

MULTIRESOLUTION REPRESENTATION OF OPERATORS WITH BOUNDARY CONDITIONS ON SIMPLE DOMAINS

GREGORY BEYLKIN^{*}, GEORGE FANN⁺, ROBERT J. HARRISON⁺,
CHRISTOPHER KURCZ^{*}, LUCAS MONZÓN^{*}

ABSTRACT. We develop a multiresolution representation of a class of integral operators satisfying boundary conditions on simple domains in order to construct fast algorithms for their application. We also elucidate some delicate theoretical issues related to the construction of periodic Green's functions for Poisson's equation.

By applying the method of images to the non-standard form of the free space operator, we obtain lattice sums that converge absolutely on all scales, except possibly on the coarsest scale. On the coarsest scale the lattice sums may be only conditionally convergent and, thus, allow for some freedom in their definition. We use the limit of square partial sums as a definition of the limit and obtain a systematic, simple approach to the construction (in any dimension) of periodized operators with sparse non-standard forms.

We illustrate the results on several examples in dimensions one and three: the Hilbert transform, the projector on divergence free functions, the non-oscillatory Helmholtz Green's function and the Poisson operator. Remarkably, the limit of square partial sums yields a periodic Poisson Green's function which is not a convolution.

Using a short sum of decaying Gaussians to approximate periodic Green's functions, we arrive at fast algorithms for their application. We further show that the results obtained for operators with periodic boundary conditions extend to operators with Dirichlet, Neumann, or mixed boundary conditions.

1. Introduction

The primary goal of this paper is to develop a multiresolution representation of a class of integral operators satisfying boundary conditions on simple domains and construct fast algorithms for their application. As a practical consequence of our approach, we show that a minor modification of the fast algorithms for free space operators in [24, 9, 6], yields a fast algorithm (of the same complexity) for the operator satisfying boundary conditions.

Another goal of this paper is to elucidate some delicate theoretical issues related to the method

In our approach we apply the method of images not to the free space operator itself but to its non-standard form. The non-standard form splits the action of the operator to an infinite set of scales and, for appropriate classes of operators, yields a sparse representation [7]. For operators with kernels whose partial derivatives decay faster than the kernel itself (e.g., the Calderon-Zygmund operators), the non-standard form is sparse on all scales, except for the coarsest scale. We use the rapid decay of the coefficients of the non-standard form to construct its periodized version and to show that, on all scales except possibly the coarsest scale, the lattice sums converge absolutely and require no further analysis. On the coarsest scale, for some of the coefficients, the lattice sums may be only conditionally convergent and, thus, allow for some freedom in their definition. For such coefficients a summation convention needs to be specified and we choose the limit of square partial sums for that purpose. In this way, we obtain a systematic, simple approach to the construction (in any dimension) of periodized operators with sparse non-standard forms. We illustrate the results on several examples in dimensions one and three: the Hilbert transform, the projector on divergence free functions (the so-called Leray projector), the non-oscillatory Helmholtz Green's function and the Poisson operator.

The Poisson Green's function appears in many fields including electrostatics, material sciences, and

for Green's functions with boundary conditions is essentially the same as that for the free space case. Indeed, we show that the operators effectively coincide on the wavelet scales which are those dominating the computational cost.

We start in Section 2 by introducing the non-standard form for convolution operators in dimension d using multiwavelet bases [1, 2, 3]. In this case only one term may require an appropriate interpretation and we illustrate this using the Hilbert transform as an example. In Section 3 we construct the non-standard form in dimension d for operators with periodic boundary conditions. As examples, we then analyze the projector on divergence free functions, the non-oscillatory Helmholtz Green's function and, in Section 4, the Poisson Green's function. In Section 5 we describe a fast algorithm for applying these operators using separated representations. In Section 6, we construct Green's functions which incorporate Dirichlet, Neumann, or mixed boundary conditions on simple domains. Finally, we provide some closing remarks in Section 7 and collect most proofs in the appendix.

2. Preliminaries

2.1. Multiresolution and non-standard form. In this section we review a multiresolution approach for representing and applying operators in one dimension. Since we use multiwavelets as the underlying basis for the multiresolution representation, we briefly describe their properties (see also [1, 3, 9, 6]). We then turn to the non-standard form of operators in multiwavelet bases and describe a class of operators which becomes effectively sparse in this representation (see also [7, 6]). We then construct an operator with periodic boundary conditions by applying the method of images to the components of the non-standard form and illustrate the result with the Hilbert transform. The notation used below deviates slightly from usual wavelet notation, however, its introduction facilitates the higher dimensional description presented in later sections.

