_2}(y)\,d(x,y)\\ &- h\frac{(-i)\sqrt{\pi}}{2\alpha}\sum_{k=-N}^{N}kh\,e^{-(4\alpha)^{-1}(kh)^2}\Big(\overline{\mathcal{F}(\psi'_{\nu_1}\psi_{\mu_1})(kh)}\mathcal{F}(\psi_{\nu_2}\psi_{\mu_2})(kh)\\ &\qquad-\overline{\mathcal{F}(\psi_{\nu_1}\psi_{\mu_1})(kh)}\mathcal{F}(\psi'_{\nu_2}\psi_{\mu_2})(kh)\Big)\Big|\le\varepsilon\,.\end{aligned}$$

Proof. In this case, the integrand reads

$$u_3(\xi) := -\frac{i\sqrt{\pi}}{2\alpha}\xi e^{-(4\alpha)^{-1}\xi^2}\left(\overline{\mathcal{F}(\psi'_{\nu_1}\psi_{\mu_1})(\xi)}\mathcal{F}(\psi_{\nu_2}\psi_{\mu_2})(\xi) - \overline{\mathcal{F}(\psi_{\nu_1}\psi_{\mu_1})(\xi)}\mathcal{F}(\psi'_{\nu_2}\psi_{\mu_2})(\xi)\right).$$

For $\xi = \xi_1 + i\xi_2$, $\xi_1, \xi_2 \in \mathbb{R}$ with $|\xi_2| \le d$, we have

$$\left|\overline{\mathcal{F}(\psi'_{\nu_1}\psi_{\mu_1})(\xi)}\mathcal{F}(\psi_{\nu_2}\psi_{\mu_2})(\xi)\right| + \left|\overline{\mathcal{F}(\psi_{\nu_1}\psi_{\mu_1})(\xi)}\mathcal{F}(\psi'_{\nu_2}\psi_{\mu_2})(\xi)\right| \le \pi^{-1}\, b_\psi\, e^{L_{\nu\mu}d}\,.$$

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 2 we can apply Lemma 2 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

$$\left|\int_{\mathbb{R}} u_3(\xi)\, d\xi - h\sum_{k\in\mathbb{Z}} u_3(kh)\right| \le \frac{\varepsilon}{2}$$

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 4,

$$h\sum_{|k|>N} |u_3(kh)| \le \frac{4b_\psi\sqrt{2\alpha}}{\sqrt{\pi}Nh} e^{-(8\alpha)^{-1}(Nh)^2}\,. \tag{32}$$

The choice of N as in (31) ensures that the right hand side in (32) is bounded by $\varepsilon/2$; note that $\sqrt{\alpha}\,\delta < 1$ by our assumptions on ε. For the second part of (31), we use Proposition 6 to obtain

$$|u(\xi)| \lesssim \alpha^{-1} 2^{\frac{1}{2}(||\nu_1|-|\mu_1||+||\nu_2|-|\mu_2||)} 2^{\max\{|\nu_1|,|\mu_1|\}+\max\{|\nu_2|,|\mu_2|\}} \\ \times (1 + 2^{-\frac{1}{2}\max\{|\nu_1|,|\mu_1|\}-\frac{1}{2}\max\{|\nu_2|,|\mu_2|\}}|\xi|)^{-2(\eta-1)}\,,$$

with a multiplicative constant depending on η and the wavelet basis, and Lemma 5 therefore yields

$$h\sum_{|k|>N} |u_3(kh)| \lesssim \alpha^{-1} 2^{\frac{1}{2}(||\nu_1|-|\mu_1||+||\nu_2|-|\mu_2||)} 2^{\frac{3}{2}(\max\{|\nu_1|,|\mu_1|\}+\max\{|\nu_2|,|\mu_2|\})} \\ \times (1 + 2^{-\frac{1}{2}\max\{|\nu_1|,|\mu_1|\}-\frac{1}{2}\max\{|\nu_2|,|\mu_2|\}}|\xi|)^{-\tilde{\eta}_3}\,.$$

Choosing N such that the latter is bounded by $\varepsilon/2$ leads to the second part of (31). □

3 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 $\int x^n \varphi(x)\,\varphi(x-l)\,dx$ 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

$$\int x^n \varphi(x)\,\varphi(x-l)\,dx = \sum_m \int x^n \tilde{\eta}(x-m)\,dx \int \eta(x-m)\,\varphi(x)\,\varphi(x-l)\,dx\,.$$

