

# Multiresolution separated representations of singular and weakly singular operators <sup>☆</sup>

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## Abstract

For a finite but arbitrary precision, we construct efficient low separation rank representations for the Poisson kernel and for the projector on the divergence free functions in the dimension  $d = 3$ . Our construction requires computing only one-dimensional integrals. We use scaling functions of multiwavelet bases, thus making these representations available for a variety of multiresolution algorithms. Besides having many applications, these two operators serve as examples of weakly singular and singular operators for which our approach is applicable. Our approach provides a practical implementation of separated representations of a class of weakly singular and singular operators in dimensions  $d \geq 2$ .

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## 1. Introduction

It has been clear for some time [1] that a multiresolution representation of certain classes of elliptic convolution operators should lead to fast and accurate numerical algorithms. However, the straightforward transition from multiresolution algorithms in one spatial dimension to those in dimensions two, three and higher yielded algorithms that are too costly for practical applications. Recent results using separated representations of multidimensional operators [2,3] provide us with a method for a practical multidimensional construction.

These representations have been already incorporated into fast algorithms for computing electronic structure [4–7] giving rise to multiresolution quantum chemistry. In this paper we derive the necessary estimates leading to accurate

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separated multiresolution representation for a class of convolution operators. These estimates provide the analytic foundation for accuracy control within the framework of separated representations of operators in high dimensions.

The kernels of operators of this class are non-oscillatory and include weakly singular and singular operators which are ubiquitous in problems of physics. The Poisson kernel and the projector on the divergence free functions provide two important examples with a wide range of applications in computational chemistry, computational electro-magnetics and fluid dynamics. However, these operators are rarely used directly for computing. For example, one typically solves the Poisson equation in the differential form as a step in solving the Navier–Stokes equations rather than apply the projector on divergence free functions. The reason for avoiding integral operators (that typically are much better conditioned than their differential counterparts) is the apparent computational complexity of their use. Such perception began to change with the wider use of the fast multipole method (FMM) (see, e.g., [8]) and introduction of wavelet based algorithms [1]. To advance the use of multidimensional integral operators, we show how to evaluate these operators on functions using only one-dimensional integrals.

In this paper we use multiwavelet bases to describe our construction. The main reason for this choice is that in many problems a basis should accommodate not only the integral operators but also differential operators and boundary conditions. It turns out that the multiwavelet bases developed in [9] satisfy many of the requirements of applications [10,11]. On one hand, multiwavelet bases retain some properties of wavelet bases, such as vanishing moments, orthogonality, and compact support. The basis functions do not overlap on a given scale and are organized in small groups of several functions (thus, *multiwavelets*) sharing the same support. Due to the vanishing moments of the basis functions, a wide class of integro-differential operators has *effectively sparse* representations in these bases, i.e., these operators are well approximated (in the operator norm) by sparse matrices. On the other hand, high order representations of operators with boundary conditions are available [10], whereas such representations with the compactly supported Daubechies' wavelets [12] are numerically unstable.

It was shown in [13] that not only singular but also the hypersingular operators have their most natural representation in multiresolution bases. Using bases of compactly supported Daubechies' wavelets [14] (or their variations) and the two-scale difference equations, the problem of discretization of weakly singular, singular and hypersingular kernels is reduced to solving a linear system of algebraic equations for the coefficients of the representation. By solving this linear system we completely avoid the otherwise difficult issue of discretization of singular and hypersingular kernels.

For multiwavelet bases, similar results are summarized in [15]. In contrast to wavelets with regularity, some of the basis functions of multiwavelet bases are discontinuous, similar to those of the Haar basis. This lack of regularity of multiwavelet bases prevents the straightforward extension of results in [13] to hypersingular operators. However, the difficulty does not arise for weakly singular and singular operators which we consider here using the Poisson kernel and the projector on the divergence free functions as examples.

We construct separated representations for the Poisson kernel in the dimension  $d = 3$  in Section 3, and for the kernel of the projector on the divergence free functions in Section 4. We note that the same approach is applicable for non-homogeneous Green's functions [5] and, without significant changes, in dimensions  $d > 3$  and  $d = 2$ . Our derivation of representations with low separation rank in multiwavelet bases makes them accessible for a variety of applications. We briefly consider algorithms for applying the resulting operators to functions and refer to [4–7] for further details. A fully adaptive algorithm for applying multiresolution separated representations of operators to functions will be described elsewhere [16].

## 2. Preliminary considerations

### 2.1. Separated representations of radial functions

Let us start by considering approximating the function  $1/r^\alpha$  with a collection of Gaussians. Remarkably, the number of terms needed for this purpose is mercifully small. We have [17]

**Proposition 1.** For any  $\alpha > 0$ ,  $0 < \delta \leq 1$ , and  $0 < \epsilon \leq \min\{\frac{1}{2}, \frac{8}{\alpha}\}$ , there exist positive numbers  $p_m$  and  $w_m$  such that

$$\left| r^{-\alpha} - \sum_{m=1}^M w_m e^{-p_m r^2} \right| \leq r^{-\alpha} \epsilon \quad \text{for all } \delta \leq r \leq 1 \quad (1)$$

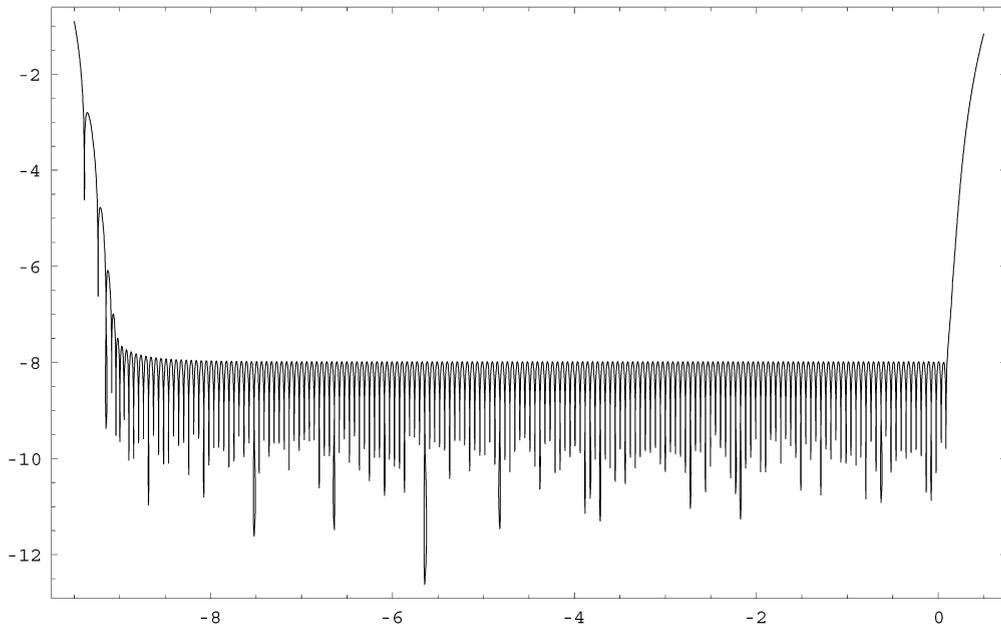


Fig. 1. Error ( $\log_{10}$ ) of approximating the Poisson kernel using Proposition 1 with consequent optimization, where  $\epsilon \approx 10^{-8}$ ,  $10^{-9} \leq \|\mathbf{x}\| \leq 1$  and  $M = 89$ .

with

$$M = \log \epsilon^{-1} [c_0 + c_1 \log \epsilon^{-1} + c_2 \log \delta^{-1}], \tag{2}$$

where  $c_k$  are constants that only depend on  $\alpha$ . For fixed power  $\alpha$  and accuracy  $\epsilon$ , we have  $M = \mathcal{O}(\log \delta^{-1})$ .

For singular operators, we will need a different measure of error in such approximations. Let us select  $\epsilon = \epsilon_0 \delta^{\alpha-2}$  in Proposition 1 and arrive at

**Proposition 2.** For any  $\alpha > 0$ ,  $0 < \delta \leq 1$ , and  $0 < \epsilon \leq \min\{\frac{1}{2}, \frac{8}{\alpha}\}$ , there exist positive numbers  $p_m$  and  $w_m$  such that

$$\left| r^{-\alpha} - \sum_{m=1}^M w_m e^{-p_m r^2} \right| \leq \epsilon_0 r^{-2} \quad \text{for all } \delta \leq r \leq 1, \tag{3}$$

where

$$M = \log \epsilon^{-1} [c_0 + c_1 \log \epsilon^{-1} + c_2 \log \delta^{-1}]. \tag{4}$$

Propositions 1 and 2 provide an initial approximation that we optimized further to reduce the number of terms via the approach in [17]. The errors of such approximation are illustrated in Figs. 1 and 2.

We note that approximations of the function  $1/r$  via sums of Gaussians have been also considered in [18–20]. In [18] it was used to approximate the Coulomb potential.

Using  $r = \|\mathbf{x}\|$ , where  $\mathbf{x} = (x_1, x_2, x_3)$ , and  $\alpha = 1$  in (1) and (3), we arrive at a separated representation for the Poisson kernel. Using  $\alpha = 3$  in (3), we obtain a separated representation that we use to compute the projector on the divergence free functions. We describe how to use approximations in Propositions 1 and 2 in the following sections.

