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Efficient convolution with the Newton potential  
in  $d$  dimensions

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# Efficient convolution with the Newton potential in $d$ dimensions

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## Abstract

The paper is concerned with the evaluation of the convolution integral  $\int_{\mathbb{R}^d} \frac{1}{\|x-y\|} f(y) dy$  in  $d$  dimensions (usually  $d = 3$ ), when  $f$  is given as piecewise polynomial of possibly large degree, i.e.,  $f$  may be considered as an  $hp$ -finite element function. The underlying grid is locally refined using various levels of dyadically organised grids. The result of the convolution is approximated in the same kind of mesh. If  $f$  is given in tensor product form, the  $d$ -dimensional convolution can be reduced to one-dimensional convolutions.

Although the details are given for the kernel  $1/\|x\|$ , the basis techniques can be generalised to homogeneous kernels, e.g., the fundamental solution  $const \cdot \|x\|^{2-d}$  of the  $d$ -dimensional Poisson equation.

## 1 Introduction

We consider the mapping of  $f \in L^2(\mathbb{R}^d)$  onto  $u \in L^2(\mathbb{R}^d)$  by means of

$$u(x) := (\mathcal{K}f)(x) := \int_{\mathbb{R}^d} \frac{1}{\|x-y\|} f(y) dy \quad \text{for } x \in \mathbb{R}^d. \quad (1.1)$$

The integral represents the convolution of the Newton (or Coulomb) potential  $1/\|\cdot\|$  with  $f$ . For  $d = 3$  the kernel  $1/4\pi\|x-y\|$  (cf. [5, §2.2]) is the fundamental solution of the Laplace operator  $\Delta$  in  $\mathbb{R}^3$ . Hence, up to a factor,  $u$  from (1.1) is the solution of the Poisson equation  $\Delta u = f$  in  $\mathbb{R}^3$  (cf. [5, Theorem 3.2.11]).

Although the details are given for the kernel  $1/\|x\|$ , the basis techniques can be generalised to homogeneous kernels, e.g., the fundamental solution  $const \cdot \|x\|^{2-d}$  of the  $d$ -dimensional Poisson equation. The homogeneity is used by the hierarchical quadrature in §4.2.4.

The solution of (1.1) is the primary goal. Here, we are interested in the case where  $f$  is smooth except of some local singularities. Furthermore,  $f$  is assumed to have bounded support<sup>1</sup>. In particular,  $f$  may represent the electron density of a many-particle in electronic structure calculations. In that case,  $f$  is rather smooth except in the neighbourhood of the atom centres. The most efficient representation of such a function  $f$  is an  $hp$ -approach using local refinements as well as high polynomial degrees.

A second goal is the evaluation of integrals of the form

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{g(x)f(y)}{\|x-y\|} dx dy, \quad (1.2)$$

which reduces to the scalar product  $\langle g, u \rangle_{L^2(\mathbb{R}^d)}$  with  $u$  from (1.1). Again, integrals of the form (1.2) appear in electronic structure calculations.

The integrals (1.1) are not computed exactly. Instead, a subspace  $S \subset L^2(\mathbb{R}^d)$  is defined which contains the discretisations of  $f$  and of the result<sup>2</sup>  $u$ . In the following, we always assume that  $f \in S$ . The optimal result would be  $u_S := P_S \mathcal{K}f$ , where  $P_S$  is the  $L^2(\mathbb{R}^d)$ -orthogonal projection onto  $S$ . However, further discretisation errors are introduced in order to get a fast evaluation.

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<sup>1</sup>The “true” function  $f$  may have unbounded support, but should decay fast enough so that it can be well approximated by a function of bounded support.

<sup>2</sup>Only for ease of notation we assume identical ansatz spaces for  $f$  and  $u$ . Since  $u$  is smoother than  $f$ ,  $u$  does not need a more refined grid, but  $u$  may decay less strongly than  $f$  and therefore require a more extended grid.

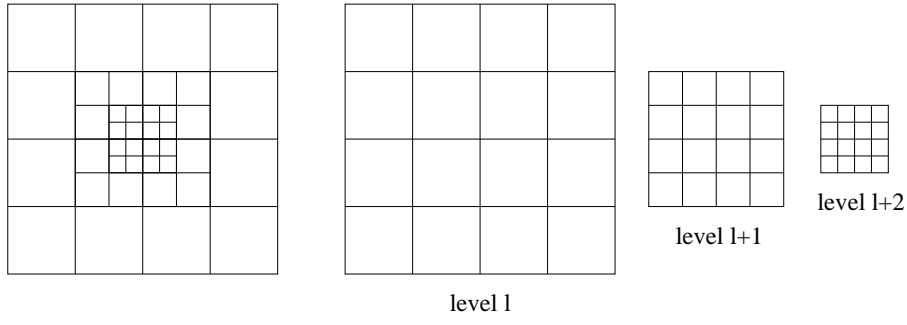


Figure 1.1: Left: regular grid refinement. Right: refinement zones  $B_\ell$  with involved uniform grids.