2.1.1. Multiwavelets. Let $\mathcal{P}_{[a,b]}$ denote the space of polynomials of degree less than l restricted to the interval $[a, b]$. Let us define subspaces

$$V_j = \mathcal{P}_{[-j, -j+1]} \quad l \in \mathbb{Z}$$

for $j \in \mathbb{N}$, where \mathbb{N} denotes all non-negative integers. These subspaces are nested

$$V_0 \subset V_1 \subset \dots \subset V_j \subset \dots$$

and $\overline{\bigcup_{j=0}^{\infty} V_j} = L^2(\mathbb{R})$. We select scaling functions to form an orthonormal basis of V_j , $\{\phi_{i;0}^{j;l}(\mathbf{x})\}_{i;0}^{j;l}$, $j \in \mathbb{N}$, $l \in \mathbb{Z}$, where

$$(1) \quad \phi_{i;0}^{j;l}(\mathbf{x}) = \begin{cases} \overline{P_i(\mathbf{x} - \phi)} & \mathbf{x} \in \phi \\ \text{otherwise} & \mathbf{x} \in \{ \dots, - \} \end{cases}$$

and P_i are the i -th order Legendre polynomials. We will need the cross-correlation functions of the scaling functions,

$$(2) \quad \int_{\mathbb{R}} \phi_{i;0}^{j;l}(\mathbf{x}) \phi_{i';0}^{j;l}(\mathbf{y}) d\mathbf{y}$$

where $\text{supp} \phi_{i;0}^{j;l} = \phi$, for $i, i' \in \{ \dots, - \}$. Due to orthogonality of the scaling functions in (1), these functions have vanishing moments (see [9, §2.2]),

$$(3) \quad \int_{\mathbb{R}} \phi_{i;0}^{j;l}(\mathbf{x}) \mathbf{x}^k d\mathbf{x} = 0 \quad \text{for } i \neq i', \text{ and } k \in \{ \dots, - \}.$$

We define the wavelet subspaces W_j as

$$W_j \oplus V_j = V_{j+1},$$

so that

$$V_{j+1} = V_0 \oplus W_0 \oplus \dots \oplus W_j.$$

We denote the multiwavelets, an orthonormal basis of W_j , as $\phi_{i;j}^{j,l}$ for $i \in \{0, \dots, M-1\}$ and $l \in \mathbb{Z}$. We do not need an explicit expression for the multiwavelets and only use their vanishing moments property,

$$(4) \quad \int_{\mathbb{R}} \phi_{i;j}^{j,l}(x) x^k dx = 0 \quad \text{for } i, k = 0, \dots, M-1, l \in \mathbb{Z}, \text{ and } j \in \mathbb{N},$$

which follows from orthogonality of the subspaces W_j and V_j . Also we need the cross-correlation functions of the wavelets,

$$(5) \quad \int_{\mathbb{R}} \phi_{i';s'}(x) \phi_{i;s}(x-y) dy = \delta_{i',i} \delta_{s',s},$$

where $s, s' = 0, \dots, M-1$ and $i, i' \in \{0, \dots, M-1\}$. In this notation $\int_{\mathbb{R}} \phi_{i';0}(x) \phi_{i;0}(x) dx = \delta_{i',i}$

2.1.3. Example in one dimension. Let K be the kernel of the convolution operator

$$(9) \quad Tf(x) = \int_{\mathbb{R}} K(x-y)f(y)dy.$$

the entries outside the band may be discarded resulting in a representation of the operator in terms of banded matrices and, therefore, yielding a fast algorithm for its application (see e.g. [7]).

2.2. Operators with periodic boundary conditions. Given a convolution operator T of the form (9), the method of images is the standard approach to construct an associated operator \mathcal{T} satisfying a periodic boundary condition. Specifically,

$$(13) \quad \mathcal{T}f(x) = \int_{-\infty}^{\infty} \left[\sum_{n \in \mathbb{Z}} K(x - y - nL) \right] f(y) dy,$$

where $\mathcal{T}f(x) = \mathcal{T}f(x - L)$ for $x \in \mathbb{R}$,

Remark 3.

3.1. **Non-standard form in dimension three.** Let us consider integral operators given by a convolution kernel in dimension $d = 3$,

$$(17) \quad T f(x) = \int_{\mathbb{R}^3} K(x-y) f(y) dy$$

for $x, y \in \mathbb{R}^3$. The basis functions (both scaling and multiwavelet) are the tensor product of the one-dimensional basis functions described in Section 2.1.1 and are denoted as

$$(18) \quad \Psi_{i;s}^{j;l}(\mathbf{x}) = \psi_{i_1;s_1}^{j;l_1}(x_1) \psi_{i_2;s_2}^{j;l_2}(x_2) \psi_{i_3;s_3}^{j;l_3}(x_3)$$

where $\mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$, $j \in \mathbb{N}$, $l = (l_1, l_2, l_3) \in \mathbb{Z}^3$, $i = (i_1, i_2, i_3) \in \{0, \dots, M-1\}$ and $s = (s_1, s_2, s_3) \in \mathbb{Z}^3$ with $s_1, s_2, s_3 \neq 0$. Thus, in this notation, the scaling functions correspond to $\Psi_{i;0}^{j;l}$. We also use the cross-correlation functions of the wavelets,

$$(19) \quad \Phi_{ii';ss'}(\mathbf{x}, \mathbf{t})$$

Remark.