As in [4] and [5], the approximations illustrated in Figs. 1 and 2 were obtained in two stages. First, we discretize the integral

$$\frac{1}{r^\alpha} = \frac{2}{\Gamma(\alpha/2)} \int_{-\infty}^{\infty} e^{-r^2 e^{2s} + \alpha s} ds \tag{5}$$

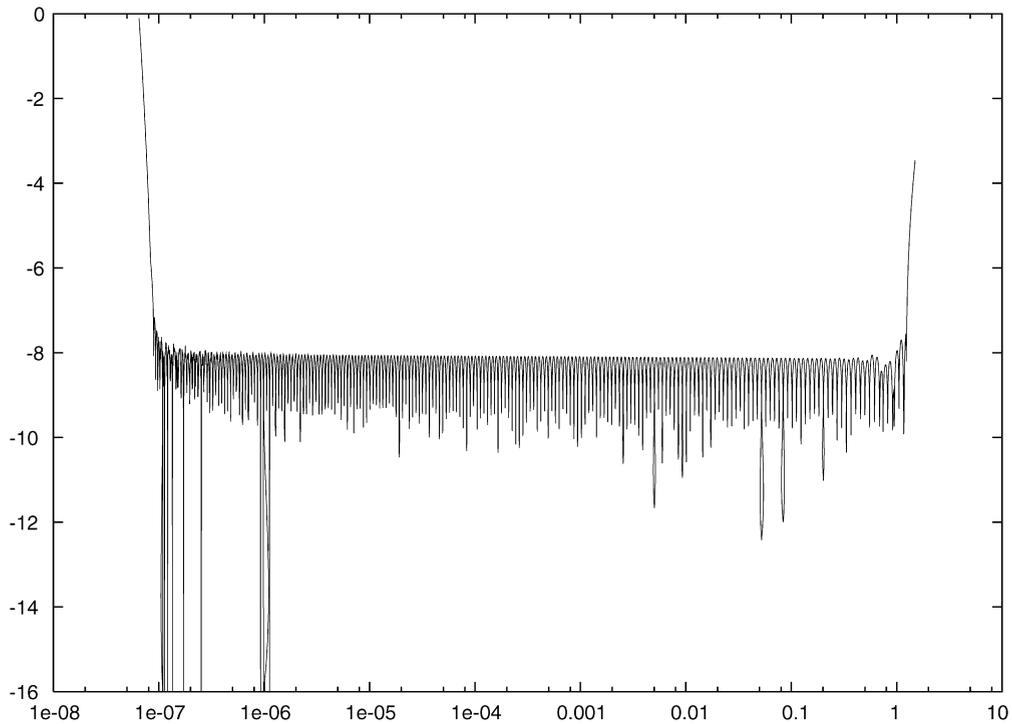


Fig. 2. Error ( $\log_{10}$ ) of approximating  $1/\|\mathbf{x}\|^3$  using Proposition 2 with consequent optimization, where  $\epsilon \approx 10^{-8}$ ,  $10^{-7} \leq \|\mathbf{x}\| \leq 1$  and  $M = 110$ .

by the trapezoidal rule, namely, setting  $p_m = e^{2s_m}$  and  $w_m = 2\Delta s e^{\alpha s_m} / \Gamma(\alpha/2)$ , where  $s_m = s_0 + (m - 1)\Delta s$ ,  $m = 1, \dots, M$ . For a given accuracy  $\epsilon$  and range  $0 < \delta \leq r \leq 1$ , we select  $s_0$  and  $s_M = s_0 + (M - 1)\Delta s$ , the end points of the interval of integration replacing the real line in (5), so that at these points the function  $f(s) = e^{-r^2 e^{2s} + \alpha s}$  and a sufficient number of its derivatives are close to zero (to within the desired accuracy). We also select  $M$ , the number of points in the quadrature, so that the accuracy requirement is satisfied.

Such approximation is easy to obtain but it is not optimal. Further reduction of the number of terms using the approach in [17] yields either an optimized approximation in (1) or an approximation in (3) with a different relative norm. We note the remarkable range,  $[\delta, 1]$ , over which the approximation is valid for these singular functions. For the details on the optimization algorithm, we refer to [17].

### 2.2. The cross-correlation functions

We use the scaling functions of the multiwavelet bases developed in [9]. For a brief review of the multiwavelet bases see also [10]. The scaling functions  $\phi_i$  are the normalized Legendre polynomials on the interval  $[0, 1]$ ,

$$\phi_i(x) = \begin{cases} \sqrt{2i+1} P_i(2x-1), & x \in [0, 1], \\ 0, & x \notin [0, 1], \end{cases} \tag{6}$$

where  $P_i$  are the Legendre polynomials on  $[-1, 1]$ ,  $i = 0, \dots, m - 1$ , and  $m$  is the order of the basis.

For convolution operators we only need to compute integrals with the cross-correlation functions of the scaling functions, namely,

$$\Phi_{ii'}(x) = \int_{-\infty}^{\infty} \phi_i(x+y)\phi_{i'}(y) dy. \tag{7}$$

Since the supports of the scaling functions are restricted to  $[0, 1]$ , the functions  $\Phi_{ii'}$  are zero outside the interval  $[-1, 1]$  and are polynomials on  $[-1, 0]$  and  $[0, 1]$  of degree  $i + i' + 1$ ,

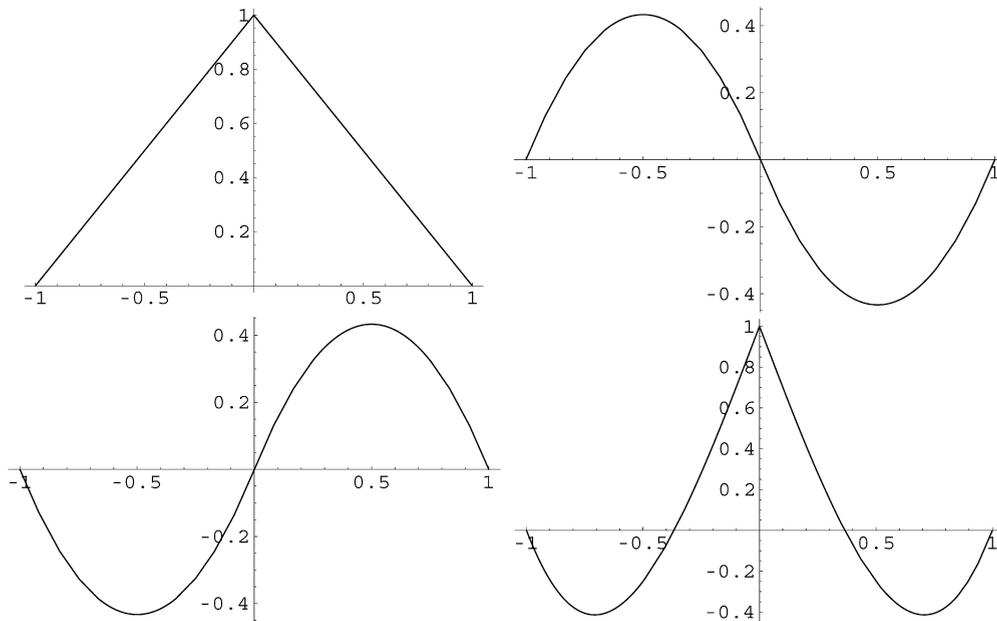


Fig. 3. The first four cross-correlation functions  $\Phi_{00}$ ,  $\Phi_{01}$ ,  $\Phi_{10}$ , and  $\Phi_{11}$ .

$$\Phi_{ii'}(x) = \begin{cases} \Phi_{ii'}^+(x), & 0 \leq x \leq 1, \\ \Phi_{ii'}^-(x), & -1 \leq x < 0, \\ 0, & 1 < |x|, \end{cases} \tag{8}$$

where  $i, i' = 0, \dots, m - 1$  and

$$\Phi_{ii'}^+(x) = \int_0^{1-x} \phi_i(x+y)\phi_{i'}(y) dy, \quad \Phi_{ii'}^-(x) = \int_{-x}^1 \phi_i(x+y)\phi_{i'}(y) dy. \tag{9}$$

The first four cross-correlation functions are illustrated in Fig. 3.

We summarize relevant properties of the cross-correlation functions  $\Phi_{ii'}$  in

- Proposition 3.** (1) *Transposition of indices:*  $\Phi_{ii'}(x) = (-1)^{i+i'} \Phi_{i'i}(x)$ .  
 (2) *Relations between  $\Phi^+$  and  $\Phi^-$ :*  $\Phi_{i,i'}^-(x) = (-1)^{i+i'} \Phi_{i,i'}^+(x)$  for  $0 \leq x \leq 1$ .  
 (3) *Values at zero:*  $\Phi_{ii'}(0) = 0$  for  $i \neq i'$ , and  $\Phi_{ii}(0) = 1$  for  $i = 0, \dots, m - 1$ .  
 (4) *Upper bound:*  $\max_{x \in [-1,1]} |\Phi_{ii'}(x)| \leq 1$  for  $i, i' = 0, \dots, m - 1$ .  
 (5) *Connection with the Gegenbauer polynomials:*  $\Phi_{00}^+(x) = \frac{1}{2} C_1^{(-1/2)}(2x - 1) + \frac{1}{2}$  and  $\Phi_{i0}^+(x) = \frac{1}{2} \sqrt{2i + 1} \times C_{i+1}^{(-1/2)}(2x - 1)$  for  $i = 1, 2, \dots$ , where  $C_{i+1}^{(-1/2)}$  are the Gegenbauer polynomials.  
 (6) *Linear expansion:* if  $i' \geq i$  then we have

$$\Phi_{ii'}^+(x) = \sum_{l=i'-i}^{i'+i} c_{ii'}^l \Phi_{i0}^+(x), \tag{10}$$

where

$$c_{ii'}^l = \begin{cases} 4l(l+1) \int_0^1 \Phi_{ii'}^+(x)\Phi_{i0}^+(x)(1 - (2x - 1)^2)^{-1} dx, & i' > i, \\ 4l(l+1) \int_0^1 (\Phi_{ii}^+(x) - \Phi_{00}^+(x))\Phi_{i0}^+(x)(1 - (2x - 1)^2)^{-1} dx, & i' = i, \end{cases} \tag{11}$$

for  $l \geq 1$  and  $c_{ii'}^0 = \delta_{ii'}$ .

- (7) *Vanishing moments:* we have  $\int_{-1}^1 \Phi_{00}(x) dx = 1$  and  $\int_{-1}^1 x^k \Phi_{ii'}(x) dx = 0$  for  $i + i' \geq 1$  and  $0 \leq k \leq i + i' - 1$ .

We use properties of the cross-correlation functions in computing multiresolution representations of operators in multiwavelet bases. A brief proof of these properties is given in Appendix A.