The moments of $\tilde{\eta}$ can be evaluated by the recursion

$$\int x^n \tilde{\eta}(x-k)\,dx = \frac{1}{(2^n-1)\sqrt{2}} \sum_{i=0}^{n-1} \binom{n}{i} \int x^i \tilde{\eta}(x-k)\,dx \sum_m h_m (m+k)^{n-i}\,.$$

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 (8) 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 $\mathcal{F}(\varphi_{0,0}\,\varphi_{0,l})(\xi)$, to which all other combinations of scaling functions and wavelets on different levels can be reduced; this expression vanishes for all ξ unless $l \in \{L-U+1, \ldots, U-L-1\}$. Using the scaling relation for φ, we obtain the recursion

$$\begin{aligned}\int \varphi(x)\,\varphi(x-l)\,e^{-ix\xi}\,dx &= \sum_{n,m} h_n h_m e^{-i\xi n/2} \int \varphi(x)\,\varphi(x+n-m-2l)\,e^{-ix\xi/2}\,dx \\ &= \sum_{m,n} h_{m-n+2l} h_m e^{-i\xi(m-n+2l)/2} \int \varphi(x)\,\varphi(x-n)\,e^{-ix\xi/2}\,dx\,. \end{aligned} \tag{33}$$

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

$$\int \varphi(x)\,\varphi(x-l)\,e^{-ix\xi}\,dx = \sum_n A_{l,n}(\xi) \int \varphi(x)\,\varphi(x-n)\,e^{-ix\xi/2}\,dx\,. \tag{34}$$

For obtaining an approximation of $\mathcal{F}(\varphi_{0,0}\,\varphi_{0,l})(\xi)$ for arbitrary ξ, we still need suitable starting values for the recursion (34). For $J \in \mathbb{N}$, let $\xi_J := 2^{-J}\xi$, then for J sufficiently large,

$$\int \varphi(x)\,\varphi(x-l)\,e^{-i\xi_J x}\,dx \;\approx\; \sum_{n=0}^{N} \frac{(-i\xi_J)^n}{n!} \int x^n \varphi(x)\,\varphi(x-l)\,dx\,. \tag{35}$$

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 (35) can be estimated by

$$\frac{\kappa^N}{N!} \max_{|x|\le\kappa} \max\bigl\{\bigl|\partial_x^N \cos(|\xi_J|x)\bigr|, \bigl|\partial_x^N \sin(|\xi_J|x)\bigr|\bigr\} \le \frac{|\kappa\xi_J|^N}{N!}\,.$$

Recall that, as discussed in the beginning of this section, the quantities $\int x^n\varphi(x)\,\varphi(x-l)\,dx$ can be precomputed up to any desired value of n. Applying (34) J times, with J large enough in relation to N, we can thus obtain approximations for $\mathcal{F}(\varphi_{0,0}\,\varphi_{0,l})(\xi)$ from the approximations of the corresponding $\mathcal{F}(\varphi_{0,0}\,\varphi_{0,l})(\xi_J)$ provided by (35).

Similarly, the expressions $\mathcal{F}(\psi_\nu'\,\psi_\mu)(\xi)$, which are required for the modified integrals (7), can be obtained from $\mathcal{F}(\varphi_{0,0}'\,\varphi_{0,l})(\xi)$. The latter can be evaluated by the recursion

$$\int \varphi'(x)\,\varphi(x-l)\,e^{-ix\xi}\,dx = 2\sum_n A_{l,n}(\xi) \int \varphi'(x)\,\varphi(x-n)\,e^{-ix\xi/2}\,dx$$

in place of (34). We restrict our following discussion to the computation of $\mathcal{F}(\psi_\nu\,\psi_\mu)(\xi)$, but the evaluation of $\mathcal{F}(\psi_\nu'\,\psi_\mu)(\xi)$ 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 4, no problems in this regard are observed in numerical practice, and integration errors close to machine precision can be achieved.