where δ_{ij} , δ_{ij} , and δ_{ij} denotes the Kronecker delta function (see e.g. [17] for more details). This operator may be obtained using the Riesz transform, see the derivation in, e.g., [25]. Observing that the first term in (27) is the identity operator (if δ_{ij}), it is sufficient to consider the non-standard forms of the free space operators [9],

$$(28) \quad T_{ij} f(x) = \text{p.v.} \int_{\mathbb{R}^3} \frac{\delta_{ij}}{|x-y|} f(y) dy$$

3.4. Non-oscillatory Helmholtz Green's function with periodic boundary conditions.

Let us consider the problem

$$(30) \quad (-\Delta - \mu) u(x) = f(x)$$

$$(31) \quad u(x+n) = u(x)$$

for $x \in \mathbb{R}$, $\mu > 0$, $n \in \mathbb{Z}$, and $f \in L^2(\mathbb{R})$. Although this problem is easily handled by the standard method of images, we apply our approach in order to show that the limit as $\mu \rightarrow \infty$ does not cover all possible constructions available for the case $\mu > 0$.

We consider the solution to (30) and (31)

$$u(x) = \int_{[0,1]^3} G_H^\mu(x-y) f(y) dy,$$

where G_H^μ satisfies

$$\begin{aligned} (-\Delta - \mu) G_H^\mu(x-y) &= \delta(x-y) \\ G_H^\mu(x-y+n) &= G_H^\mu(x-y). \end{aligned}$$

We obtain G_H^μ

See Appendix 8.6 for the proof. The formulas derived in the proof may be used to explicitly compute other elements of the non-standard form.

4. Poisson Green's function with periodic boundary conditions

In this section we consider the problem

$$(34) \quad -\Delta u(x) = f(x) \quad \text{in } \mathbb{R}^3$$

$$(35) \quad u(x+n) = u(x) \quad \text{for } x \in \mathbb{R}^3, n \in \mathbb{Z}^3$$

for $x \in \mathbb{R}^3$, $n \in \mathbb{Z}^3$ and $f \in L^2(\mathbb{R}^3)$, $\int_{\mathbb{R}^3} f(x) dx = 0$ satisfying the mean-free condition

$$(36) \quad \int_{[0,1]^3} f(x) dx = 0.$$

(ii) For $|i - i'| \geq 1$, the lattice sums defining the scaling part elements of the periodized non-standard form (25) converge absolutely.

$$(40) \quad \mathcal{T}_{ii';00}^{0;0} = \sum_{\mathbf{n} \in \mathbb{Z}^3} \int_{[-L, L]^3} \frac{\Phi_{ii'}(\mathbf{x}) \phi(\mathbf{x} - \mathbf{n})}{|\mathbf{x} - \mathbf{n}|} d\mathbf{x},$$

converge absolutely.

(iii) For $|i - i'| = 0$, the lattice sums in (39) for the scaling part of the periodized non-standard form

$$(41) \quad \mathcal{T}_{ii';00}^{0;0} = \lim_{N \rightarrow \infty} \sum_{\|\mathbf{n}\| \leq N} \int_{[-L, L]^3} \frac{\Phi_{ii'}(\mathbf{x}) \phi(\mathbf{x} - \mathbf{n})}{|\mathbf{x} - \mathbf{n}|} d\mathbf{x},$$

converge conditionally.

(iv) For $|i - i'| = 0$, with the summation convention (iii), the lattice sum for the element $\mathcal{T}_{00;00}^{0;0}$ diverges. By setting it to zero, $\mathcal{T}_{00;00}^{0;0} = 0$, we effectively restrict the domain of the periodized operator to the class of functions with zero mean $\int_{[0, L]^3} \mathbf{f}(\mathbf{x}) d\mathbf{x} = 0$.

See Appendix 8.4 for the proof.

Remark 9. The fact that only a few elements of the non-standard form are given by conditionally convergent sums permits a characterization of all possible versions of the periodic Poisson Green's function. Our approach offers a unified way of constructing such Green's functions and, perhaps, explains difficulties encountered in their usual interpretation. Some of these different periodic Green's functions may be found in the literature [19, 15, 30]. The fact that in computing the periodic Poisson Green's function one encounters conditionally convergent sums is well known. Assigning

multi-indices $i' = (i'_1, i'_2, i'_3)$, $i'' = (i''_1, i''_2, i''_3)$ and $i' = (i'_1, i'_2, i'_3)$. Hence, we obtain

$$\int_{[0, L]^3} u(x) dx = \sum_{i' \in \mathbb{Z}^3} \int_{[0, L]^3} f(x, x, x) \phi_{i'}(x - x_{i'}) P_{i'}(x - x_{i'}) dx dx dx .$$