### 3. The Poisson kernel in 3D

Let us consider the Poisson kernel,

$$K(\mathbf{x}) = \frac{1}{4\pi} \frac{1}{\|\mathbf{x}\|}, \quad (12)$$

where  $\mathbf{x} \in \mathbb{R}^3$  and  $\|\cdot\|$  denotes the Euclidean distance. The function  $K$  satisfies  $-\Delta K(\mathbf{x}) = \delta(\mathbf{x})$ , and the Poisson operator is a convolution with the kernel  $K$ . In order to represent this operator in multiwavelet bases, we need to compute the integrals

$$t_{ii',jj',kk'}^{n;I,I'} = \int K(\mathbf{x} - \mathbf{y}) \phi_{i,l_1}^n(x_1) \phi_{i',l_1'}^n(y_1) \phi_{j,l_2}^n(x_2) \phi_{j',l_2'}^n(y_2) \phi_{k,l_3}^n(x_3) \phi_{k',l_3'}^n(y_3) \, d\mathbf{x} \, d\mathbf{y}, \quad (13)$$

where  $\mathbf{x} = (x_1, x_2, x_3)$ ,  $\mathbf{y} = (y_1, y_2, y_3)$ ,  $I = (l_1, l_2, l_3)$  and  $I' = (l_1', l_2', l_3')$ . The integration in (13) is over the support of the product of one-dimensional scaling functions,

$$\phi_{i,l}^n(x) = 2^{n/2} \phi_i(2^n x - l), \quad (14)$$

where  $\phi_i$  are defined in (6),  $i = 0, \dots, m-1$ , and  $m$  is the order of the basis. We note that the total number of coefficients in (13),  $m^6$  for each  $I$  and  $I'$ , is too large for a practical method of applying this kernel. To reduce the cost of using coefficients (13), we construct their separated representation for a finite but arbitrary accuracy  $\epsilon$ . As a result, the computation of coefficients (13) reduces to the evaluation of a small number of one-dimensional integrals.

By changing variables of integration and taking advantage of  $K$  being a convolution, we obtain  $t_{ii',jj',kk'}^{n;I,I'} = t_{ii',jj',kk'}^{n;I-I'}$  and

$$t_{ii',jj',kk'}^{n;I} = 2^{-3n} \int_B K(2^{-n}(\mathbf{x} + I)) \Phi_{ii'}(x_1) \Phi_{jj'}(x_2) \Phi_{kk'}(x_3) \, d\mathbf{x}, \quad (15)$$

where  $\Phi_{ii'}(x)$  are the cross-correlation of the scaling functions (9) and  $B = [-1, 1]^3$ . Furthermore, due to the homogeneity of the Poisson kernel, we have

$$t_{ii',jj',kk'}^{n;I} = 2^{-2n} t_{ii',jj',kk'}^I, \quad (16)$$

where

$$t_{ii',jj',kk'}^I = t_{ii',jj',kk'}^{l_1, l_2, l_3} = \int_B K(\mathbf{x} + I) \Phi_{ii'}(x_1) \Phi_{jj'}(x_2) \Phi_{kk'}(x_3) \, d\mathbf{x}. \quad (17)$$

We prove

**Theorem 4.** For any  $\epsilon > 0$  and  $0 < \delta \leq 1$  the coefficients  $t_{ii',jj',kk'}^I$  in (17) have an approximation with a low separation rank,

$$r_{ii',jj',kk'}^I = \frac{1}{4\pi} \sum_{m=1}^M \frac{w_m}{b} F_{ii'}^{m,l_1} F_{jj'}^{m,l_2} F_{kk'}^{m,l_3}, \quad (18)$$

such that if  $\max_i |l_i| \geq 2$ , then

$$|t_{ii',jj',kk'}^I - r_{ii',jj',kk'}^I| \leq \frac{2\epsilon}{\pi}, \quad (19)$$

and if  $\max_i |l_i| \leq 1$ , then

$$|t_{ii',jj',kk'}^I - r_{ii',jj',kk'}^I| \leq C\delta^2 + \frac{2\epsilon}{\pi}, \quad (20)$$

where  $b = \sqrt{3} + \|\mathbf{l}\|$ ,

$$F_{ii'}^{m,l} = \int_{-1}^1 e^{-p_m(x+l)^2/b^2} \Phi_{ii'}(x) dx, \tag{21}$$

and  $\delta, M, p_m, w_m, m = 1, \dots, M$  are described in Propositions 1 or 2 for  $\alpha = 1$ .

**Proof.** For  $\mathbf{x} \in B, b = \sqrt{3} + \|\mathbf{l}\| \geq \|\mathbf{x} + \mathbf{l}\| \geq \delta b$ , we have from Proposition 1

$$\left| \frac{1}{\|\mathbf{x} + \mathbf{l}\|} - \sum_{m=1}^M \frac{w_m}{b} e^{-p_m \|\mathbf{x} + \mathbf{l}\|^2/b^2} \right| \leq \frac{\epsilon}{\|\mathbf{x} + \mathbf{l}\|}. \tag{22}$$

If  $\max_i |l_i| \geq 2$ , then  $\min_{\mathbf{x} \in B} \|\mathbf{x} + \mathbf{l}\| = 1$  and the integral in (17) has no singularities. We then obtain by using (22) in (17),

$$|l_{ii',jj',kk'}^l - r_{ii',jj',kk'}^l| \leq \frac{\epsilon}{4\pi} \int_B \frac{d\mathbf{x}}{\|\mathbf{x} + \mathbf{l}\|} \leq \frac{\epsilon}{4\pi} \int_B d\mathbf{x} \leq \frac{2\epsilon}{\pi}. \tag{23}$$

If  $\max_i |l_i| \leq 1$ , we split the domain of integration in (17) into the neighborhood around the singularity  $D_\rho = \{\mathbf{x}: \|\mathbf{x} + \mathbf{l}\| \leq \rho\}$ , where  $\rho = \delta b$ , and  $B \setminus D_\rho$ . The estimate for the integral over  $B \setminus D_\rho$  is the same as in (23). However, in addition, we need to estimate the integrals over  $D_\rho$  for both the kernel and its approximation. Using  $|\Phi_{ii'}| \leq 1$  and changing variables  $\mathbf{y} = \mathbf{x} + \mathbf{l}$ , we have

$$\left| \frac{1}{4\pi} \int_{D_\rho} \frac{1}{\|\mathbf{x} + \mathbf{l}\|} \Phi_{ii'}(x_1) \Phi_{jj'}(x_2) \Phi_{kk'}(x_3) d\mathbf{x} \right| \leq \frac{1}{4\pi} \int_{\|\mathbf{y}\| \leq \rho} \frac{1}{\|\mathbf{y}\|} d\mathbf{y} \leq \frac{\rho^2}{2}. \tag{24}$$

For the approximation of the kernel in (22), we have

$$\begin{aligned} \left| \frac{1}{4\pi} \int_{D_\rho} \sum_{m=1}^M \frac{w_m}{b} e^{-p_m \|\mathbf{x} + \mathbf{l}\|^2/b^2} \Phi_{ii'}(x_1) \Phi_{jj'}(x_2) \Phi_{kk'}(x_3) d\mathbf{x} \right| &\leq \frac{1}{4\pi b} \sum_{m=1}^M w_m e^{-p_m \delta^2} \int_{D_\rho} d\mathbf{x} \\ &\leq \frac{\rho^3}{3b} \sum_{m=1}^M w_m e^{-p_m \delta^2}. \end{aligned} \tag{25}$$

Using (22) for  $\delta b = \|\mathbf{x} + \mathbf{l}\|$ , we have  $|1 - \delta \sum_{m=1}^M w_m e^{-p_m \delta^2}| \leq \epsilon$ , so that

$$\frac{\rho^3}{3b} \sum_{m=1}^M w_m e^{-p_m \delta^2} \leq \frac{\delta^2 b^2}{3} \left| \delta \sum_{m=1}^M w_m e^{-p_m \delta^2} - 1 \right| + \frac{\delta^2 b^2}{3} \leq \delta^2 \frac{b^2}{3} (1 + \epsilon). \tag{26}$$

Combining (24), (25), and (26), we obtain (20).  $\square$

**Remark 5.** The statement of the theorem continues to hold if instead of Proposition 1 we use the exponents and weights in Proposition 2 for  $n = 1$  and its weaker estimate

$$\left| \frac{1}{r} - \sum_{m=1}^M w_m e^{-p_m r^2} \right| \leq \frac{\epsilon}{r^2}. \tag{27}$$

Then, instead of (20), we obtain

$$|l_{ii',jj',kk'}^l - r_{ii',jj',kk'}^l| \leq C\delta + \frac{2\epsilon}{\pi}. \tag{28}$$

**Remark 6.** Not all terms are needed in the derived approximations. In practical computations terms in (18) that are below the threshold of accuracy  $\epsilon$  may be removed. The near-optimality of expansion of  $1/r$  via Gaussians does not

imply the same for (18). In fact for  $\mathbf{l}$  with  $\max_i |l_i| \geq 2$ , the contribution of most of the terms in (18) is below the threshold of accuracy  $\epsilon$  due to a limited range of (22) needed in (23). We also note that the separation rank of the representation in (18) can be reduced further by using algorithms in [2,3].

#### 4. Projector on the divergence-free functions in 3D

The projector on the divergence-free vector functions in  $\mathbb{R}^3$ , the so-called Leray projector, is a singular homogeneous operator of order zero. As an integral operator, it is a convolution with the kernel acting on vector functions in  $\mathbb{R}^3$ ,

$$P_{qq'}(\mathbf{x}) = \delta_{qq'}\delta(\mathbf{x}) - \frac{1}{4\pi} \frac{\partial^2}{\partial x_q \partial x_{q'}} \left( \frac{1}{\|\mathbf{x}\|} \right) = \delta_{qq'}\delta(\mathbf{x}) - \frac{1}{4\pi} \left[ \frac{\delta_{qq'}}{\|\mathbf{x}\|^3} - \frac{3x_q x_{q'}}{\|\mathbf{x}\|^5} \right], \tag{29}$$

where  $q, q' = 1, 2, 3$ ,  $\delta_{qq'}$  is the Kronecker delta, and  $\delta(\mathbf{x})$  is the three-dimensional delta function. It appears in many applications, notably in fluid dynamics, and can be found in a variety of forms in mathematical literature, see, e.g., [21]. Although this operator has long been used in analysis, its use in numerical applications has been limited. A multiresolution representation of the kernel (29) using compactly supported wavelets can be found in [13] and in multiwavelet bases in [15]. In this paper we construct a multiresolution *separated* representation of the projector on the divergence-free functions necessary for its accurate and efficient numerical implementation.