Remark 7. *An alternative to the above recursive scheme is to use the identity*

$$\int_{\mathbb{R}} \varphi(x)\,\varphi(x-l)\,e^{-ix\xi}\,dx = \int_{\mathbb{R}} (\mathcal{F}\varphi)(\xi-\eta)\,(\mathcal{F}\varphi)(\eta)\,e^{-il\eta}\,d\eta\,,$$

and apply the trapezoidal rule to the integral on the right hand side, where $\mathcal{F}\varphi$ 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 3 applies in this case as well. Due to the algebraic decay of $\mathcal{F}\varphi$, the resulting convergence is only algebraic in the number of integration points[2]*. Using this approach, the overall asymptotic complexity of the integration scheme would therefore deteriorate substantially.*

The combination of (34) and (35) enables the evaluation of $\mathcal{F}(\varphi_{0,0}\,\varphi_{0,l})(\xi)$ for any $l \in \mathbb{Z}$ and $\xi \in \mathbb{R}$. For any $j, J, k, l \in \mathbb{Z}$ with $J \ge j$, we also have

$$\mathcal{F}(\varphi_{j,k}\varphi_{J,l})(\xi) = \mathcal{F}(\varphi_{0,k}\,\varphi_{J-j,l})(2^{-j}\xi) = e^{-ik2^{-j}\xi}\mathcal{F}(\varphi_{0,0}\,\varphi_{J-j,l-2^{J-j}k})(2^{-j}\xi)\,.$$

It thus suffices to consider $\mathcal{F}(\varphi_{0,0}\,\varphi_{j,l})(\xi)$ for $j > 0$. By j steps of the recursion

$$\int \varphi(x)\varphi(2^j x - l)\,e^{-ix\xi}\,dx = \frac{1}{\sqrt{2}} \sum_n h_n e^{-in\xi/2} \int \varphi(x)\varphi(2^{j-1}x + 2^{j-1}n - l)\,e^{-ix\xi/2}\,dx\,,$$

this case can again be reduced to the evaluation of $\mathcal{F}(\varphi_{0,0}\,\varphi_{0,n})(\xi)$ for $n = L-U+1,\dots,U-L-1$. The number of intermediate results required in each step stays bounded by $2U-2L-1$: for each $0 \le \iota < j$, it suffices to compute the intermediate values

$$\int \varphi(x)\,\varphi(2^\iota x - (l_\iota - 2^\iota n_\iota))\,e^{-ix(2^{j-\iota}\xi)}\,dx\,,$$

[2]The substitutions mentioned in Remark 6 that would guarantee exponential decay turn out to give no improvement in the overall convergence estimate in this case either.

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

$$\int \psi(x)\,\psi(x-l)\,e^{-ix\xi}\,dx = \sum_{m,n} g_{m-n+2l}\,g_m\,e^{-i\xi(m-n+2l)/2} \int \varphi(x)\,\varphi(x-n)\,e^{-ix\xi/2}\,dx\,. \tag{36}$$

Combining the above recursions, we are therefore able to approximately evaluate $\mathcal{F}(\psi_\nu\psi_\mu)(\xi)$ for any $\xi \in \mathbb{R}$ and $\nu, \mu \in \nabla$.

4 Numerical Realization

We now turn to the practical realization of the quadrature scheme. For instance, additionally exploiting symmetries, for (2) we have a quadrature scheme of the form

$$\begin{aligned}\sqrt{\alpha}\int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}(\psi_{\nu_1}\otimes\psi_{\nu_2})\,(\psi_{\mu_1}\otimes\psi_{\mu_2})\,dx \;\approx\; & h\sqrt{\pi}\,\overline{\mathcal{F}(\psi_{\nu_1}\psi_{\mu_1})(0)}\mathcal{F}(\psi_{\nu_2}\psi_{\mu_2})(0) \\ & + 2h\sum_{k=1}^{N}\sqrt{\pi}\,e^{-(4\alpha)^{-1}(kh)^2}\overline{\mathcal{F}(\psi_{\nu_1}\psi_{\mu_1})(kh)}\mathcal{F}(\psi_{\nu_2}\psi_{\mu_2})(kh)\,.\end{aligned}$$

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 3 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 $\mathcal{F}(\varphi_{0,0}\,\varphi_{0,l})(2^{-j}k\,\tau_0)$. This can yield a substantial gain in efficiency because, by the recursions discussed in Section 3, 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 $\mathcal{F}(\psi_\nu\,\psi_\mu)(\xi)$ for further combinations of $\nu, \mu \in \nabla$ and integration points ξ.

The matrix in the recursion (33) 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 (33) was consistently faster for values of M up to 46, even when using the optimized FFT library, FFTW [10].

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.