Expanding $P_{i'}(x - x_{i'}) = \sum_{i'' \in \mathbb{Z}^3} t_{i''} t_{i''}$ and using that f is mean-free, the last equation is equivalent to

$$(45) \quad \int_{[0, L]^3} u(x) dx = \sum_{i' \in \mathbb{Z}^3} \int_{[0, L]^3} f(x, x, x) \phi_{i'}(x - x_{i'}) (x - x_{i'} - x - x - x) dx dx dx .$$

This last condition is also derived in the literature (but with more restrictive assumptions on the function f). See, e.g., [5, Eq. 29], [26, Eq. 38] or [29, Eq. 8].

Further analysis of (45) leads us to consider the weak formulation of the problem (46)-(47),

$$(46) \quad \int_{[0, L]^3} u(x) \phi_{i'}(x) dx = \int_{[0, L]^3} f(x) \phi_{i'}(x) dx$$

$$(47) \quad \int_{[0, L]^3} u(x) \phi_{i'}(x) dx = \int_{[0, L]^3} u(x) \phi_{i'}(x) dx$$

Since the periodicity of G_0 yields

$$\int_{[0, 1]^3} G_0(x - y) \phi dx = \int_{[0, 1]^3} G_0(x) \phi dx$$

we also have that the solution u is mean-free. We now modify G_0 as to obtain a Green's function G yielding the boundary condition (49). Note that for $y = (y_1, y_2, y_3) \in \mathbb{R}^3$,

$$(52) \quad \int_{\partial([0, 1]^3)} G_0(x - y) \phi dx = \sum_{j=1}^3 \frac{e^{-\pi i n_j y_j}}{n_j} (y_j - y_{j+1}) / \phi - p_0(y) \phi$$

where p_0 is the polynomial in (48). Let's define for $x, y \in \mathbb{R}^3$,

$$G(x, y) = G_0(x - y) + G(x, y)$$

where

$$G(x, y) = \sum_{j=1}^3 \left(x_j - y_j - \sum_{j=1}^3 x_j y_j \right)$$

which we extend periodically as $G(x + n, y) = G(x, y)$ and $G(x, y + n) = G(x, y)$ for $x, y \in \mathbb{R}^3$ and any $n \in \mathbb{Z}$. Although $G(x, y) = \sum_{n \in \mathbb{Z}} G_0(x - y + n)$

where α and μ are non-negative parameters, both not simultaneously zero, and p_γ is a polynomial, $\gamma \in \mathbb{R}$, $\gamma > 0$. We note that both, $\|x\|^{-\beta}$ and $e^{-\mu\|x\|_2}$, or $\|x\|^{-\beta} e^{-\mu\|x\|_2}$, may be efficiently approximated by short sums of Gaussians for any user selected accuracy ϵ and distance from the origin (see Theorem 6 and Proposition 8 of [14]). In fact, the number

Thus, in order to compute $\hat{T}_{ii;ss}^{j;l-1}$, it is sufficient to evaluate one dimensional integrals with the cross-correlations of the scaling functions (see (20)),

$$\hat{t}_{ii;00;m;\gamma}^{j;l-1} = \int_{\mathbb{R}} \rho_{\gamma}(x) e^{-\tau_m x^2} \hat{t}_{ii}^{j+l-1}(x-l) dx$$

and then apply the quadrature mirror filters for the multiwavelets (see [3, eq 3.25a 3.25b 3.25c 3.25d]) to construct all the coefficients $\hat{t}_{ii;ss;m;\gamma}^{j;l-1}$ for $s = 1, 2, 3$. We note that to apply the operator we may also use the modified non-standard form [6] which only requires the projection of the operator onto cross-correlation functions of the scaling functions.

Applying the method of images to (60), we obtain the coefficients of the non-standard form of the operator with periodic boundary conditions,

$$(62) \quad \hat{\mathcal{T}}_{ii;ss}^{j;l-1} = \sum_{m=1}^M \mathbf{W}_m \hat{t}_{i_1 i_1; s_1 s_1; m}^{j;l_1-l_1} \hat{t}_{i_2 i_2; s_2 s_2; m}^{j;l_2-l_2} \hat{t}_{i_3 i_3; s_3 s_3; m}^{j;l_3-l_3},$$

where in each direction

$$(63) \quad \hat{t}_{ii;ss;m;\gamma}^{j;l-1} = \sum_{n \in \mathbb{Z}} \hat{t}_{ii;ss;m;\gamma}^{j;l-1 + jn}$$

with $\hat{t}_{ii;ss;m;\gamma}^{j;l-1 + jn}$ defined in (61). Clearly (62) is in separated form with the same separation rank as its free space counterpart (60) and, moreover, (63) provides a simple recipe for computing its components.