Using essentially the same derivation as for the Poisson kernel, we obtain a representation of  $P_{qq'}(\mathbf{x})$  by computing integrals formally written as

$$t_{ii'jj'kk'}^{l,qq'} = -\frac{1}{4\pi} \int_B \left[ \frac{\delta_{qq'}}{\|\mathbf{x} + \mathbf{l}\|^3} - \frac{3(x_q + l_q)(x_{q'} + l_{q'})}{\|\mathbf{x} + \mathbf{l}\|^5} \right] \Phi_{ii'}(x_1) \Phi_{jj'}(x_2) \Phi_{kk'}(x_3) \, d\mathbf{x}, \tag{30}$$

where  $B = [-1, 1]^3$ ,  $\mathbf{l} = (l_1, l_2, l_3)$  and  $q, q' = 1, 2, 3$ . Some of these integrals are only conditionally convergent and their meaning will be clarified later. The fact that the operator is singular results in different error estimates (in comparison with Theorem 4) and expressions for terms affected by the singularity. We will use the approximation of  $1/\|\mathbf{x}\|^3$  by Gaussians to construct the separated representation of the components of this matrix kernel.

Since the operator is homogeneous of degree zero, for the coefficients on scale  $n$  we have

$$t_{ii'jj'kk'}^{n;l,qq'} = t_{ii'jj'kk'}^{l,qq'}. \tag{31}$$

We consider separately the diagonal  $t_{ii'jj'kk'}^{l,qq}$ , and the off-diagonal  $t_{ii'jj'kk'}^{l,qq'}$ ,  $q \neq q'$ ,  $q, q' = 1, 2, 3$  terms in (30) and obtain that for any  $\epsilon > 0$  the coefficients  $t_{ii'jj'kk'}^{l,qq'}$  in (30) have an approximation with a low separation rank. We summarize our results as

**Theorem 7.** *Let  $\delta$ ,  $M$ ,  $p_m$ ,  $w_m$  and  $\epsilon$  be as in Proposition 2 for  $\alpha = 3$ . Then we have:*

(1) *With the exception of  $\mathbf{l} = \mathbf{0}$  and  $i = i'$ ,  $j = j'$ , and  $k = k'$ , the diagonal terms in (30) are approximated as*

$$r_{ii'jj'kk'}^{l,11} = \frac{1}{4\pi} \sum_{m=1}^M \frac{w_m}{b^3} G_{ii'}^{m,l_1} F_{jj'}^{m,l_2} F_{kk'}^{m,l_3}, \tag{32}$$

$$r_{ii'jj'kk'}^{l,22} = \frac{1}{4\pi} \sum_{m=1}^M \frac{w_m}{b^3} F_{ii'}^{m,l_1} G_{jj'}^{m,l_2} F_{kk'}^{m,l_3}, \tag{33}$$

$$r_{ii'jj'kk'}^{l,33} = \frac{1}{4\pi} \sum_{m=1}^M \frac{w_m}{b^3} F_{ii'}^{m,l_1} F_{jj'}^{m,l_2} G_{kk'}^{m,l_3}, \tag{34}$$

where  $b = \sqrt{3} + \|\mathbf{l}\|$ ,

$$F_{jj'}^{m,l} = \int_{-1}^1 e^{-p_m(x+l)^2/b^2} \Phi_{jj'}(x) \, dx \tag{35}$$

and

$$r_{ii'}^{m,l} = \frac{2p_m}{b^2} \int_{-1}^1 e^{-p_m(x+l)^2/b^2} (x+l)^2 \Phi_{ii'}(x) dx - F_{ii'}^{m,l}. \tag{36}$$

(2) If  $l = \mathbf{0}$  and  $i = i', j = j',$  and  $k = k',$  then the approximation is of the form

$$r_{ijjkk}^{\mathbf{0},11} = \frac{1}{4\pi} \sum_{m=1}^M \frac{w_m}{b^3} G_{ii}^{m,0} F_{jj}^{m,0} F_{kk}^{m,0} - \frac{1}{4\pi} \sum_{m=1}^M \frac{w_m}{b^3} G_{00}^{m,0} F_{00}^{m,0} F_{00}^{m,0}, \tag{37}$$

$$r_{ijjkk}^{\mathbf{0},22} = \frac{1}{4\pi} \sum_{m=1}^M \frac{w_m}{b^3} F_{ii}^{m,0} G_{jj}^{m,0} F_{kk}^{m,0} - \frac{1}{4\pi} \sum_{m=1}^M \frac{w_m}{b^3} F_{00}^{m,0} G_{00}^{m,0} F_{00}^{m,0}, \tag{38}$$

$$r_{ijjkk}^{\mathbf{0},33} = \frac{1}{4\pi} \sum_{m=1}^M \frac{w_m}{b^3} F_{ii}^{m,0} F_{jj}^{m,0} G_{kk}^{m,0} - \frac{1}{4\pi} \sum_{m=1}^M \frac{w_m}{b^3} F_{00}^{m,0} F_{00}^{m,0} G_{00}^{m,0}. \tag{39}$$

(3) The off-diagonal terms are approximated as

$$r_{ii'jj'kk'}^{l,12} = \frac{1}{4\pi} \sum_{m=1}^M \frac{2p_m w_m}{b^5} T_{ii'}^{m,l_1} T_{jj'}^{m,l_2} F_{kk'}^{m,l_3}, \tag{40}$$

$$r_{ii'jj'kk'}^{l,13} = \frac{1}{4\pi} \sum_{m=1}^M \frac{2p_m w_m}{b^5} T_{ii'}^{m,l_1} F_{jj'}^{m,l_2} T_{kk'}^{m,l_3}, \tag{41}$$

$$r_{ii'jj'kk'}^{l,23} = \frac{1}{4\pi} \sum_{m=1}^M \frac{2p_m w_m}{b^5} F_{ii'}^{m,l_1} T_{ii'}^{m,l_1} T_{kk'}^{m,l_3}, \tag{42}$$

where

$$T_{jj'}^{m,l} = \int_{-1}^1 e^{-p_m(x+l)^2/b^2} (x+l) \Phi_{jj'}(x) dx. \tag{43}$$

(4) For any  $\epsilon > 0$  and for  $\max_i |l_i| \geq 2,$  we have

$$|t_{ii'jj'kk'}^{l,qq'} - r_{ii'jj'kk'}^{l,qq'}| \leq \epsilon, \tag{44}$$

and, for  $\max_i |l_i| \leq 1,$

$$|t_{ii'jj'kk'}^{l,qq'} - r_{ii'jj'kk'}^{l,qq'}| \leq \epsilon + C\delta. \tag{45}$$

**Proof.** (1) First let us consider the case  $l \neq \mathbf{0}.$  We use

$$\partial_{x_q} \left( \frac{x_q + l_q}{\|\mathbf{x} + \mathbf{l}\|^3} \right) = \frac{1}{\|\mathbf{x} + \mathbf{l}\|^3} - \frac{3(x_q + l_q)(x_q + l_q)}{\|\mathbf{x} + \mathbf{l}\|^5} \tag{46}$$

to integrate by parts the diagonal and

$$\partial_{x_q} \frac{1}{\|\mathbf{x} + \mathbf{l}\|^3} = -\frac{3(x_q + l_q)}{\|\mathbf{x} + \mathbf{l}\|^5} \tag{47}$$

the off-diagonal terms in (30).

We start with the diagonal terms and, without loss of generality, consider only the term with  $q = q' = 1.$  Since the cross-correlation functions  $\Phi_{ii'}(x_1)$  are continuous at  $x_1 = 0$  and  $\Phi_{ii'}(\pm 1) = 0,$  the integration by parts yields

$$t_{ii'jj'kk'}^{l,11} = \frac{1}{4\pi} \int_B \frac{x_1 + l_1}{\|\mathbf{x} + \mathbf{l}\|^3} \Phi_{ii'}(x_1) \Phi_{jj'}(x_2) \Phi_{kk'}(x_3) dx. \tag{48}$$

Here and in what follows, the integration by parts involving the cross-correlation functions is performed by first splitting the interval of their support  $[-1, 1]$  as  $[-1, 0]$  and  $[0, 1]$  on which these functions are polynomials, integrating by parts, and then writing the result as a single integral where possible.

As long as  $\mathbf{l} \neq \mathbf{0}$  and the singularity is not at  $\mathbf{x} = \mathbf{0}$ , the boundary term in the integration by parts vanishes either directly or as a limit. The same properties of the cross-correlation functions also makes (48) integrable. We note that  $\Phi'_{ii'}(x_1)$  in (48) may be discontinuous at  $x_1 = 0$ .

For  $b = \sqrt{3} + \|\mathbf{l}\| \geq \|\mathbf{x} + \mathbf{l}\| \geq \delta b$  for  $x \in B$ , we obtain using (3),

$$\left| \frac{1}{\|\mathbf{x} + \mathbf{l}\|^3} - \sum_{m=1}^M \frac{w_m}{b^3} e^{-p_m \|\mathbf{x} + \mathbf{l}\|^2 / b^2} \right| \leq \frac{\epsilon}{b \|\mathbf{x} + \mathbf{l}\|^2}. \tag{49}$$

Using (48) and the approximation in (49), we arrive at (32), where

$$G_{ii'}^{m,l} = \int_{-1}^1 e^{-p_m(x+l)^2/b^2} (x+l) \Phi'_{ii'}(x) dx, \tag{50}$$

and  $F_{jj'}^{m,l}$  is given by (35). Integrating by parts in (50) and, again, using the continuity of  $\Phi_{ii'}(x_1)$  at zero and  $\Phi_{ii'}(\pm 1) = 0$ , we obtain (36).

(2) If  $\mathbf{l} = \mathbf{0}$  and at least one of the three pairs of indices,  $i \neq i'$ , or  $j \neq j'$ , or  $k \neq k'$ , then the derivation above holds since for at least one of the variables the cross-correlation functions vanish at zero. Again, the integration by parts is done separately on subintervals  $[-1, 0]$  and  $[0, 1]$  and, for the boundary term, a limit taken as  $x_1 \rightarrow 0$  to verify that it vanishes.