4.1 Numerical Experiments

For our numerical tests, we use a variant of Daubechies wavelets constructed by Ojanen [21], with has slightly less vanishing moments for a given support size than the Daubechies wavelets, but instead has higher regularity; this property is of interest because it leads to better compressibility of operators. The particular scaling function and wavelet we use, shown in Figure 1, have support length 19 with 6 vanishing moments and are in $H^s(\mathbb{R})$ for $s \approx 4.32$, see [21].

We consider, with u_2 as in (29), the integrals

$$\sqrt{\alpha}\int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\,(\psi_{\nu_1}\otimes\psi_{\nu_2})\,(\psi_{\mu_1}\otimes\psi_{\mu_2})\,dx = \int_{\mathbb{R}} u_2(\xi)\,d\xi\,, \tag{37}$$

for the six different combinations of $\nu_1, \nu_2, \mu_1, \mu_2$ which are listed in Table 1, and for

$$\alpha = 10^0,\, 10^2,\, 10^4,\, 10^6,\, 10^8,\, 10^{16}\,.$$

For comparing numerical errors, reference values for the integrals were computed using the completely different scheme of Subsection 1.2 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 1, this

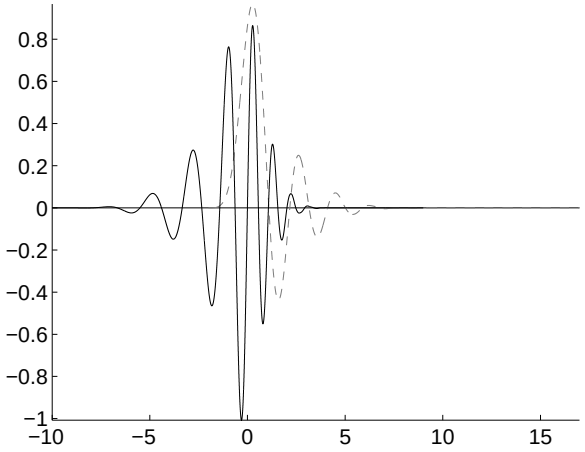

Figure 1: Wavelet ψ (solid line) and scaling function φ (dashed line) used in the numerical tests.

	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 1: Combinations of wavelet indices $\nu_1, \nu_2, \mu_1, \mu_2 \in \nabla$ used in (37) 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	$6.445564928603676 \times 10^{-01}$	$3.087756935213937 \times 10^{-07}$
10^2	$1.044688765938243 \times 10^{+00}$	$3.280482098078684 \times 10^{-08}$
10^4	$1.055320499670092 \times 10^{+00}$	$3.182372092623544 \times 10^{-08}$
10^6	$1.055428713601353 \times 10^{+00}$	$3.181395966734626 \times 10^{-08}$
10^8	$1.055429795933709 \times 10^{+00}$	$3.181386205984803 \times 10^{-08}$
10^{16}	$1.055429806866383 \times 10^{+00}$	$3.181386107391438 \times 10^{-08}$
α	Integral 3	Integral 4
10^0	$-4.072379711218127 \times 10^{-06}$	$1.867098215486562 \times 10^{-02}$
10^2	$1.798985688973480 \times 10^{-03}$	$-8.269936318309225 \times 10^{-03}$
10^4	$2.420502335354703 \times 10^{-03}$	$-3.494643176839263 \times 10^{-02}$
10^6	$2.426105327025463 \times 10^{-03}$	$-3.525196817558028 \times 10^{-02}$
10^8	$2.426161253646409 \times 10^{-03}$	$(-3.525502876165434 \times 10^{-02})$
10^{16}	$2.426161818551820 \times 10^{-03}$	$(-3.525505967720674 \times 10^{-02})$
α	Integral 5	Integral 6
10^0	$9.995156344291690 \times 10^{-01}$	$-8.216257535442750 \times 10^{-13}$
10^2	$9.556600670183798 \times 10^{+00}$	$1.876368135997672 \times 10^{-09}$
10^4	$3.421268763593881 \times 10^{+01}$	$-1.572584027194289 \times 10^{-04}$
10^6	$5.377733435130575 \times 10^{+01}$	$-2.812674495013307 \times 10^{-04}$
10^8	$(5.557894638574768 \times 10^{+01})$	$(-2.832442081084854 \times 10^{-04})$
10^{16}	$(5.559816312094642 \times 10^{+01})$	$(-2.832642840672890 \times 10^{-04})$

Table 2: Reference values for integrals (37) with wavelet indices as in Table 1.