The subspace  $S$  consists of piecewise (high-degree) polynomials. The underlying geometric grid is a family of regular tensor grids of step size  $h_\ell = 2^{-\ell}$  ( $\ell \in \mathbb{Z}$ ). Like for wavelet bases, this construction easily allows local refinements around singularities of  $f$ . Large step sizes  $h_\ell = 2^{-\ell}$  ( $\ell < 0$ ) can be used to approximate smooth parts in the far field<sup>3</sup>. Figure 1.1 shows a possible locally refined grid<sup>4</sup> combining regular grids of size  $h_\ell = 2^{-\ell}$  in the refinement zones<sup>5</sup>  $B_\ell := [-2h_\ell \mathbf{1}, 2h_\ell \mathbf{1}] := \{x \in \mathbb{R}^d : -2h_\ell \leq x_j \leq 2h_\ell \text{ for } 1 \leq j \leq d\} \subset B_{\ell-1}$ . In the paper, we introduce only one family of refinement zones  $B_\ell$  around  $x = x_0$ . But the generalisation to refinement zones around several singularity points is obvious.

The chosen approach allows to use basis functions with the smallest possible support (one cube). This advantage is lost if a corresponding multi-wavelet setting is used, while wavelets have other positive properties (cf. [8]). Note that the method in [1] relies on the multi-resolution analysis.

Since for  $d = 3$   $u$  from (1.1) satisfies the Poisson equation, one may compare the present approach with Poisson solvers. First, because of the unbounded domain, Poisson solvers are not as easy in  $\mathbb{R}^d$ . Second, we aim at approximations with high-degree polynomials in order to get high accuracy, whereas the order of Poisson solvers is usually limited. Third, the present approach allows the use of piecewise approximations which are discontinuous functions across the faces of the cubes. This fact leads to the smallest possible support of the basis functions.

The method from [4] applies to the 2D Poisson in the square. It also allows high order approximations of  $f$ , but is based on the multipole method and does not rely on discrete convolutions.

Since the grid is a combination of regular grids of step size  $h_\ell$ , also  $S$  has contributions  $S \cap S_\ell$  to several levels  $\ell$  ( $S_\ell$  is the space of piecewise polynomials on the infinite grid of size  $h_\ell$ , the functions of  $S \cap S_\ell$  have their support only in the refinement zone  $B_\ell$ ). The subspace

$$S_{\leq \ell} := S \cap \bigcup_{\lambda \leq \ell} S_\lambda$$

describes the refinement up to level  $\ell$ . Details of levels  $\lambda > \ell$  corresponding to finer step size than  $h_\ell$  are missing. Like in wavelet approaches, a function  $f \in S$  can be written as  $f = \sum_\ell f_\ell$  with  $f_\ell \in S \cap S_\ell$ . The true Galerkin approach in  $S$  maps all  $f_\ell$  into  $P_S \mathcal{K} f_\ell$  ( $P_S$ :  $L^2(\mathbb{R}^d)$ -orthogonal projection onto  $S$ ). Instead we use the projection onto  $S_{\leq \ell}$ :  $u_\ell := P_{S_{\leq \ell}} \mathcal{K} f_\ell$  and compute  $u := \sum_\ell u_\ell$ . This extra discretisation simplifies the computation essentially and is discussed in §3.1. A precise analysis of the addition discretisation error is subject of ongoing work. The local refinement in §2.3 introduces a condition (2.9) enforcing a soft change in the step size. Therefore, the introduced errors can be considered as approximations in the far field.

The above modification allows to reduce the convolution to grids of uniform step size. The involved integration with  $1/\|x - y\|$  can be performed rather accurately. In particular, the arising weakly singular integrals introduce no extra error (see §4.2). Finally, when discrete convolutions have to be performed, one can apply the Fast Fourier Transform. If the data size is as small as in Figure 1.1 (5 grid points in each direction), even the naive summation may be used.

<sup>3</sup>Even if  $f$  is rather concentrated around a point with fast decay in the far field (like the Gaussian  $\exp(-\alpha\|x - y\|^2)$ ), the induced function  $u = \mathcal{K}f$  may decay more slowly like  $1/\|x\|$ . This fact, however, is no drawback, if the integral (1.2) is to be evaluated and also  $g$  has fast decay. The latter case often occurs in electronic structure calculations.

<sup>4</sup>Note that the refinement is required by the function  $f$ , not by the kernel function  $1/\|x - y\|$ .

<sup>5</sup>The bold number “**1**” is the multi-index  $\mathbf{1} = (1, \dots, 1) \in \mathbb{Z}^d$ .

In the first approach of §4, the convolution problem in  $\mathbb{R}^d$  is solved in the original form. The drawback is that for  $d \geq 3$  the data size may become large because of the exponent  $d$ . Therefore, special emphasise is laid on the tensor product variant. Here we assume that the function  $f$  has the tensor product form

$$f = \sum_{\mu=1}^r f_1^{(\mu)}(x_1) \cdot \dots \cdot f_d^{(\mu)}(x_d)$$

(more precise description in (5.4)) with hopefully small  $r$ . Such representation are, e.g., possible for the electron density of molecules. In that case, the  $d$ -dimensional convolutions can be split into  $d$  one-dimensional convolutions. The data size and the computational work increase only proportionally to  $d$  if the spatial dimension increases. The tensor approximation of  $1/\|x\|$  together with the involved approximation is described in §5.2.

The paper is organised as follows.

In Section 2 we introduce the notations for the geometric grid (the one-dimensional case in §2.1, for general  $d$  in §2.2, the grid refinement in §2.3). Therein, also the basis functions  $\Phi_{\nu,\alpha}^\ell$  are defined. The representation of  $f \in S$  is discussed in §2.4. Subsection 2.5 introduces notations for projections, prolongations and restrictions. Finally, in §2.6, the convolution is expressed by means of the basis functions.