If  $\mathbf{l} = \mathbf{0}$  and  $i = i'$ ,  $j = j'$ , and  $k = k'$ , then we cannot integrate by parts in (30) since the function  $\Phi_{ii}(x_1)\Phi_{jj}(x_2) \times \Phi_{kk}(x_3)$  is equal to 1 at  $\mathbf{x} = \mathbf{0}$ . In this case let us first consider (30) for the diagonal terms and  $i = i' = j = j' = k = k' = 0$ ,

$$t_{000000}^{\mathbf{0},11} = -\frac{1}{4\pi} \int_B \frac{x_2^2 + x_3^2 - 2x_1^2}{\|\mathbf{x}\|^5} \Phi_{00}(x_1)\Phi_{00}(x_2)\Phi_{00}(x_3) d\mathbf{x}. \tag{51}$$

We note that this integral is only conditionally convergent and equal to zero if the limit is arranged symmetrically with respect to the variables  $x_1, x_2$ , and  $x_3$ , as the definition of this singular operator requires. For computing  $t_{ii'jj'kk}^{\mathbf{0},11}$  with the non-zero indices, let us replace  $\Phi_{ii}(x_1)\Phi_{jj}(x_2)\Phi_{kk}(x_3)$  in (30) by  $\Phi_{ii}(x_1)\Phi_{jj}(x_2)\Phi_{kk}(x_3) - \Phi_{00}(x_1)\Phi_{00}(x_2)\Phi_{00}(x_3)$ . This combination vanishes at the singularity  $\mathbf{x} = \mathbf{0}$  since both products are equal to 1 at that point. This allows us to integrate by parts and use the approximation in (49) to obtain (37).

(3) Without loss of generality, we consider the off-diagonal term with  $q = 1$  and  $q' = 2$ . After integrating by parts, we have

$$r_{ii'jj'kk'}^{l,12} = \frac{1}{4\pi} \int_B \frac{x_2 + l_2}{\|\mathbf{x} + \mathbf{l}\|^3} \Phi'_{ii'}(x_1)\Phi_{jj'}(x_2)\Phi_{kk'}(x_3) d\mathbf{x}, \tag{52}$$

and, using the approximation in (49), arrive at

$$r_{ii'jj'kk'}^{l,12} = \frac{1}{4\pi} \sum_{m=1}^M \frac{w_m}{b^3} \tilde{T}_{ii'}^{m,l_1} T_{jj'}^{m,l_2} F_{kk'}^{m,l_3}, \tag{53}$$

with (35) and

$$\tilde{T}_{ii'}^{m,l} = \int_{-1}^1 e^{-p_m(x+l)^2/b^2} \Phi'_{ii'}(x) dx. \tag{54}$$

Integrating by parts in (54) yields  $\tilde{T}_{ii'}^{m,l} = 2p_m/b^2 T_{ii'}^{m,l}$ , and, thus, (40).

If  $\mathbf{l} = \mathbf{0}$  and  $i = i', j = j',$  and  $k = k',$  then for the off-diagonal terms we have

$$t_{ii'jj'kk'}^{0,12} = \frac{1}{4\pi} \int_B \frac{3x_1x_2}{\|\mathbf{x}\|^5} \Phi_{ii'}(x_1)\Phi_{jj'}(x_2)\Phi_{kk'}(x_3) \, d\mathbf{x} = 0, \tag{55}$$

as the conditional limit of corresponding integrals for all  $i, j, k.$

(4) If  $\max_i |l_i| \geq 2,$  then  $\min_{\mathbf{x} \in B} \|\mathbf{x} + \mathbf{l}\| = 1$  and the integral in (30) has no singularities. The estimate (44) is then obtained by using (49),

$$|t_{ii'jj'kk'}^{l,qq'} - \tilde{t}_{ii'jj'kk'}^{l,qq'}| \leq \frac{\epsilon}{4\pi b} \int_B \frac{d\mathbf{x}}{\|\mathbf{x} + \mathbf{l}\|^2} \leq \frac{\epsilon}{4\pi\sqrt{3}} \int_{\|\mathbf{x}\| \leq \sqrt{3}} \frac{d\mathbf{x}}{\|\mathbf{x}\|^2} = \epsilon. \tag{56}$$

If  $\max_i |l_i| \leq 1,$  we split the domain of integration for  $t_{ii'jj'kk'}^{l,qq'}$  into the neighborhood around the singularity  $D_\delta = \{\mathbf{x}: \|\mathbf{x} + \mathbf{l}\| \leq \delta\}$  and the rest of the domain,  $B \setminus D_\delta.$  The estimate for the integral over  $B \setminus D_\delta$  is the same as in (56). We need, however, to estimate the integrals over  $D_\delta$  for both the kernel and its approximation. Using  $|\Phi_{ii'}| \leq 1$  and  $|\Phi'_{ii'}| \leq \tilde{C}$  for some constant  $\tilde{C}$  (except at zero), and changing variables to  $\mathbf{y} = \mathbf{x} + \mathbf{l},$  we have for the diagonal term with  $q = q' = 1,$

$$\left| \frac{1}{4\pi} \int_{D_\delta} \frac{x_1 + l_1}{\|\mathbf{x} + \mathbf{l}\|^3} \Phi'_{ii'}(x_1)\Phi_{jj'}(x_2)\Phi_{kk'}(x_3) \, d\mathbf{x} \right| \leq \frac{\tilde{C}}{4\pi} \int_{\|\mathbf{y}\| \leq \delta} \frac{|y_1|}{\|\mathbf{y}\|^3} \, d\mathbf{y} = \frac{\tilde{C}\pi\delta}{4}. \tag{57}$$

This estimate holds also in the case  $\mathbf{l} = \mathbf{0}$  and  $i = i', j = j',$  and  $k = k',$  since we use  $\Phi_{ii'}(x_1)\Phi_{jj'}(x_2)\Phi_{kk'}(x_3) - \Phi_{00}(x_1)\Phi_{00}(x_2)\Phi_{00}(x_3)$  in the definition of non-zero terms. Also it holds for the off-diagonal terms as follows from the structure of (52). For the expression approximating the kernel, we have

$$\begin{aligned} & \left| \frac{1}{4\pi} \int_{D_\delta} \sum_{m=1}^M \frac{w_m}{b^3} e^{-p_m/b^2\|\mathbf{x}+\mathbf{l}\|^2} (x_1 + l_1)\Phi'_{ii'}(x_1)\Phi_{jj'}(x_2)\Phi_{kk'}(x_3) \, d\mathbf{x} \right| \\ & \leq \frac{\tilde{C}}{4\pi} \sum_{m=1}^M \frac{w_m}{b^3} e^{-p_m\delta^2} \int_{D_\delta} |x_1 + l_1| \, d\mathbf{x} \leq \frac{\tilde{C}}{4\pi} \sum_{m=1}^M \frac{w_m}{b^3} e^{-p_m\delta^2} \int_{\|\mathbf{y}\| \leq \delta} |y_1| \, d\mathbf{y} = \frac{\tilde{C}\pi\delta^4}{16b^3} \sum_{m=1}^M w_m e^{-p_m\delta^2}. \end{aligned} \tag{58}$$

Using (49) for  $\delta b = \|\mathbf{x} + \mathbf{l}\|,$  we have  $|1 - \delta^3 \sum_{m=1}^M w_m e^{-p_m\delta^2}| \leq \epsilon\delta,$  so that

$$\frac{\tilde{C}\pi\delta^4}{16b^3} \sum_{m=1}^M w_m e^{-p_m\delta^2} = \frac{\tilde{C}\pi\delta}{16b^3} \left( \delta^3 \sum_{m=1}^M w_m e^{-p_m\delta^2} - 1 \right) + \frac{\tilde{C}\pi\delta}{16b^3} \leq \left( \frac{\tilde{C}\pi\epsilon\delta}{16b^3} + \frac{\tilde{C}\pi}{16b^3} \right) \delta. \tag{59}$$

Using (59), (58), and (57), we obtain (45).  $\square$

**Remark 8.** For some shifts  $\mathbf{l},$  the estimate in (45) can be improved with respect to  $\delta.$  If  $|l_1| + |l_2| + |l_3| = 3$  or  $|l_1| + |l_2| + |l_3| = 2,$  then a more careful estimate shows that this term is  $\mathcal{O}(\delta^2).$  If  $|l_1| + |l_2| + |l_3| = 1,$  then for the off-diagonal terms the estimate is also  $\mathcal{O}(\delta^2).$  In all of these cases the effective singularity of the integrand turns out to be weaker than that prescribed by the kernel since the cross-correlation functions are zero at the point of singularity.

In the next section we show how to remove the error due to the singularity by using explicit asymptotic estimates of the coefficients.

### 5. Improving representation near the singularity

The estimates (20) and (45) depend on the range of validity of the separated representations in Propositions 1 and 2; in particular, on the distance  $\delta$  from the singularity of the kernel. We observe (see Section 2.1) that there is a correspondence between  $\delta$  and the upper range of the exponents  $p_m$  in (1) and (3), namely, the exponents grow rapidly as  $\delta \rightarrow 0.$  For large exponents we can compute integrals that define the coefficients in Theorems 4 and 7 by

using asymptotic expansions and, as a result, obtain for them simple analytic expressions. Moreover, if we combine the contributions of the terms with large exponents, we effectively remove the dependence on the parameter  $\delta$  altogether. In the process of accounting for the singularity in this manner, we also reduce the separation rank of the representation. Although the separation rank in Propositions 1 and 2 is near optimal, the resulting representation for operators in Theorems 4 and 7, however reasonable, may not have the same property since the terms with large exponents yield almost the same coefficients (up to a multiplicative factor) and are easily combined to reduce the separation rank further. We note that a simplification also occurs for the terms with very small exponents. This may be easily verified by using the Taylor expansion of the exponential in appropriate integrals and is not considered here.