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 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 2.

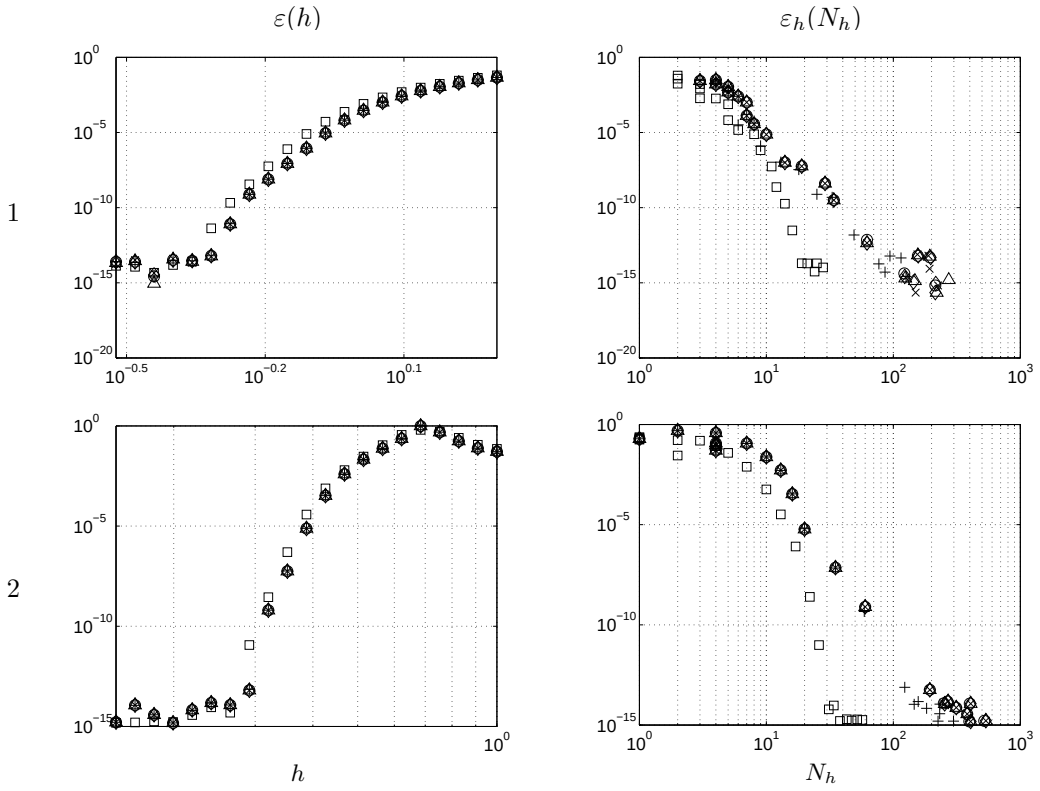

Figure 2: Integration error in dependence of given h and corresponding N_h, with markers corresponding to values of α: $\square$ 1, + 10^2, $\circ$ 10^4, $\times$ 10^6, $\diamond$ 10^8, $*$ 10^{16}.

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 4.

We first study the numerical errors that can be achieved in principle by the integration of Section 2 combined with the recursive evaluation of Fourier transforms as in Section 3. For this first test, we thus take an approach similar to the basic strategy of the convergence analysis: for given h we first approximate

$$\varepsilon(h) = \left| \int_{\mathbb{R}} u_2(\xi)\, d\xi - h \sum_{k \in \mathbb{Z}} u_2(hk) \right|$$

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

$$\varepsilon_h(N_h) := h \sum_{|k| > N_h} |u_2(hk)| \leq \varepsilon(h)\,,$$

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 2, 3, and 4. In each case, errors close to machine precision are achieved; an exception is case 5 in Figure 4, where the minimum errors are of order $\approx 10^{-13}$. This is not surprising since, for instance,

$$\int_{\mathbb{R}} e^{-(4\alpha)^{-1}\xi^2} |\mathcal{F}(\psi_{j,0} \otimes \psi_{j,0})|^2\, d\xi = 2^j \int_{\mathbb{R}} e^{-(4\alpha)^{-1} 2^{2j} \xi^2} |\mathcal{F}(\psi_{0,0} \otimes \psi_{0,0})|^2\, d\xi\,,$$