Section 3 introduces the approximation of  $\mathcal{K}f$ , when  $f$  belongs to level  $\ell$ . This treatment is important for the algorithm described in §3.2. Possible modifications are mentioned in §3.3.

Section 4 describes the computation of the integrals  $N_{\mathbf{i}-\mathbf{j},\alpha,\beta}^\ell = \iint \Phi_{\mathbf{i},\alpha}^\ell(x) \Phi_{\mathbf{j},\beta}^\ell(y) / \|x-y\| dx dy$ . It turns out that in the far field well-known approximations can be applied (§4.2.3), while the near field contributions can be determined without further approximation errors (§4.2.4).

Section 5 discusses the tensor product approximations. In particular, in §5.2 the tensor product approximation of the kernel  $1/\|x\|$  is described. Then the convolution leads to one-dimensional problems (§5.3). The algorithm is given in §5.4.

The Appendix contains additional remarks about examples for the tensor approximation of  $1/\|x\|$  (§A.1), the recursions for the Galerkin matrix computation (§A.2 for the one-dimensional and §A.3 for the multi-dimensional case), and finally the recursions for the coefficients  $\xi_{\mathbf{x},\alpha}$  (§A.4).

## 2 Setting of the problem

### 2.1 Notation in the univariate case

Before we introduce the  $d$ -dimensional quantities, we start with the 1D case. Let

$$h_\ell := 2^{-\ell} \quad \text{for } \ell \in \mathbb{Z} \quad (2.1)$$

be the step sizes corresponding to the  $\ell$ th level. Note that also negative level numbers  $\ell < 0$  associated with large step sizes  $h_\ell$  are allowed. The real axis  $\mathbb{R}$  is divided into intervals

$$I_\nu^\ell := [\nu h_\ell, (\nu+1) h_\ell) \quad \text{for } \nu, \ell \in \mathbb{Z}, \quad (2.2)$$

which form the grid

$$\mathcal{M}_\ell := \{I_\nu^\ell : \nu \in \mathbb{Z}\} \quad \text{for } \ell \in \mathbb{Z}.$$

The function  $f$  from (1.1) is approximated by piecewise polynomials. For that purpose we define the basis functions

$$\Phi_{\nu,\alpha}^\ell \quad (\ell, \nu \in \mathbb{N}_0, 0 \leq \alpha \leq p)$$

as Legendre polynomials of degree  $\alpha$  mapped from  $[-1, 1]$  onto  $I_\nu^\ell$ , extended by zero outside of  $I_\nu^\ell$ , and normalised by  $\|\Phi_{\nu,\alpha}^\ell\|_{L^2} = 1$ . Hence, for all  $\ell \in \mathbb{Z}$ ,  $\{\Phi_{\nu,\alpha}^\ell : \nu \in \mathbb{Z}, 0 \leq \alpha \leq p\}$  is an orthonormal system.

**Lemma 2.1** *The basis functions  $\Phi_{\nu,\alpha}^\ell$  of subsequent levels satisfy the relation*

$$\Phi_{\nu,\mathbf{x}}^\ell = \sum_{\alpha=0}^{\mathbf{x}} (\xi_{\mathbf{x},\alpha,0} \Phi_{2\nu,\alpha}^{\ell+1} + \xi_{\mathbf{x},\alpha,1} \Phi_{2\nu+1,\alpha}^{\ell+1}) \quad \text{with } \xi_{\mathbf{x},\alpha,0} := (-1)^{\mathbf{x}+\alpha} \xi_{\mathbf{x},\alpha}, \quad \xi_{\mathbf{x},\alpha,1} := \xi_{\mathbf{x},\alpha},$$

where the coefficients  $\xi_{\mathbf{x},\alpha}$  are independent of  $\ell$  and  $\nu$  and can easily be computed (cf. §A.4).

## 2.2 Uniform grids in the multidimensional case

Using the step sizes  $h_\ell$  in all directions, we define multidimensional intervals (cubes) by

$$\mathbf{I}_\nu^\ell := [\nu h_\ell, (\nu + \mathbf{1}) h_\ell] := I_{\nu_1}^\ell \times \dots \times I_{\nu_d}^\ell \quad \text{for } \nu \in \mathbb{Z}^d, \ell \in \mathbb{Z}, \quad (2.3)$$

where now the position index  $\nu = (\nu_1, \dots, \nu_d)$  is a multi-index. This defines the mesh

$$\mathbf{M}_\ell := \{\mathbf{I}_\nu^\ell : \nu \in \mathbb{Z}^d\} \quad \text{for } \ell \in \mathbb{Z}. \quad (2.4)$$

The basis functions (piecewise polynomials of coordinatewise degree  $\leq p$ ) are defined as tensor products of the univariate basis functions. The degree is given by a multi-index  $\alpha \in \{0, \dots, p\}^d$ :

$$\Phi_{\nu, \alpha}^\ell(x_1, \dots, x_d) = \prod_{\delta=1}^d \Phi_{\nu_\delta, \alpha_\delta}^\ell(x_\delta) \quad (\ell \in \mathbb{Z}, \nu \in \mathbb{Z}^d, \mathbf{0} \leq \alpha \leq p\mathbf{1}) \quad (2.5)$$