To motivate this section consider (5) for  $\alpha = 1$ , and split the integral into two, over  $(-\infty, \bar{s}]$  and  $[\bar{s}, \infty)$ , with some  $\bar{s} > 0$ . Let us consider

$$f(r) = \frac{2}{\sqrt{\pi}} \int_{\bar{s}}^{\infty} e^{-r^2 e^{2s} + s} ds,$$

and use this expression to compute its contribution to the representation of the Poisson kernel. Let us consider the terms with  $\mathbf{l} = \mathbf{0}$  and we obtain

$$\frac{2}{\sqrt{\pi}} \int_{\bar{s}}^{\infty} \int_B e^{-\|\mathbf{x}\|^2 e^{2s} + s} \Phi_{ii'}(x_1) \Phi_{jj'}(x_2) \Phi_{kk'}(x_3) d\mathbf{x} ds = \frac{2}{\sqrt{\pi}} \int_{\bar{s}}^{\infty} e^s I_{ii'}(s) I_{jj'}(s) I_{kk'}(s) ds,$$

where

$$I_{ii'}(s) = \int_{-1}^1 e^{-x^2 e^{2s}} \Phi_{ii'}(x) dx. \tag{60}$$

Let us select  $\bar{s}$  so that  $e^{2\bar{s}}$  is large enough so that in (60) we can approximate  $\Phi_{ii'}(x) \approx \Phi_{ii'}(0) = \delta_{ii'}$ . We have  $I_{ii'}(s) = \sqrt{\pi} e^{-s} \delta_{ii'}$  and the dominant contribution then amounts to

$$\pi e^{-2\bar{s}} \delta_{ii'} \delta_{jj'} \delta_{kk'}.$$

Since the interval  $[\bar{s}, \infty)$  in (5) accounts for the singularity at  $r = 0$ , its full contribution is evaluated explicitly. For practical purposes it is convenient to account for such contribution after the discretization of the integral (5) as in Proposition 1. We formulate our observations as

**Theorem 9.** *Let us write the separated representation (18) obtained using Proposition 1 as*

$$r_{ii',jj',kk'}^{\mathbf{l}} = \tilde{r}_{ii',jj',kk'}^{\mathbf{l}} + \tilde{r}_{ii',jj',kk'}^{\mathbf{l}}, \tag{61}$$

by splitting the sum in Proposition 1 into two parts  $\sum_{m=1}^{M_0-1}$  and  $\sum_{m=M_0}^M$  (respectively), where  $M \rightarrow \infty$  and  $M_0$  is selected given the desired accuracy  $\epsilon$ .

For  $\mathbf{l} = \mathbf{0}$  we have

$$\tilde{r}_{ii',jj',kk'}^{\mathbf{0}} = q_0 \delta_{ii'} \delta_{jj'} \delta_{kk'} + \mathcal{O}(e^{-3s(M_0)}), \tag{62}$$

where  $q_0 = b^2 \pi [2h/(1 - e^{-2h})] e^{-2s(M_0)}$  and  $s(M_0) = s_0 + (M_0 - 1)h$  is the length of a subinterval in the trapezoidal rule approximation of (5) for  $\alpha = 1$ .

For  $\mathbf{l} \neq \mathbf{0}$  we have

$$\tilde{r}_{ii',jj',kk'}^{\mathbf{l}} = \mathcal{O}(e^{-3s(M_0)}). \tag{63}$$

We note that the error in the approximation (62) does not depend on the parameter  $\delta$  in Proposition 1. Also,  $s(M_0)$  in this theorem corresponds to  $\bar{s}$  in the motivating discussion above.

**Proof.** To demonstrate (62), let us consider (21) as a function of the exponent  $p$ ,

$$F_{ii'}^{\mathbf{l}}(p) = \int_{-1}^1 e^{-p(x-l)^2} \Phi_{ii'}(x) dx, \tag{64}$$

where  $F_{ii'}^{m,l} = F_{ii'}^{-l}(p_m/b^2)$ . The function  $\Phi_{ii'}(x)$  is a polynomial on subintervals  $[0, 1]$  and  $[-1, 0]$ . Using the Taylor expansion in  $[0, 1]$  at points  $l = 0, 1$ , we have

$$\Phi_{ii'}^+(x) = \Phi_{ii'}^+(l) + \Phi_{ii'}^{\prime+}(l)(x - l) + \Phi_{ii'}^{\prime\prime+}(l)\frac{(x - l)^2}{2} + \dots, \tag{65}$$

where the one-sided derivatives are computed at the end points in directions from the interior of the interval  $[0, 1]$  (outer derivative), and set  $\Phi_{ii'}^+(x) = \Phi_{ii'}^{\prime+}(x) = \Phi_{ii'}^{\prime\prime+}(x) = \dots = 0$  for all  $x$  outside  $[0, 1]$ . Similarly, we have expansion for  $\Phi_{ii'}^-(x)$  in  $[-1, 0]$  at points  $l = -1, 0$ ,

$$\Phi_{ii'}^-(x) = \Phi_{ii'}^-(l) + \Phi_{ii'}^{\prime-}(l)(x - l) + \Phi_{ii'}^{\prime\prime-}(l)\frac{(x - l)^2}{2} + \dots, \tag{66}$$

and set  $\Phi_{ii'}^-(x) = \Phi_{ii'}^{\prime-}(x) = \Phi_{ii'}^{\prime\prime-}(x) = \dots = 0$  for all  $x$  outside  $[-1, 0]$ .

For large  $p$  (say,  $p > 100$ ), we replace  $e^{-p}$ ,  $\text{erf}(\sqrt{p})$  and  $\text{erf}(-\sqrt{p})$  by their limits. Here  $\text{erf}(\cdot)$  denotes the error function,

$$\text{erf}(s) = \frac{2}{\sqrt{\pi}} \int_0^s e^{-t^2} dt. \tag{67}$$

Since  $\text{erf}(-s) = -\text{erf}(s)$ ,  $\text{erf}(0) = 0$  and  $\text{erf}(\sqrt{p}) \rightarrow 1$  for large  $p$ , we have for  $l = 0, 1$ ,

$$\begin{aligned} \int_0^1 e^{-p(x-l)^2} dx &= \sqrt{\pi}[\text{erf}(l\sqrt{p}) - \text{erf}((l-1)\sqrt{p})]/2p^{1/2} \rightarrow \sqrt{\pi}/2p^{1/2}, \\ \int_0^1 (x-l)e^{-p(x-l)^2} dx &= [e^{-l^2p} - e^{-(l-1)^2p}]/2p \rightarrow \begin{cases} 1/2p, & l=0, \\ -1/2p, & l=1, \end{cases} \\ \int_0^1 (x-l)^2 e^{-p(x-l)^2} dx &= [(l-1)e^{-(l-1)^2p} - le^{-l^2p}]/2p + \sqrt{\pi}[\text{erf}(l\sqrt{p}) - \text{erf}((l-1)\sqrt{p})]/4p^{3/2} \\ &\rightarrow \sqrt{\pi}/4p^{3/2}. \end{aligned} \tag{68}$$

For  $l = -1$  and large  $p$  these integrals approach zero exponentially fast and are set to zero. Similarly, for  $l = -1, 0$ , we have

$$\begin{aligned} \int_{-1}^0 e^{-p(x-l)^2} dx &\rightarrow \sqrt{\pi}/2p^{1/2}, \\ \int_{-1}^0 (x-l)e^{-p(x-l)^2} dx &\rightarrow \begin{cases} -1/2p, & l=0, \\ 1/2p, & l=-1, \end{cases} \\ \int_{-1}^0 (x-l)^2 e^{-p(x-l)^2} dx &\rightarrow \sqrt{\pi}/4p^{3/2} \end{aligned} \tag{69}$$

and set integrals to zero for  $l = 1$ . Combining (64)–(66), (68), and (69), we obtain for  $l = -1, 0, 1$ ,

$$F_{ii'}^l(p) = \sqrt{\pi} \frac{\Phi_{ii'}(l)}{p^{1/2}} + (-1)^l \frac{\Phi_{ii'}^{\prime+}(l) - \Phi_{ii'}^{\prime-}(l)}{2p} + \frac{\sqrt{\pi}}{8} \frac{\Phi_{ii'}^{\prime\prime+}(l) + \Phi_{ii'}^{\prime\prime-}(l)}{p^{3/2}} + \mathcal{O}\left(\frac{1}{p^2}\right). \tag{70}$$

This expansion allows us to compute explicitly a portion of the separated representation near the singularity. In Proposition 1, we use the trapezoidal rule as the first step in approximating the kernel. Let us choose the range  $[\delta, 1]$  over which such approximation is valid. We have

$$\left| \frac{1}{\|\mathbf{x}\|} - \sum_{m=1}^M \frac{w_m}{b} e^{-p_m \|\mathbf{x}\|^2/b^2} \right| \leq \frac{\epsilon}{\|\mathbf{x}\|}, \tag{71}$$

where  $M \rightarrow \infty$  as  $\delta \rightarrow 0$  and  $p_m = e^{2s_m}$ ,  $w_m = 2he^{s_m}/\sqrt{\pi}$ , and  $s(m) = s_0 + (m - 1)h$  (see Section 2.1 for criteria in choosing  $s_0$  and  $h$ ). We split the sum in (71) into two parts,  $\sum_{m=1}^{M_0-1}$  and  $\sum_{m=M_0}^M$ , and consider  $M \rightarrow \infty$ . For sufficiently large  $M_0$ , we obtain the main term

$$\tilde{r}_{ii',jj',kk'}^0 = \sum_{m=M_0}^{\infty} \frac{w_m}{b} F_{ii'}^{m,0} F_{jj'}^{m,0} F_{kk'}^{m,0} = q_0 \Phi_{ii'}(0) \Phi_{jj'}(0) \Phi_{kk'}(0) + \mathcal{O}(e^{-3s(M_0)}), \tag{72}$$

where

$$q_0 = \sum_{m=M_0}^{\infty} \frac{w_m}{b} \left( \frac{b\sqrt{\pi}}{\sqrt{p_m}} \right)^3 = 2hb^2\pi \sum_{m=M_0}^{\infty} e^{-2s(m)} = b^2\pi \frac{2h}{1 - e^{-2h}} e^{-2s(M_0)}, \tag{73}$$

and the next term yields  $\mathcal{O}(e^{-3s(M_0)})$ . Using property (3) of the cross-correlation functions, we obtain (62), a purely diagonal contribution in the separated representation.  $\square$

Using the same approach for the projector on the divergence free functions, we demonstrate

**Theorem 10.** We write the separated representations in (32)–(34), (37)–(39), and (40)–(42) obtained using Proposition 1 as

$$r_{ii',jj',kk'}^{l,qq} = \tilde{r}_{ii',jj',kk'}^{l,qq} + \tilde{r}_{ii',jj',kk'}^{l,qq}, \tag{74}$$

by splitting the sum in Proposition 1 into two parts  $\sum_{m=1}^{M_0-1}$  and  $\sum_{m=M_0}^M$ , where  $M \rightarrow \infty$  and  $M_0$  is selected given the desired accuracy  $\epsilon$ .