Remark 14. By first computing the blocks $\hat{T}_{ii;ss}^{j;l-1 + jn}$ of the non-standard form of the free space approximation \hat{K} , we have a simple way to evaluate via (63) the corresponding blocks $\hat{\mathcal{T}}_{ii;ss}^{j;l-1}$ for the approximation of the periodized operator. Since the norm of the blocks $\hat{t}_{ii;ss;m;\gamma}^{j;l-1 + jn}$ in (63) decays rapidly with n , only a few terms participate in the sum for a given accuracy. In fact, on finer scales (large j) only the term with $n = 0$ needs to be kept. We may estimate the error $|\hat{\mathcal{T}}_{ii;ss}^{j;l-1} - \hat{T}_{ii;ss}^{j;l-1}|$, where $\hat{T}_{ii;ss}^{j;l-1}$ are the blocks of the non-standard form of the original operator \mathbf{K} , by using Proposition 4 together with the estimates for $|\hat{T}_{ii;ss}^{j;l-1 + jn} - \hat{T}_{ii;ss}^{j;l-1 + jn}|$ given in [9, Theorem 4]. However, an exception to using (63) for computing operator blocks has to be made for conditionally convergent elements on the coarsest scale whose definition requires special attention (see Proposition 10).

Remark 15. Our approach applies to any Bravais lattice. We note that for a non-rectangular lattice the non-standard form does not separate along each coordinate and further approximations are required.

6. Dirichlet, Neumann and mixed boundary conditions

Using the results for the periodic case, we now have the necessary tools to efficiently apply operators with Dirichlet, Neumann or mixed boundary conditions on simple domains. We note that although the resulting integral operators are no longer convolutions, they have a simple algebraic structure and, as a result, the algorithm for applying these operators is similar to those described in the previous section.

As an example, let us consider the problem

$$(64) \quad (-\Delta_x^\mu) u(x) = f(x) \text{ for } x \in D$$

$$(65) \quad u(x) = 0 \text{ for } x \in \partial D,$$

where $\mu > 0$ and $D =]0, 1[\times]0, 1[\times \dots \times]0, 1[$. A solution to (64) which satisfies (65) is given by

$$u(x) = \int_D G^\mu(x, y) f(y) dy,$$

where G^μ satisfies

$$(66) \quad (-\Delta_x^\mu) G^\mu(x, y) = \delta(x - y)$$

$$(67) \quad G^\mu(x, y) = 0 \text{ for } x \in \partial D$$

and Δ_x denotes the Laplacian with respect to x . Let us first consider the case where $\mu > 0$. Even though the integral operator G^μ is not a convolution, it may be written as

$$(68) \quad G^\mu(x, y) = G_H^\mu\left(\frac{x_1 - y_1}{2}, \frac{x_2 - y_2}{2}, \frac{x_3 - y_3}{2}\right) - G_H^\mu\left(\frac{x_1 - y_1}{2}, \frac{x_2 - y_2}{2}, \frac{x_3 + y_3}{2}\right) \\ - G_H^\mu\left(\frac{x_1 - y_1}{2}, \frac{x_2 + y_2}{2}, \frac{x_3 - y_3}{2}\right) - G_H^\mu\left(\frac{x_1 - y_1}{2}, \frac{x_2 + y_2}{2}, \frac{x_3 + y_3}{2}\right) \\ - G_H^\mu\left(\frac{x_1 + y_1}{2}, \frac{x_2 - y_2}{2}, \frac{x_3 - y_3}{2}\right) - G_H^\mu\left(\frac{x_1 + y_1}{2}, \frac{x_2 - y_2}{2}, \frac{x_3 + y_3}{2}\right) \\ - G_H^\mu\left(\frac{x_1 + y_1}{2}, \frac{x_2 + y_2}{2}, \frac{x_3 - y_3}{2}\right) - G_H^\mu\left(\frac{x_1 + y_1}{2}, \frac{x_2 + y_2}{2}, \frac{x_3 + y_3}{2}\right),$$

where the periodic Green's function G_H^μ is constructed as in Section 3.4 to satisfy

$$(69) \quad (-\Delta_x^\mu) G_H^\mu(x - y) = \delta(x - y).$$

The changes in the equation relative to (66) are due to the way variables appear in (68) and to the dimension of the space, $d = 3$. Since G_H^μ has period one and is even in each variable, for $x \in \partial D$ the terms in (68) cancel each other so that G^μ satisfies the Dirichlet boundary condition (67). For $x = y$ inside D , we have $(-\Delta_x^\mu) G^\mu(x, y) = \delta(x - y)$ since each of the eight terms in (68) vanishes. The only singularity is at $x = y$.