(note that  $0 \leq \alpha \leq p\mathbf{1}$  is equivalent to  $\alpha \in \{0, \dots, p\}^d$ ). The support of  $\Phi_{\nu, \alpha}^\ell$  is  $\mathbf{I}_\nu^\ell \in \mathbf{M}_\ell$ . The basis  $\{\Phi_{\nu, \alpha}^\ell : \nu \in \mathbb{Z}^d, \alpha \in \{0, \dots, p\}^d\}$  is orthonormal and spans the space

$$S_\ell := \text{span} \{\Phi_{\nu, \alpha}^\ell : \nu \in \mathbb{Z}^d, \alpha \in \{0, \dots, p\}^d\} \quad (\ell \in \mathbb{N}_0). \quad (2.6)$$

The analogue of Lemma 2.1 is

**Lemma 2.2** *The basis functions  $\Phi_{\nu, \alpha}^\ell$  of subsequent levels satisfy the relation*

$$\Phi_{\nu, \varkappa}^\ell = \sum_{\mathbf{0} \leq \alpha \leq \varkappa} \sum_{\mathbf{0} \leq \mathbf{i} \leq \mathbf{1}} \xi_{\varkappa, \alpha, \mathbf{i}} \Phi_{2\nu + \mathbf{i}, \alpha}^{\ell+1} \quad \text{with } \xi_{\varkappa, \alpha, \mathbf{i}} := (-1)^{\langle \varkappa + \alpha, \mathbf{1} - \mathbf{i} \rangle} \xi_{\varkappa, \alpha}, \quad \xi_{\varkappa, \alpha} := \prod_{\delta=1}^d \xi_{\varkappa_\delta, \alpha_\delta}. \quad (2.7)$$

## 2.3 Locally refined mesh in $\mathbb{R}^d$

In the following, we restrict the infinitely many levels  $\ell \in \mathbb{Z}$  to  $\underline{L} \leq \ell \leq \bar{L}$  and associate a sequence of nested boxes

$$\emptyset \neq B_{\underline{L}} \subset \dots \subset B_{\ell+1} \subset B_\ell \subset \dots \subset B_{\underline{L}} \subset \mathbb{R}^d \quad \text{with } B_\ell = [\mathbf{a}_\ell h_\ell, \mathbf{b}_\ell h_\ell], \quad (2.8)$$

where  $\mathbf{a}_\ell, \mathbf{b}_\ell \in 2\mathbb{Z}^d$  (even integers) and  $[\mathbf{a}_\ell h_\ell, \mathbf{b}_\ell h_\ell]$  abbreviates the  $d$ -dimensional box  $[a_{\ell,1} h_\ell, b_{\ell,1} h_\ell] \times [a_{\ell,2} h_\ell, b_{\ell,2} h_\ell] \times \dots \times [a_{\ell,d} h_\ell, b_{\ell,d} h_\ell]$ . For formal purpose we define

$$B_{\bar{L}+1} := \emptyset.$$

In order to avoid an immediate jump from a fine step size to a neighbouring coarse step size, we require that the boxes  $B_\ell$  are properly nested. The precise condition is<sup>5</sup>: There is some  $m \in \mathbb{N}$  with

$$B_\ell + [-mh_{\ell-1}\mathbf{1}, mh_{\ell-1}\mathbf{1}] = [\mathbf{a}_\ell h_\ell - mh_{\ell-1}\mathbf{1}, \mathbf{b}_\ell h_\ell + mh_{\ell-1}\mathbf{1}] \subset B_{\ell-1} \quad \text{for } \underline{L} + 1 \leq \ell \leq \bar{L}, \quad (2.9)$$

which is equivalent to  $\text{dist}_\infty(\partial B_{\ell-1}, \partial B_\ell) \geq mh_{\ell-1}$  (distance in the maximum norm).

For the approximation of  $f$  from (1.1) we use the refined mesh defined by

$$\mathbf{M} := \{\mathbf{I}_\nu^\ell \in \mathbf{M}_\ell : \mathbf{I}_\nu^\ell \subset B_\ell \setminus B_{\ell+1}\}.$$

The corresponding function space is given by

$$S := \text{span} \{\Phi_{\nu, \alpha}^\ell : \mathbf{I}_\nu^\ell \in \mathbf{M}, 0 \leq \alpha \leq p\mathbf{1}\}. \quad (2.10)$$

**Remark 2.3** *a) The basis functions in (2.10) are orthonormal.*

*b) Any function in  $S$  has a support contained in  $B_{\underline{L}}$ .*

*c) After restriction to  $B_\ell \setminus B_{\ell+1}$ , the spaces  $S$  and  $S_\ell$  (cf. (2.6)) coincide.*

*d) Any  $\mathbf{I}_\nu^\ell \subset B_\ell$  has the distance  $\text{dist}_\infty(\mathbf{I}_\nu^\ell, \partial B_{\ell'}) \geq (2 - 2^{\ell'+1-\ell})mh_{\ell-1} \geq mh_{\ell-1}$  from  $\partial B_{\ell'}$  or  $B_0 \setminus B_{\ell'}$  for  $\ell' < \ell$  with respect to the maximum norm.*

**Example 2.4** For a function decaying for  $\|x\| \rightarrow \infty$  with a less regular behaviour at  $x = 0$ , the simplest refinement structure uses

$$B_\ell = 2h_\ell [-\mathbf{1}, \mathbf{1}] = [-2h_\ell, 2h_\ell]^d.$$

Then, for  $m = 1$  the inclusion (2.9) becomes an equality. Furthermore, the cardinality of  $\mathbf{M}$  is

$$\#\mathbf{M} = 2^d (2^d (\bar{L} - \underline{L} + 1) - (\bar{L} - \underline{L})),$$

and  $\dim S = (p+1)^d \#\mathbf{M}$  hold. The covered support  $B_{\underline{L}} = 2^{1-\underline{L}}[-\mathbf{1}, \mathbf{1}]$  may be large because of  $\underline{L} < 0$ , while the smallest step size  $h_{\bar{L}} = 2^{-\bar{L}}$  in  $B_{\bar{L}}$  may be rather small.