For  $l \neq 0$  we have

$$\begin{aligned} \tilde{r}_{ii',jj',kk'}^{l,qq} &= q_1 \frac{(-1)^{l_1}}{2} (\Phi_{ii'}^{'+}(-l_1) - \Phi_{ii'}^{'-}(-l_1)) \Phi_{jj'}(-l_2) \Phi_{kk'}(-l_3) \\ &\quad + q_2 \frac{(-1)^{l_1+l_2}}{4} (\Phi_{ii'}^{'+}(-l_1) - \Phi_{ii'}^{'-}(-l_1)) (\Phi_{jj'}^{'+}(-l_2) - \Phi_{jj'}^{'-}(-l_2)) \Phi_{kk'}(-l_3) \\ &\quad + q_2 \frac{(-1)^{l_1+l_3}}{4} (\Phi_{ii'}^{'+}(-l_1) - \Phi_{ii'}^{'-}(-l_1)) \Phi_{jj'}(-l_2) (\Phi_{kk'}^{'+}(-l_3) - \Phi_{kk'}^{'-}(-l_3)) \\ &\quad + q_3 \frac{1}{2} (\Phi_{ii'}^{''+}(-l_1) + \Phi_{ii'}^{''-}(-l_1)) \Phi_{jj'}(-l_2) \Phi_{kk'}(-l_3) + \mathcal{O}(e^{-3s(M_0)}), \end{aligned} \tag{75}$$

where  $s(M_0) = s_0 + (M_0 - 1)h$  is the length of a subinterval in the trapezoidal rule approximation of (5) for  $\alpha = 3$  and

$$\begin{aligned} q_1 &= 4b\sqrt{\pi} [h/(1 - e^{-h})] e^{-s(M_0)}, & q_2 &= 2b^2 [2h/(1 - e^{-2h})] e^{-2s(M_0)}, \\ q_3 &= b^2\pi [2h/(1 - e^{-2h})] e^{-2s(M_0)}. \end{aligned} \tag{76}$$

For  $l = 0$  we have the same expression as in (75) with an additional term due to (37),

$$\begin{aligned} \tilde{r}_{ii',jj',kk'}^{0,qq} &= q_1 \frac{1}{2} (\Phi_{ii'}^{'+}(0) - \Phi_{ii'}^{'-}(0)) \delta_{jj'} \delta_{kk'} + q_2 \frac{1}{4} (\Phi_{ii'}^{'+}(0) - \Phi_{ii'}^{'-}(0)) (\Phi_{jj'}^{'+}(0) - \Phi_{jj'}^{'-}(0)) \delta_{kk'} \\ &\quad + q_2 \frac{1}{4} (\Phi_{ii'}^{'+}(0) - \Phi_{ii'}^{'-}(0)) \delta_{jj'} (\Phi_{kk'}^{'+}(0) - \Phi_{kk'}^{'-}(0)) \\ &\quad + q_3 \frac{1}{2} (\Phi_{ii'}^{''+}(0) + \Phi_{ii'}^{''-}(0)) \delta_{jj'} \delta_{kk'} + (q_1 - 2q_2) \delta_{ii'} \delta_{jj'} \delta_{kk'} + \mathcal{O}(e^{-3s(M_0)}). \end{aligned} \tag{77}$$

For the off-diagonal terms,  $q \neq q'$ , we have

$$\tilde{r}_{ii',jj',kk'}^{l,qq'} = q_3 \frac{\Phi_{ii'}'^+(-l_1) + \Phi_{ii'}'^-(-l_1)}{2} \frac{\Phi_{jj'}'^+(-l_2) + \Phi_{jj'}'^-(-l_2)}{2} \Phi_{kk'}(-l_3) + \mathcal{O}(e^{-3s(M_0)}). \tag{78}$$

**Proof.** In this case we need to estimate for large  $p$  the contribution from (36). Introducing

$$G_{ii'}^l(p) = S_{ii'}^l(p) - F_{ii'}^l(p) \tag{79}$$

with

$$S_{ii'}^l(p) = 2p \int_{-1}^1 e^{-p(x-l)^2} (x-l)^2 \Phi_{ii'}(x) dx, \tag{80}$$

we have  $G_{ii'}^{m,l} = G_{ii'}^{-l}(p_m/b^2)$ . Using (68) and (69), as well as

$$\int_0^1 (x-l)^3 e^{-p(x-l)^2} dx \rightarrow \begin{cases} 1/2p^2, & l=0, \\ -1/2p^2, & l=1, \end{cases}$$

$$\int_0^1 (x-l)^4 e^{-p(x-l)^2} dx \rightarrow 3\sqrt{\pi}/8p^{5/2}, \tag{81}$$

and

$$\int_{-1}^0 (x-l)^3 e^{-p(x-l)^2} dx \rightarrow \begin{cases} -1/2p^2, & l=0, \\ 1/2p^2, & l=-1, \end{cases}$$

$$\int_{-1}^0 (x-l)^4 e^{-p(x-l)^2} dx \rightarrow \frac{3\sqrt{\pi}}{8p^{5/2}}, \tag{82}$$

we obtain

$$S_{ii'}^l(p) = \sqrt{\pi} \frac{\Phi_{ii'}(l)}{p^{1/2}} + (-1)^l \frac{\Phi_{ii'}'^+(l) - \Phi_{ii'}'^-(l)}{p} + \frac{3\sqrt{\pi}}{8} \frac{\Phi_{ii'}''+(l) + \Phi_{ii'}''-(l)}{p^{3/2}} + \mathcal{O}\left(\frac{1}{p^2}\right), \tag{83}$$

and, combining with (70),

$$G_{ii'}^l(p) = (-1)^l \frac{\Phi_{ii'}'^+(l) - \Phi_{ii'}'^-(l)}{2p} + \frac{\sqrt{\pi}}{4} \frac{\Phi_{ii'}''+(l) + \Phi_{ii'}''-(l)}{p^{3/2}} + \mathcal{O}\left(\frac{1}{p^2}\right). \tag{84}$$

We have

$$\left| \frac{1}{\|\mathbf{x}\|^3} - \sum_{m=1}^M \frac{w_m}{b^3} e^{-p_m/b^2 \|\mathbf{x}\|^2} \right| \leq \frac{\epsilon}{b \|\mathbf{x}\|^2}, \tag{85}$$

where  $M \rightarrow \infty$  as  $\delta \rightarrow 0$ ,  $p_m = e^{2s_m}$ ,  $w_m = 4he^{3s_m}/\sqrt{\pi}$ , and  $s(m) = s_0 + (m-1)h$ . For sufficiently large  $M_0$ , by combining terms of the same order in (84) and (70), we obtain

$$q_1 = \sum_{m=M_0}^{\infty} \frac{w_m}{b^3} \frac{b^2}{p_m} \frac{b\sqrt{\pi}}{\sqrt{p_m}} \frac{b\sqrt{\pi}}{\sqrt{p_m}} = 4hb\sqrt{\pi} \sum_{m=M_0}^{\infty} e^{-s(m)} = 4hb\sqrt{\pi} \frac{e^{-s(M_0)}}{1 - e^{-h}},$$

$$q_2 = \sum_{m=M_0}^{\infty} \frac{w_m}{b^3} \frac{b^2}{p_m} \frac{b^2}{p_m} \frac{b\sqrt{\pi}}{\sqrt{p_m}} = 4hb^2 \sum_{m=M_0}^{\infty} e^{-2s(m)} = 4hb^2 \frac{e^{-2s(M_0)}}{1 - e^{-2h}},$$

$$q_3 = \sum_{m=M_0}^{\infty} \frac{w_m}{b^3} \frac{\sqrt{\pi}b^3}{2\sqrt{p_m}p_m} \frac{b\sqrt{\pi}}{\sqrt{p_m}} \frac{b\sqrt{\pi}}{\sqrt{p_m}} = 2hb^2\pi \sum_{m=M_0}^{\infty} e^{-2s(m)} = 2hb^2\pi \frac{e^{-2s(M_0)}}{1 - e^{-2h}}. \tag{86}$$

If  $l = 0$  then the additional term is obtained from (75) by setting indices to zero and evaluating the cross-correlation functions explicitly.

For computing the off-diagonal terms, we need to estimate for large  $p$

$$T_{ii'}^l(p) = \int_{-1}^1 e^{-p(x-l)^2} (x-l) \Phi_{ii'}(x) dx. \tag{87}$$

Using (68) and (69), and observing that  $\Phi_{ii'}(\pm 1) = 0$ , we obtain for  $l = -1, 0, 1$

$$T_{ii'}^l(p) = \sqrt{\pi} \frac{\Phi_{ii'}^+ + \Phi_{ii'}^-}{4p^{3/2}} + \mathcal{O}\left(\frac{1}{p^2}\right). \tag{88}$$

Combining (88) and (70), we arrive at (78), where

$$\sum_{m=M_0}^{\infty} \frac{2p_m w_m}{b^5} \frac{b^3 \sqrt{\pi}}{2p_m^{3/2}} \frac{b^3 \sqrt{\pi}}{2p_m^{3/2}} \frac{b \sqrt{\pi}}{p_m^{1/2}} = 2hb^2\pi \sum_{m=M_0}^{\infty} e^{-2s(m)} = q_3. \quad \square \tag{89}$$

### 6. On applying operators in multiresolution separated representation

The sparsity of the non-standard form induced by the vanishing moments of bases is not sufficient by itself for practical algorithms in dimensions other than  $d = 1$ . For fast practical algorithms in higher dimensions, we need an additional structure for the non-zero coefficients of the representation. This role is taken by the separated representations introduced in [2,3] and [4–7]. Once the components of the non-standard form have a separated representation within the retained bands, the numerical application of operators becomes efficient in higher dimensions.