MULTIRESOLUTION REPRESENTATION OF OPERATORS WITH BOUNDAR

and

$$\int_{\mathbb{R}^2} \tilde{t}_{ii;ss;m}^{j;l+l+j(n+)} e^{-\tau m(x+y+n)^2} \phi_{i,s}^{j,l}(y) \phi_{i,s}^{j,l}(x) dx dy$$

for $j \in \mathbb{N}$, $n \in \mathbb{Z}$, $l, l' \in \{0, \dots, j-1\}$, $i, i' \in \{1, \dots, M\}$. The integrals $\tilde{t}_{ii;ss;m}^{j;l+l+j(n+)}$ and $\tilde{t}_{ii;ss;m}^{j;l-l+j(n)}$ are simplified further and reduce to one dimensional integrals using cross and auto-correlations of wavelet and scaling functions (see Section 5). As a result, the non-standard form is given by

$$\tilde{T}_{ii;ss}^{j;ll} = \sum_{m=1}^M \mathbf{w}_m \tilde{t}_{i_1 i_1; s_1 s_1; m}^{j;l_1 l_1} \tilde{t}_{i_2 i_2; s_2 s_2; m}^{j;l_2 l_2} \tilde{t}_{i_3 i_3; s_3 s_3; m}^{j;l_3 l_3}$$

where

$$\tilde{t}_{ii;ss;m}^{j;ll} = \sum_{n \in \mathbb{Z}} \left(-\tilde{t}_{ii;ss;m}^{j;l-l+j(n)} + \tilde{t}_{ii;ss;m}^{j;l+l+j(n)} \right) \quad ii$$

Using Hölder's inequality and $\dot{H}^{j;l}_{i;0} L$

8.3. Proof of Proposition 4.

Proof. It is enough to prove the result for $1 - I'$ \bar{d} since the general result follows by

where we used $\left\| \Psi_{i;s}^{j;l} \right\|_{L^2(\mathbb{R}^d)}$ and

$$\int_{I_1} \left| \mathbf{x} - \mathbf{x}_0 \right|^\alpha \mathbf{d}\mathbf{x} = \int_{r=0}^d \int_{l_r}^{l_r+1} \left(\mathbf{t} - \mathbf{t}_r \right)^{\alpha_r} \mathbf{d}\mathbf{t} = \int_{r=0}^d \int_0^1 \left(\mathbf{u} \right)^{\alpha_r} \mathbf{d}\mathbf{u} = \frac{d - \alpha_r(j+1)}{r}.$$

Combining these estimates we obtain the result with

$$C_j = \frac{C_\alpha}{|\alpha|^\nu} - j(d-\beta).$$

It remains to prove the estimate for

$$(88) \quad T_{ii;00}^{0;l-1} = \int_{[-,]^d} \mathbf{K}(\mathbf{x}, \mathbf{l} - \mathbf{l}') \Phi_{ii}(\mathbf{x}) \mathbf{d}\mathbf{x}.$$

First assume $|\mathbf{i} - \mathbf{i}'| \leq \nu$. This time we use the Taylor expansion of $\mathbf{K}(\mathbf{x}, \mathbf{l} - \mathbf{l}')$ centered at the origin, so that

$$\mathbf{K}(\mathbf{x}, \mathbf{l} - \mathbf{l}') = \sum_{|\alpha| \leq \nu} -D^\alpha \mathbf{K}(\mathbf{l} - \mathbf{l}') \mathbf{x}^\alpha + \sum_{|\alpha| = \nu} -D^\alpha \mathbf{K}(\mathbf{l} - \mathbf{l}') \mathbf{x}^\alpha,$$

where $\nu = \min\{|\mathbf{i} - \mathbf{i}'|, \nu\}$ and $\mathbf{l} - \mathbf{l}' \in [-,]^d$. Substituting into (88) and using that Φ_{ii} have vanishing moments (3), we observe that all terms with $|\alpha| < \nu$ do vanish. For the remainder term in the Taylor expansion, using (23),

$$\left| T_{ii;00}^{0;l-1} \right| \leq \frac{C_\alpha}{|\alpha|^\nu} \int_{[-,]^d} \frac{|\mathbf{x}^\alpha \Phi_{ii}(\mathbf{x})|}{|\alpha| + \beta} \mathbf{d}\mathbf{x} = \frac{C_\alpha a_\alpha}{|\alpha|^\nu} \frac{|\alpha| + \beta}{|\alpha| + \beta},$$

where $a_\nu = \int_{[-,]^d} |\mathbf{x}^\alpha \Phi_{ii}(\mathbf{x})| \mathbf{d}\mathbf{x}$ and we estimated

which, changing variables $x_j \leftarrow x_j - n_j$ on each $j = 1, \dots, d$, yields

$$\lim_{N \rightarrow \infty} \int_{[-N, N]^3} \dots dx = \int_{\mathbb{R}^3} \dots dx = \infty.$$

Thus, the summation convention (41) yields a non-finite element $\mathcal{T}_{00;00}^{-0;0}$. To deal with this situation, we simply set the value of this element to zero which is equivalent to restrict the domain of the operator to mean-free functions. □

8.5. Auxiliary results for the computation of non-standard form elements. The vanishing moments and symmetries of the cross-correlation functions (20) allow us to explicitly compute elements of the periodized non-standard forms. The relevant properties and how we use them to compute these elements are captured on the following results.