For simplicity, we will use a fixed polynomial degree  $p$ . Instead one may adapt also the polynomial degree as usual for the  $hp$ -finite element approach.

## 2.4 Representation of $f \in S$

By definition of the space  $S$  (cf. (2.10)) there are coefficients  $f_{\mathbf{j},\beta}^\ell$  of  $f \in S$  so that

$$f = \sum_{\ell=\underline{L}}^{\bar{L}} \sum_{\mathbf{j},\beta} f_{\mathbf{j},\beta}^\ell \Phi_{\mathbf{j},\beta}^\ell.$$

This defines a level-wise decomposition

$$f = \sum_{\ell=\underline{L}}^{\bar{L}} f^\ell \quad \text{with} \quad f^\ell := \sum_{\mathbf{j},\beta} f_{\mathbf{j},\beta}^\ell \Phi_{\mathbf{j},\beta}^\ell \in S_\ell. \quad (2.11)$$

Here the summation  $\sum_{\mathbf{j},\beta}$  is taken over positions  $\mathbf{j} \in \mathbb{Z}^d$  with  $\mathbf{I}_{\mathbf{j}}^\ell \subset B_\ell \setminus B_{\ell+1}$  and degrees  $\mathbf{0} \leq \beta \leq p\mathbf{1}$  (i.e.,  $\beta \in \{0, \dots, p\}^d$ ).

**Remark 2.5** a) The unique decomposition (2.11) of  $f$  into the  $f^\ell$ -contributions leads to the supports

$$\text{supp}(f^\ell) \subset \overline{B_\ell \setminus B_{\ell+1}}. \quad (2.12)$$

b) In the following we allow a representation  $f = \sum_{\ell=\underline{L}}^{\bar{L}} f^\ell$  with  $f^\ell := \sum_{\mathbf{j},\beta} f_{\mathbf{j},\beta}^\ell \Phi_{\mathbf{j},\beta}^\ell \in S_\ell$  such that

$$\text{supp}(f^\ell) \subset \overline{B_\ell}.$$

In this case the restriction  $f|_{B_\ell \setminus B_{\ell+1}}$  may involve contributions from all levels  $\ell, \ell-1, \dots, \underline{L}$ . As a consequence, such a representation is not unique.

## 2.5 Notations: projections, restriction and prolongation

Let  $S$  and  $S_\ell$  be the subspaces of  $L^2(\mathbb{R}^d)$  introduced above. Then the corresponding  $L^2$ -orthogonal projections are denoted by

$$P : L^2(\mathbb{R}^d) \rightarrow S, \quad P_\ell : L^2(\mathbb{R}^d) \rightarrow S_\ell.$$

By the definition of an orthogonal projection, the explicit representation of  $P_\ell$  is

$$P_\ell : \varphi \in L^2(\mathbb{R}^d) \mapsto \varphi_\ell = P_\ell \varphi = \sum_{\mathbf{i},\alpha} \varphi_{\mathbf{i},\alpha}^\ell \Phi_{\mathbf{i},\alpha}^\ell \quad \text{with} \quad \varphi_{\mathbf{i},\alpha}^\ell = \langle \varphi, \Phi_{\mathbf{i},\alpha}^\ell \rangle. \quad (2.13)$$

The relation between  $P$  and  $P_\ell$  is given by the restrictions  $(Pf)|_{\overline{B_\ell \setminus B_{\ell+1}}} = (P_\ell f)|_{\overline{B_\ell \setminus B_{\ell+1}}}$  to  $\overline{B_\ell \setminus B_{\ell+1}}$ .

**Notation 2.6** The coefficients  $f_{\mathbf{j},\beta}^\ell$  of  $f^\ell := \sum_{\mathbf{j},\beta} f_{\mathbf{j},\beta}^\ell \Phi_{\mathbf{j},\beta}^\ell \in S_\ell$  give rise to the multi-indexed sequences

$$f_{\ell,\beta} := (f_{\mathbf{j},\beta}^\ell)_{\mathbf{j} \in \mathbb{Z}^d} \quad \text{for all } \mathbf{0} \leq \beta \leq p\mathbf{1}$$

which are summarised in the tuple

$$\mathbf{f}[\ell] := (f_{\ell,\beta})_{\mathbf{0} \leq \beta \leq p\mathbf{1}}.$$