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 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 shows what can at best be expected, but is 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 (10), 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 3. The results given in Table 4 show that the automatic refinement procedure reliably produces approximate

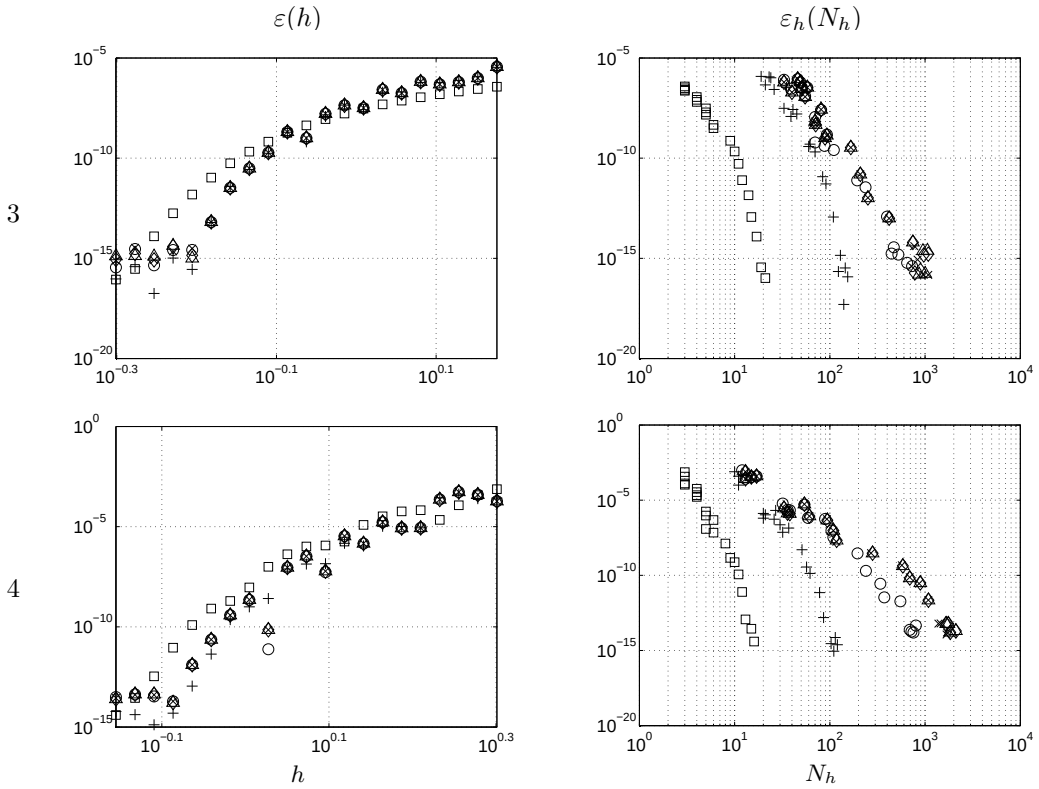

Figure 3: Integration error in dependence of given h and corresponding N_h, with markers as in Figure 2.