Lemma 19. Let ϕ be a bounded function with odd symmetry about $t = 0$

$$(95) \quad \phi(-t) = -\phi(t), \quad \phi(0) = 0.$$

Then

$$\sum_{n=-N}^N \int_0^N \phi(t-n) h(t-n) dt = \sum_{n=-N}^N \int_0^N \phi(t) h(t-N) dt,$$

for any even function h such that the integrals exist.

Proof. Let I be

$$I = \sum_{n=-N}^N \int_0^N \phi(t-n) h(t-n) dt.$$

Splitting the sum in non-negative and negative values of n and changing variables $t \leftarrow -t$ on the latter, the assumption (95) yields

$$I = \sum_{n=0}^N \int_0^N \phi(t-n) h(t-n) dt - \sum_{n=0}^N \int_0^N \phi(-t-n) h(-t-n) dt \\ = \sum_{n=0}^N \int_0^N \phi(t-n) h(t-n) dt - \sum_{n=0}^N \int_0^N \phi(t-n) h(t-n) dt + \int_0^N \phi(t) h(t-N) dt,$$

because h is even. □

Lemma 20. Let ϕ_j, ψ_j, χ_j be three bounded functions on $[-N, N]$ such that one of them, e.g. ϕ_j , is odd and let $G(x_1, x_2, x_3)$ be a locally integrable function, even on each variable. Then

$$(96) \quad \lim_{N \rightarrow \infty} \int_{\|\mathbf{n}\| \leq N} \phi_j(x_1 - n_1) \psi_j(x_2 - n_2) \chi_j(x_3 - n_3) G(x_1 - n_1, x_2 - n_2, x_3 - n_3) dx = 0$$

Proof. Let C denote a constant whose value may change along the derivation. Observe that

$$\int_{\|\mathbf{n}\| \leq N} \phi_j(x_1 - n_1) \psi_j(x_2 - n_2) \chi_j(x_3 - n_3) G(x_1 - n_1, x_2 - n_2, x_3 - n_3) dx$$

is always well defined because ϕ_j are bounded and G

over \mathbb{R}^3 and $-\mathbb{R}^3$, and changing variables $x \rightarrow -x$ in the latter yields

$$\int_{|n_1| \leq N} \int_{\mathbb{R}^3} g(x) \phi(x - n) dx = \int_{|n_1| \leq N} \int_{\mathbb{R}^3} g(x) \phi(x - n) dx - \int_{|n_1| \leq N} \int_{\mathbb{R}^3} g(-x) \phi(-x - n) dx.$$

Since in the last term the sum over n is the same as the sum over $-n$ and g is an even function, the two terms in the previous equation cancel each other and we obtain the result. \square

Proposition 21. Let f, g, h denote three bounded functions on \mathbb{R}^3 . It holds that

A: If f is odd about \mathbb{R}^3 , then

$$(97) \quad \lim_{N \rightarrow \infty} \int_{|n| \leq N} \int_{[0, 1]^3} \frac{f(x) \phi(x - n)}{|x - n|} dx = \int_0^1 \int_0^1 \int_0^1 f(t) \phi(t) dt.$$

B: If f is even about \mathbb{R}^3 and mean free, then

$$(98) \quad \lim_{N \rightarrow \infty} \int_{|n| \leq N} \int_{[0, 1]^3} \frac{f(x) \phi(x - n)}{|x - n|} dx = \int_0^1 \int_0^1 \int_0^1 f(t) \phi(t) dt.$$

C: If f is mean free, then

$$(99) \quad \lim_{N \rightarrow \infty} \int_{|n| \leq N} \int_{[0, 1]^3} \frac{f(x) \phi(x - n)}{|x - n|} dx = \int_0^1 \int_0^1 \int_0^1 f(t) \phi(t) dt.$$

For simplicity, the proposition is stated for the Poisson kernel $G(x) = \frac{1}{|x|}$, but similar results hold for any radially symmetric kernel with enough decay at infinity and, thus, to linear combination of such kernels. However, due to the slow decay of the Poisson kernel, the proof of Proposition 21 is more challenging than the one for kernels with faster decay at infinity.