Since  $S_\ell \subset S_{\ell+1}$ , any  $f^\ell \in S_\ell$  can be represented at level  $\ell$  ( $f^\ell := \sum_{\mathbf{i}, \alpha} f_{\mathbf{i}, \alpha}^\ell \Phi_{\mathbf{i}, \alpha}^\ell$ ) as well as at level  $\ell + 1$ :  $f^\ell = \sum_{\mathbf{j}, \beta} f_{\mathbf{j}, \beta}^{\ell+1} \Phi_{\mathbf{j}, \beta}^{\ell+1}$ . The respective coefficients are compactly written as  $\mathbf{f}[\ell]$  and  $\mathbf{f}[\ell + 1]$ . To characterise the *prolongation*  $\mathcal{P} : \mathbf{f}[\ell] \mapsto \mathbf{f}[\ell + 1]$ , we make use of (2.7) and obtain

$$\mathcal{P}(\mathbf{f}[\ell]) = \mathbf{f}[\ell + 1] \quad \text{with } f_{2\mathbf{i}+\mathbf{k}, \beta}^{\ell+1} := \sum_{\beta \leq \alpha \leq p\mathbf{1}} f_{\mathbf{i}, \alpha}^\ell \xi_{\alpha, \beta, \mathbf{k}} \quad \text{for all } \mathbf{0} \leq \mathbf{k} \leq \mathbf{1} \quad (2.14)$$

with the coefficients  $\xi_{\alpha, \beta, \mathbf{k}}$  from (2.7).

The opposite direction is performed by the *restriction*  $\mathcal{R} : \mathbf{f}[\ell + 1] \mapsto \mathbf{f}[\ell]$  associated to the  $L^2$ -orthogonal projection of a function  $f^{\ell+1} \in S_{\ell+1}$  onto  $f^\ell \in S_\ell$ . Note that  $f^\ell$  has the coefficients  $f_{\mathbf{i}, \alpha}^\ell = \langle f^{\ell+1}, \Phi_{\mathbf{i}, \alpha}^\ell \rangle$ . Inserting the representation  $f^{\ell+1} := \sum_{\mathbf{j}, \beta} f_{\mathbf{j}, \beta}^{\ell+1} \Phi_{\mathbf{j}, \beta}^{\ell+1}$  and the recursion formula (2.7), we get the component-wise representation

$$\mathcal{R} : \mathbf{f}[\ell + 1] \mapsto \mathbf{f}[\ell] \quad \text{with } f_{\mathbf{i}, \alpha}^\ell := \sum_{\mathbf{0} \leq \mathbf{x} \leq \alpha} \sum_{\mathbf{0} \leq \mathbf{k} \leq \mathbf{1}} \xi_{\alpha, \mathbf{x}, \mathbf{k}} f_{2\mathbf{i}+\mathbf{k}, \mathbf{x}}^{\ell+1}. \quad (2.15)$$

## 2.6 Convolution with $1/\|x\|$

The convolution with the Newton<sup>6</sup> potential defines the operator

$$(\mathcal{K}f)(x) := \int_{\mathbb{R}^d} \frac{f(y)}{\|x - y\|} dy.$$

Instead of general  $f$  we consider ansatz functions  $f \in S$ . The Galerkin approximation of  $\mathcal{K}$  is given by  $PKP$  ( $P$  from §2.5). Therefore, for  $f \in S$ , the function

$$u := PKf \in S \quad (f \in S)$$

is to be determined. Thanks to Remark 2.3a, the coefficients of  $u \in S$  can be characterised explicitly:

$$u = \sum_{\ell'=\underline{L}}^{\overline{L}} \sum_{\substack{\mathbf{i} \in \mathbb{Z}^d \text{ with} \\ \mathbf{I}_i^\ell \subset B_\ell \setminus B_{\ell+1}}} \sum_{\mathbf{0} \leq \alpha \leq p\mathbf{1}} u_{\mathbf{i}, \alpha}^{\ell'} \Phi_{\mathbf{i}, \alpha}^{\ell'} \quad \text{with } u_{\mathbf{i}, \alpha}^{\ell'} := \langle \mathcal{K}f, \Phi_{\mathbf{i}, \alpha}^{\ell'} \rangle.$$

Since  $f \in S$  is a linear combination of certain  $\Phi_{\mathbf{j}, \beta}^\ell$ , the quantities

$$\langle \mathcal{K} \Phi_{\mathbf{j}, \beta}^\ell, \Phi_{\mathbf{i}, \alpha}^{\ell'} \rangle = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\Phi_{\mathbf{i}, \alpha}^{\ell'}(x) \Phi_{\mathbf{j}, \beta}^\ell(y)}{\|x - y\|} dx dy \quad (2.16)$$

need to be computed. In the following we will discuss the case  $\ell' = \ell$ .

**Remark 2.7** *In principle, the general case  $\ell' \neq \ell$  can be reduced to  $\ell' = \ell$  as follows. Let, e.g.,  $\ell' > \ell$ . Using (2.7), we can replace  $\Phi_{\mathbf{j}, \beta}^\ell(y)$  by basis functions of level  $\ell + 1$ . Repeating this process  $(\ell' - \ell)$ -times, only expressions of the form  $\langle \mathcal{K} \Phi_{\mathbf{j}, \beta}^{\ell'}, \Phi_{\mathbf{i}, \alpha}^{\ell'} \rangle$  appear. In practice, this procedure requires that  $f|_{B_\ell \setminus B_{\ell+1}} \in S_\ell$  must be expressed by basis functions from level  $\ell'$  which increases the data size by  $2^{\ell' - \ell}$ .*

Because of the last mentioned disadvantage, we will introduce an *approximation* of  $PKP$  which requires (2.16) for equal levels  $\ell = \ell'$  only. Note that

$$\mathcal{K}_\ell := P_\ell \mathcal{K} P_\ell$$

is the Galerkin approximation of  $\mathcal{K}$  in  $S_\ell$ . Its matrix entries are the quantities from (2.16) with  $\ell = \ell'$ .