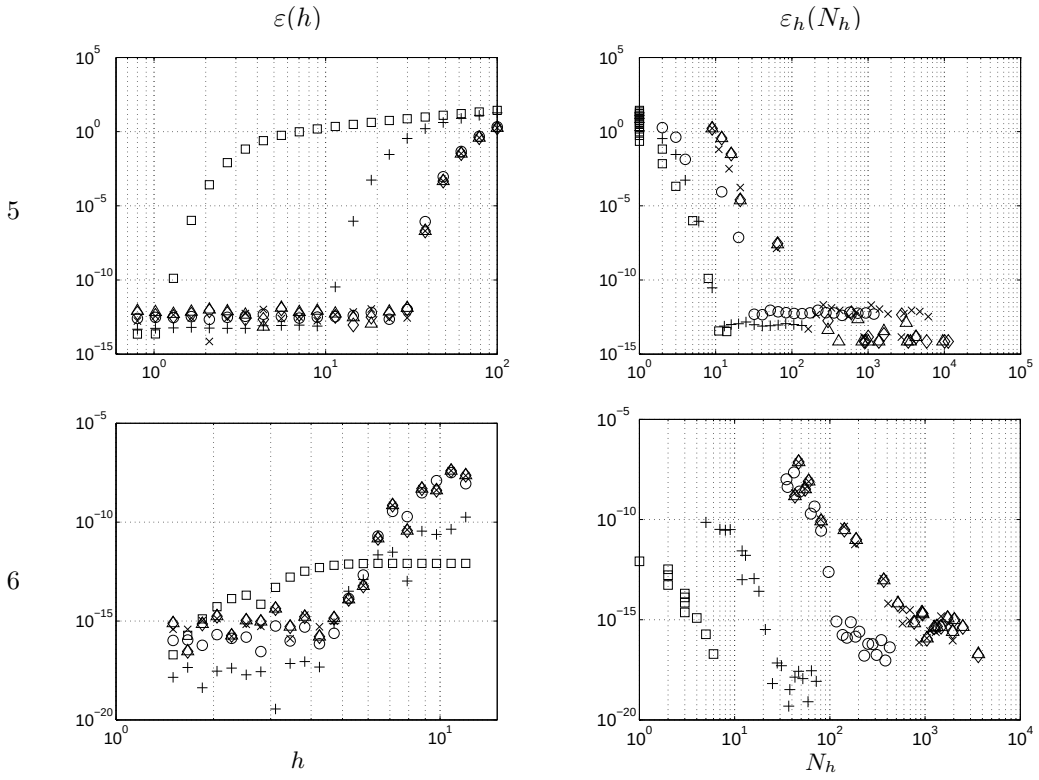

Figure 4: Integration error in dependence of given h and corresponding N_h, with markers as in Figure 2.

		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 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 2, rescaled by the factors given in Table 3.

		10^{-6}	10^{-8}	10^{-10}	10^{-12}	# stored values (memory)
$\xi_0 = 1$,	1 thread	4254.5	6212.1	9125.9	14808.5	865 (501 KB)
$\xi_0 = 1$,	4 threads	1196.4	1768.5	2578.9	4123.7	
$\xi_0 = 10^3$,	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 5: Times in seconds for evaluation of the 153664 integrals with parameters as in (38), run on a Xeon E5450 system at 3 GHz, for different prescribed target accuracies, where values of $\mathcal{F}(\varphi_{0,l}\,\varphi_{0,0})(2^{-j}k)$ for $0 \le 2^{-j}k \le \xi_0$ are stored and reused. In addition, in each case 1.57 seconds are spent on preprocessing.

integrals with prescribed error, requiring in each case a number of points only slightly larger than the minimum possible according to Figures 2, 3, and 4.

We finally consider CPU times for the evaluation of the integrals (37) in the range of parameters

$$\alpha \in \left\{1, 10^4, 10^8, 10^{12}\right\}, \quad \nu_1, \nu_2, \mu_1, \mu_2 \in \left\{(0, k, s)\colon\ k = -3, \ldots, 3\,,\ s = 0, 1\right\}. \tag{38}$$

This amounts to a total number of 153664 integrals[3]. Here we consider the acceleration of the Fourier-based scheme by two strategies: On the one hand, by storing and reusing computed values of $\mathcal{F}(\varphi_{0,l}\,\varphi_{0,0})(2^{-j}k)$, 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 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. In summary, our practical tests show that the quadrature scheme allows the evaluation of the integrals under consideration with a reasonable number of integration points, even for very large exponents in the Gaussian term and high

[3]Note that in practice, due to the symmetries of the integrand, not all of these integrals would need to be evaluated separately.

wavelet levels, and the quadrature can be performed with prescribed accuracy by a reliable automatic refinement procedure.

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A Analysis of the Reference Scheme

Proof of Proposition 1. We prove the proposition for the two-dimensional case; the one-dimensional integrals can be treated analogously. By the direct estimate for $\{\theta_{J,k}\}_k$,

$$\Big\|\sqrt{\alpha}e^{-\alpha(x_1-x_2)^2} - \sum_{k\in\mathbb{Z}^2} \langle \sqrt{\alpha}e^{-\alpha(\tilde{x}_1-\tilde{x}_2)^2}, \tilde{\theta}_{J,k_1}\otimes\tilde{\theta}_{J,k_2}\rangle \theta_{J,k_1}\otimes\theta_{J,k_2}\Big\|_\infty \\ \leq 2^{-pJ}\sqrt{\alpha} \max_{\substack{i_1,i_2\geq 0\\ i_1+i_2=p}} \|\partial_{x_1}^{i_1}\partial_{x_2}^{i_2} e^{-\alpha(x_1-x_2)^2}\|_\infty .$$