Proof. We use the same notation as in the proof of Lemma 20. Note that, the same argument given in that proof shows that

$$(100) \quad \lim_{N \rightarrow \infty} \int_{|n| \leq N} \int_{\mathbb{R}^3} f(x) \phi(x - n) dx = \int_{\mathbb{R}^3} f(x) \phi(x) dx.$$

Hence, substituting (103) into (100) yields

$$(104) \quad \mathbf{S}_N^+ \Big|_{|n_2| \leq N, |n_3| \leq N} [0,]^3 \mathbf{x} \Big|_{\mathbb{Z}^3} \mathbf{N} \phi [] \mathbf{x} \phi, \mathbf{x} \phi \quad \mathbf{x} \phi$$

and hence I

the term corresponding to $n = N$ in S_N^+ leads to a sequence which tends to ∞ as $N \rightarrow \infty$. Setting $n = -N$ leads to a similar estimate yielding

$$S_\infty^+ \underset{N \rightarrow \infty}{\sim} S_N,$$

where

$$S_N = \int_{n_1=-N}^N \int_{n_2=-N}^{N-n_1} \int_{n_3=-N}^{N-n_1-n_2} \frac{\mathbf{x} \cdot \boldsymbol{\phi}}{[\dots]^3}$$

and, since $\int_{-N}^N a_N(x) \phi(x) dx = \int_{-N}^N a_N(x) \phi(x) dx$,

$$\int_{-N}^N a_N(x) \phi(x) dx = \int_{-N}^N a_N(x) \phi(x) dx - \int_{-N}^N \frac{d}{dx} a_N(x) \phi(x) dx$$

The result follows observing that

$$(113) \quad \int_{-N}^N \frac{d}{dx} a_N(x) \phi(x) dx = \frac{1}{N} \int_{-N}^N \frac{d}{dx} a_N(x) \phi(x) dx$$

it is a Riemann Sum in the interval $[-1, 1]$, for the continuous function $\frac{1}{(1+x^2)\sqrt{1+x^2}}$. As $N \rightarrow \infty$, the sum (113) converges to

$$\int_{-1}^1 \frac{1}{(1+x^2)\sqrt{1+x^2}} dx = \frac{\pi}{2}$$

For part C, given a mean free function $\phi(x)$ we write it as $\phi(x) = \phi_{\text{odd}}(x) + \phi_{\text{even}}(x)$, where

$$(114) \quad \phi_{\text{odd}}(x) = \frac{\phi(x) - \phi(-x)}{2} \quad \text{and} \quad \phi_{\text{even}}(x) = \frac{\phi(x) + \phi(-x)}{2}$$

Since both ϕ_{odd} and ϕ_{even} are mean free, the same holds for ϕ_{even} . Using parts A and B and the definitions of ϕ_{odd} and ϕ_{even} , the result follows adding

$$\int_0^1 t \phi_{\text{odd}}(t) dt = \int_0^1 (t - (-t)) \phi_{\text{odd}}(t) dt = \int_0^1 t \phi_{\text{odd}}(t) dt$$

and

$$\int_0^1 t \phi_{\text{even}}(t) dt = \int_0^1 (t - (-t)) \phi_{\text{even}}(t) dt = \int_0^1 (t - t) \phi_{\text{even}}(t) dt$$

□

8.6. Proof of Proposition 7.

Proof. Since from (72) we have that $\mathcal{T}_{ii}^{0;0}(x) = \phi^{j+i}(\mathcal{T}_{ii}^{0;n}(x))$, it is enough to show the result for $\mathcal{T}_{ii}^{0;0}$.

By (26) and (22),

$$\mathcal{T}_{ii}^{0;0}(\mu) \stackrel{N \rightarrow \infty}{\|n\| \leq N} \mathcal{T}_{ii}^{0;n}(\mu) \stackrel{N \rightarrow \infty}{\|n\| \leq N} [-1, 1]^3 \mathbf{G}_{\text{free}}^\mu(x) \phi_{i_1 i_1}(x) \phi_{i_2 i_2}(x) \phi_{i_3 i_3}(x) dx.$$

Therefore, Lemma 20 implies that $\mathcal{T}_{ii}^{0;0}(\mu)$ vanishes whenever any of the functions $\phi_{i_j i_j}$, $j = 1, 2, 3$, is odd, which, by (73), is the case if i_j and i_j have different parity. We have proved part (ii). Next consider the case of i_j and i_j having the same parity for all j . In this case all the functions $\phi_{i_j i_j}$, $j = 1, 2, 3$, are even and

$$\mathcal{T}_{ii}^{0;0}(\mu) \stackrel{N \rightarrow \infty}{\|n\| \leq N} [0, 1]^3 \mathbf{G}_{\text{free}}^\mu(x) \phi_{i_1 i_1}(x) \phi_{i_2 i_2}(x) \phi_{i_3 i_3}(x) dx$$

$$[0, 1]^3 \phi_{i_1 i_1}(x) \phi_{i_2 i_2}(x) \phi_{i_3 i_3}(x) \mathbf{G}_H^\mu(x) dx.$$

For part (iii), by symmetry of the kernel, it is sufficient to consider only one of the elements listed on each of the three cases. The case $i = \dots, \dots, \phi$ and $i' = \dots, \dots, \phi$