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<sup>6</sup>In connection with electrical fields, the Newton potential is also called Coulomb potential.



### 3 Approximation of the convolution

The reasoning is as follows: The image  $\mathcal{K}\varphi$  is smoother than  $\varphi$ . In particular the mapping of the part  $\varphi|_{\Omega_1}$  to  $(\mathcal{K}\varphi)|_{\Omega_2}$  has smoothing character. If the grid size  $h_{\ell-1}$  is sufficient to approximate  $f^{\ell-1}$  in  $\Omega_1$  it should also be sufficient to approximate  $u = \mathcal{K}f^{\ell-1}$  by  $u^{\ell-1} = P_{\ell-1}\mathcal{K}f^{\ell-1}$ .

#### 3.1 Definition of the approximation

Consider  $f^\ell \in S_\ell$  with support  $B_\ell$ . The image  $u := P\mathcal{K}f^\ell \in S$  is the exact Galerkin result. Fix a level  $\lambda$  and consider the restriction  $u^\lambda := u|_{B_\lambda \setminus B_{\lambda+1}}$ . This function extended by zero outside belongs to  $S_\lambda$ . Hence,

$$u^\lambda = P_\lambda \mathcal{K} P_\ell f^\ell$$

holds, where  $\underline{L} \leq \lambda \leq \overline{L}$ . As mentioned before, the computation of  $P_\lambda \mathcal{K} P_\ell$  for  $\lambda \neq \ell$  is possible, but costly. Instead we introduce a further approximation error and replace  $P_\lambda \mathcal{K} P_\ell$  by  $P_{\min\{\lambda, \ell\}} \mathcal{K} P_{\min\{\lambda, \ell\}}$ . The verbal justification is as follows. A more formal justification will follow in §3.4.

If  $\lambda \geq \ell$ , the result  $u^\lambda$  requires the finer step size  $h_\lambda \leq h_\ell$ . However, since  $\mathcal{K}f^\ell$  is smoother than  $f^\ell \in S_\ell$ , also the image should be well approximated in  $S_\ell$ . Therefore, we replace  $P_\lambda$  by  $P_\ell = P_{\min\{\lambda, \ell\}}$ .

If  $\lambda = \ell - 1$ , the support  $B_{\ell-1} \setminus B_\ell$  is disjoint from the support of  $f^\ell$ , which is contained in  $B_\ell$ . This leads to a further smoothing effect by  $\mathcal{K}$  and allows to neglect the difference  $P_{\ell-1}\mathcal{K}(P_\ell - P_{\ell-1})f^\ell$ , i.e., to replace  $P_\lambda \mathcal{K} P_\ell f^\ell$  by  $P_\lambda \mathcal{K} P_\lambda f^\ell$ .

If  $\lambda < \ell - 1$ , the support  $B_\lambda \setminus B_{\lambda+1}$  has a distance of at least  $mh_{\lambda+1}$  from the support of  $f^\ell$ . This increased the smoothing effect again and allows to use  $P_\lambda \mathcal{K} P_\lambda f^\ell$ .

The described replacements lead to the following approximation.

**Definition 3.1** Represent  $f \in S$  in the form

$$f = \sum_{\ell} f^\ell \quad \text{with } f^\ell \in S_\ell, \text{ supp}(f^\ell) \subset \overline{B_\ell} \quad (3.1a)$$

(cf. Remark 2.5b). Approximate each term  $P\mathcal{K}f^\ell \in S$  by  $u_\ell = \sum_{\lambda=\underline{L}}^{\ell} u^{\lambda, \ell}$  with

$$u^{\ell, \ell} := (P_\ell \mathcal{K} P_\ell f^\ell)|_{B_\ell}, \quad (3.1b)$$

$$u^{\lambda, \ell} := (P_\lambda \mathcal{K} P_\lambda f^\ell)|_{B_\lambda \setminus B_{\lambda+1}} \quad \text{for } \underline{L} \leq \lambda < \ell. \quad (3.1c)$$

Altogether the approximation of  $\mathcal{K}f$  is

$$u := \sum_{\ell=\underline{L}}^{\overline{L}} \sum_{\lambda=\underline{L}}^{\ell} u^{\lambda, \ell}. \quad (3.1d)$$

**Remark 3.2** Note that the result  $u$  in (3.1d) depends on the representation (3.1a) of  $f$ . The most accurate result is to be expected for the representation from Remark 2.5a.

#### 3.2 Algorithm

The algorithmic description of Definition 3.1 reads as follows:

```

 $F := 0; u := 0;$ 
for  $\ell := \overline{L}$  downto  $\underline{L}$  do
begin  $F := P_\ell F;$ 
 $u|_{B_\ell} := u|_{B_\ell} + (P_\ell \mathcal{K} P_\ell f^\ell)|_{B_\ell};$ 
 $u|_{B_\ell \setminus B_{\ell+1}} := (P_\ell \mathcal{K} P_\ell F)|_{B_\ell \setminus B_{\ell+1}};$ 
 $F := F + f^\ell;$ 
end;
```

(3.2)

The function  $F$  from line 3 is  $F = P_\ell \sum_{\lambda=\ell+1}^{\overline{L}} f^\lambda \in S_\ell$ . Its support is in  $B_{\ell+1}$ . In line 4, the new term  $u^{\ell, \ell}$  from (3.1b) is added. Line 5 contains  $\sum_{\lambda=\ell+1}^{\overline{L}} u^{\ell, \lambda}$  from (3.1c).