The separated representations in Theorems 4, 7, 9, and 10 yield *multiresolution* separated representations, which are suitable for fast and adaptive application of operators to functions. Using such representations for the Poisson kernel and for the kernel  $e^{-\mu\|\mathbf{x}\|/\|\mathbf{x}\|}$ , where  $\mu > 0$  and  $\mathbf{x} \in \mathbb{R}^3$  (obtained via the same approach), led to algorithms of multiresolution quantum chemistry for electronic structure computations [4–7]. Since solving equations of quantum chemistry involves multiple applications of operators to functions in  $\mathbb{R}^3$ , the speed of these algorithms determines the overall speed of the computation.

We note that alternative algorithms for applying such operators are based on the fast multipole method (FMM), see, e.g., [22]. The approximation that assures the speed of FMM also uses a separated representation [8]. The approximation used in [8] is valid within a solid angle, thus requiring separate approximations along different directions. The number of directions grows exponentially with the dimension  $d$  of the space, although for  $d = 2, 3$  the cost is affordable. In our approach the separated representation is valid within a ball and, thus, does not require separate approximations in different directions. In addition, our approach provides not only the speed but also a convenient general setup for electronic structure computations.

We use the separable multiwavelet transform in combination with separated representations to reduce all computations to repeated applications of operators in dimension one. The multiresolution constructions using multiwavelet transform are now fairly standard [9,10]. The main feature of wavelet bases is the vanishing moments property of the basis functions that (for a finite but arbitrary accuracy) leads to a sparse representation for a large class of operators [1], certainly including those considered in this paper. Although wavelet representations are banded in any dimension, it is the combination of the multiresolution approach with the separated representations developed in Theorems 4, 7, 9, and 10 that allows us to avoid still very significant computational cost of the straightforward extension of the multiresolution approach to multiple dimensions.

The algorithms in [4–7] are based on an implementation of the non-standard form of operators [1] in multiwavelet bases. Consider the multiresolution analysis as a decomposition of  $L^2(\mathbb{R}^d)$  (or  $L^2([0, 1]^d)$ ) into a chain of subspaces

$$\mathbf{V}_0 \subset \mathbf{V}_1 \subset \mathbf{V}_2 \subset \dots \subset \mathbf{V}_n \subset \dots,$$

so that  $L^2(\mathbb{R}^d) = \overline{\bigcup_{j=0}^{\infty} \mathbf{V}_j}$ . On each subspace  $\mathbf{V}_n$ , we use the tensor product basis of scaling functions obtained using the functions  $\phi_{i,j}^n$  in (14). The wavelet subspaces  $\mathbf{W}_j$  are defined as the orthogonal complements of  $\mathbf{V}_j$  in  $\mathbf{V}_{j-1}$ , thus

$$\mathbf{V}_n = \mathbf{V}_0 \bigoplus_{j=0}^n \mathbf{W}_j.$$

Introducing the orthogonal projector on  $\mathbf{V}_n$ ,  $P_n : L^2(\mathbb{R}^d) \rightarrow \mathbf{V}_n$  and considering an operator  $T : L^2(\mathbb{R}^d) \rightarrow L^2(\mathbb{R}^d)$ , we define its projection  $T_n : \mathbf{V}_n \rightarrow \mathbf{V}_n$  as  $T_n = P_n T P_n$ . This projection is written explicitly in (13) in dimension  $d = 3$  for convolution operators with the kernel  $K(\mathbf{x} - \mathbf{y})$ .

We also consider the orthogonal projector  $Q_n : L^2(\mathbb{R}^d) \rightarrow \mathbf{W}_n$ , defined as  $Q_n = P_{n+1} - P_n$ . The non-standard form of the operator  $T$  is the collection of components of the telescopic expansion

$$T_n = (T_n - T_{n-1}) + (T_{n-1} - T_{n-2}) + \dots + T_0 = T_0 + \sum_{j=0}^{n-1} (A_j + B_j + C_j),$$

where  $A_j = Q_j T Q_j$ ,  $B_j = Q_j T P_j$ , and  $C_j = P_j T Q_j$ . The main property of this telescopic expansion is that the rate of decay of the matrix elements of operators  $A_j$ ,  $B_j$ , and  $C_j$  away from the diagonal is controlled by the number of vanishing moments of the basis and, for a finite but arbitrary accuracy  $\epsilon$ , the matrix elements outside a certain band can be set to zero resulting in an error of the norm less than  $\epsilon$ . Such behavior of the matrix elements becomes clear if we observe that the derivatives of the kernels under consideration decay faster than the kernel itself and, in our case, the rate of decay corresponds to the number of derivatives taken. If we use the Taylor expansion of the kernel to estimate the matrix elements away from the diagonal, then the size of these elements is controlled by a high derivative of the kernel since the vanishing moments remove the lower order terms [1].

Applying the non-standard form to a function, we write

$$T_n f = T_0 f + \sum_{j=0}^{n-1} (A_j(Q_j f) + B_j(P_j f) + C_j(Q_j f)), \tag{90}$$

where the operators  $P_j$  and  $Q_j$  are inserted to indicate the necessary projections of the function  $f$ . The advantage of the non-standard form is that it accounts for the interaction between different scales via an operator-independent projection applied after evaluating all of the components in (90). Namely, we observe that although the components  $A_j f + C_j f \in \mathbf{W}_j$ , are a part of the multiwavelet expansion, the components  $B_j f \in \mathbf{V}_j$  need to be projected on the appropriate wavelet subspaces [1] to obtain the final result.

We note that there are several ways to implement the application of the non-standard form to functions. Using Theorems 9 and 10, a new adaptive algorithm has been developed recently and will be described elsewhere [16].

### 7. Conclusions

Using the Poisson kernel and the projector on the divergence free function as examples, we have constructed separated representations of these kernels in multiwavelet bases. A similar approach is applicable to non-homogeneous convolutions, for example kernels  $e^{-\mu\|\mathbf{x}\|} / \|\mathbf{x}\|$ , where  $\mu > 0$  and  $\mathbf{x} \in \mathbb{R}^3$ , used in [4] and [5]. The key to these computations are separated approximations described in Section 2.1. Our approach also reveals the structure of operators on fine scales depicted in Theorems 9 and 10.

### Appendix A

Let us provide a brief proof of properties of the cross-correlation functions in Proposition 3.

(1) Since  $P_i(-x) = (-1)^i P_i(x)$ , we have from (6)  $\phi_i(-x + 1) = (-1)^i \phi_i(x)$ . Setting  $x + y = -z + 1$  in (7), we obtain

$$\Phi_{ii'}(x) = \int_{-\infty}^{\infty} \phi_i(-z + 1) \phi_{i'}(-z - x + 1) dz = (-1)^{i+i'} \int_{-\infty}^{\infty} \phi_i(z) \phi_{i'}(z + x) dz.$$

(2) The relations between  $\Phi^+$  and  $\Phi^-$  follow from the direct examination of (8) and (9).

(3) Since

$$\Phi_{ii'}^+(0) = \int_0^1 \phi_i(x + y) \phi_{i'}(y) dy,$$

the values at zero are obtained using the orthonormality of the scaling functions  $\phi_i$ .

(4) Let us obtain the upper bound for  $\Phi_{i'i'}^+$  using (9). We have

$$\int_0^{1-x} |\phi_i(x+y)| |\phi_{i'}(y)| dy \leq \left( \int_0^{1-x} |\phi_i(x+y)|^2 dy \right)^{1/2} \left( \int_0^{1-x} |\phi_{i'}(y)|^2 dy \right)^{1/2}, \quad (\text{A.1})$$

and, maximizing the interval of integration by setting  $x = 0$  in (A.1) and using orthonormality of the scaling functions, arrive at

$$|\Phi_{i'i'}^+(x)| \leq \left( \int_0^1 |\phi_i(y)|^2 dy \right)^{1/2} \left( \int_0^1 |\phi_{i'}(y)|^2 dy \right)^{1/2} \leq 1.$$

(5) From (9) we obtain  $\frac{d}{dx} \Phi_{l_0}^+(x) = -\phi_l(x) = -\sqrt{2l+1} P_l(2x-1)$ . Using  $P_l(x) = C_l^{1/2}(x)$  from [23, Eq. 22.5.36] and differentiating the Gegenbauer polynomials,  $\frac{d}{dx} C_{l+1}^{-1/2}(x) = -C_l^{1/2}(x)$ , we find that the cross-correlation functions  $\Phi_{l_0}^+$  are, in fact, rescaled Gegenbauer polynomials as stated in Proposition 3.

(6) Since  $\Phi_{l_0}^+(x)$ ,  $l = 0, \dots, 2m-1$ , are orthogonal polynomials on  $[0, 1]$ , we have (10). The coefficients  $c_{i'i'}^m$  are then easily evaluated via (11).

(7) Let us evaluate the moments,

$$I_{i'i'}^m = \int_{-\infty}^{\infty} x^m \Phi_{i'i'}(x) dx = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} x^m \phi_i(x+y) \phi_{i'}(y) dy dx,$$

where integration is limited to the support of the integrands. By changing variables  $z = x + y$ , we obtain

$$I_{i'i'}^m = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} (z-y)^m \phi_i(z) \phi_{i'}(y) dy dz.$$

Since  $\phi_i$  are orthogonal polynomials on  $[0, 1]$ , we have  $\int_{-\infty}^{\infty} z^j \phi_i(z) dz = 0$  for  $j \leq i-1$ . Using the binomial expansion,

$$I_{i'i'}^m = \sum_{j=0}^m \frac{m!(-1)^m}{j!(m-j)!} \left( \int_{-\infty}^{\infty} z^j \phi_i(z) dz \right) \left( \int_{-\infty}^{\infty} y^{m-j} \phi_{i'}(y) dy \right),$$

we obtain that  $I_{i'i'}^m = 0$  if  $m \leq i + i' - 1$ .

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