Furthermore, by Cramér's inequality (cf. [18]), we have

$$\|\partial_{x_1}^{i_1}\partial_{x_2}^{i_2} e^{-\alpha(x_1-x_2)^2}\|_\infty \lesssim \alpha^{p/2}\|e^{-(\alpha/2)(x_1-x_2)^2}\|_\infty , \quad i_1+i_2=p . \tag{39}$$

We use the direct estimate for $\{\tilde{\theta}_{J,k}\}_k$ to obtain

$$\Big\|\psi_{\nu_1}\,\psi_{\mu_1}\otimes\psi_{\nu_2}\,\psi_{\mu_2} - \sum_{k\in\mathbb{Z}^2} \langle \psi_{\nu_1}\,\psi_{\mu_1}\otimes\psi_{\nu_2}\,\psi_{\mu_2}, \theta_{J,k_1}\otimes\theta_{J,k_2}\rangle \tilde{\theta}_{J,k_1}\otimes\tilde{\theta}_{J,k_2}\Big\|_\infty \\ \leq 2^{-qJ} \max_{\substack{i_1,i_2\geq 0\\ i_1+i_2=q}} \|\partial_{x_1}^{i_1}\partial_{x_2}^{i_2}(\psi_{\nu_1}\,\psi_{\mu_1}\otimes\psi_{\nu_2}\,\psi_{\mu_2})\|_\infty ,$$

where $\|\partial_{x_1}^{i_1}\partial_{x_2}^{i_2}(\psi_{\nu_1}\,\psi_{\mu_1}\otimes\psi_{\nu_2}\,\psi_{\mu_2})\|_\infty \lesssim 2^{\frac{1}{2}(|\nu_1|+|\mu_1|+|\nu_2|+|\mu_2|)}2^{q\max\{|\nu_1|,|\mu_1|,|\nu_2|,|\mu_2|\}}$. As a consequence, the error in the expansion (12) 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

$$J \geq \min\Big\{ \tfrac{1}{p}\log_2 c\varepsilon^{-1} + \tfrac{1}{2}\big(1+\tfrac{1}{p}\big)\log_2\alpha, \\ \tfrac{1}{q}\log_2 c\varepsilon^{-1} + \max\{|\nu_1|,|\mu_1|,|\nu_2|,|\mu_2|\} + \tfrac{1}{2q}(|\nu_1|+|\mu_1|+|\nu_2|+|\mu_2|)\Big\} . \tag{40}$$

Let

$$\mathcal{K}_{J,\varepsilon}^{(2)} := \Big\{ k\in\mathbb{Z}^2 :\ |x_1-x_2| \leq \alpha^{-\frac{1}{2}}(\max\{\tfrac{1}{4}, \ln\varepsilon^{-1}\})^{\frac{1}{2}} \ \text{ for all } (x_1,x_2)\in \operatorname{supp}\tilde{\theta}_{J,k_1}\otimes\tilde{\theta}_{J,k_2}\Big\} ,$$

and assume that ε is sufficiently small such that $\ln\varepsilon^{-1} > \frac{1}{4}$. By the estimate

$$\int_y^\infty \sqrt{\alpha}\, e^{-\alpha x^2}\, dx \leq e^{-\alpha y^2} \ \text{ for } y \geq \frac{1}{2}\alpha^{-\frac{1}{2}}$$

we thus obtain

$$\Big| \int_{\mathbb{R}^2} e^{-\alpha(x_1-x_2)^2}\,(\psi_{\nu_1}\otimes\psi_{\nu_2})\,(\psi_{\mu_1}\otimes\psi_{\mu_2})\,dx \\ - \sum_{k\in\mathcal{K}_{J,\varepsilon}^{(2)}} \int \sqrt{\alpha}e^{-\alpha(x_1-x_2)^2}\tilde{\theta}_{J,k_1}\otimes\tilde{\theta}_{J,k_2}\,dx \int_{\mathbb{R}} \theta_{J,k_1}\,\psi_{\nu_1}\,\psi_{\mu_1}\,dx \int_{\mathbb{R}} \theta_{J,k_2}\,\psi_{\nu_2}\,\psi_{\mu_2}\,dx \Big| \lesssim \varepsilon$$

for J as in (40), with a constant independent of ε, assuming that $\ln\varepsilon^{-1} > \frac{1}{4}$. □