If one wants to follow the lines of Remark 3.2, Algorithm (3.2) is to be preceded by

$$\boxed{\begin{array}{l} \text{for } \ell := \underline{L} \text{ to } \overline{L} - 1 \text{ do} \\ \text{begin } \mathbf{f}[\ell + 1] := \mathbf{f}[\ell + 1] + \mathcal{P}(\mathbf{f}[\ell]|_{B_{\ell+1}}); \mathbf{f}[\ell]|_{B_{\ell+1}} := 0 \text{ end;} \end{array}} \quad (3.3)$$

$\mathcal{P}$  is the prolongation from (2.14). The notation  $\mathbf{f}[\ell]|_{B_{\ell+1}}$  is used for the coefficients of the restriction  $f^\ell|_{B_{\ell+1}}$ , i.e.  $f_{\mathbf{i},\alpha}^\ell = 0$  for  $\mathbf{I}_\mathbf{i}^\ell \cap B_{\ell+1} = \emptyset$ . This part is represented with respect to the basis of level  $\ell + 1$ . The subtraction of this part from level  $\ell$  is described by replacing all coefficients corresponding to  $\mathbf{I}_\mathbf{i}^\ell \subset \overline{B_{\ell+1}}$  by zero.

It remains to described the performance of  $\mathcal{K}_\ell f^\ell$  for  $\mathcal{K}_\ell := P_\ell \mathcal{K} P_\ell$ , which is the discrete convolution with the Newton potential.

### 3.3 Possible improvements and modifications

The approximation errors introduced in §3.1 can be reduced as follows. The truncation of  $u^\lambda = P_\lambda \mathcal{K} P_\ell f^\ell$  from a coarse level  $\lambda < \ell$  to  $P_\lambda \mathcal{K} P_\lambda f^\ell$  happens if  $\text{supp}(f^\ell) \subset \overline{B_\ell}$  and if the result is to be evaluated in  $B_\lambda \setminus B_{\lambda+1}$ . For  $\lambda = \ell - 1$ , these support are directly neighboured, otherwise ( $\lambda < \ell - 1$ ) there is a distance of at least  $m h_{\ell-1} = 2m h_\ell$  (cf. Remark 2.3d). Increasing  $m$  improves the accuracy for  $\lambda < \ell - 1$ . To include the case  $\lambda = \ell - 1$ , one may split  $A := B_\lambda \setminus B_{\lambda+1} = [\mathbf{a}_\lambda h_\lambda, \mathbf{b}_\lambda h_\lambda] \setminus [\mathbf{a}_{\lambda+1} h_{\lambda+1}, \mathbf{b}_{\lambda+1} h_{\lambda+1})$  into

$$\begin{aligned} A' &:= [\mathbf{a}_\lambda h_\lambda, \mathbf{b}_\lambda h_\lambda] \setminus [\mathbf{a}_{\lambda+1} h_{\lambda+1} - m' h_{\lambda+1} \mathbf{1}, \mathbf{b}_{\lambda+1} h_{\lambda+1} + m' h_{\lambda+1} \mathbf{1}), \\ A'' &:= [\mathbf{a}_{\lambda+1} h_{\lambda+1} - m' h_{\lambda+1} \mathbf{1}, \mathbf{b}_{\lambda+1} h_{\lambda+1} + m' h_{\lambda+1} \mathbf{1}) \setminus [\mathbf{a}_{\lambda+1} h_{\lambda+1}, \mathbf{b}_{\lambda+1} h_{\lambda+1}), \end{aligned}$$

assuming  $\mathbf{a}_\lambda h_\lambda \leq \mathbf{a}_{\lambda+1} h_{\lambda+1} - m' h_{\lambda+1} \mathbf{1}$  and  $\mathbf{b}_\lambda h_\lambda \geq \mathbf{b}_{\lambda+1} h_{\lambda+1} + m' h_{\lambda+1} \mathbf{1}$ . The restriction  $u^\lambda|_{A'} = P_\lambda \mathcal{K} P_\ell f^\ell|_{A'} \approx P_\lambda \mathcal{K} P_\lambda f^\ell|_{A'}$  is treated as before, whereas in  $A''$  we determine  $u^\ell|_{A''} = P_\ell \mathcal{K} P_\ell f^\ell|_{A''}$  on the finer level and prolongate this result to level  $\lambda = \ell - 1$ .

As mentioned in Remark 2.5b, we may allow contributions to  $B_\ell$  from all levels  $\lambda \leq \ell$ . In the (multi-) wavelet setting this is the common approach with the difference that for increasing levels the data contain details which are orthogonal to previous contributions, i.e.,

$$f = \sum_{\ell=\underline{L}}^{\overline{L}} f^\ell \quad \text{with} \quad f^\ell \in S_\ell \text{ and } f^\ell \perp S_\lambda \text{ for } \lambda < \ell. \quad (3.4)$$

The advantage of this representation is that the size of the details can be used to estimate errors or to adapt the mesh. Given any representation  $f = \sum_{\ell=\underline{L}}^{\overline{L}} f^\ell$  with  $f^\ell \in S_\ell$  organised by the data  $\mathbf{f}[\ell]$ , the algorithm

$$\boxed{\begin{array}{l} \text{for } \ell = \overline{L} \text{ downto } \underline{L} + 1 \text{ do} \\ \text{begin } \mathbf{d}[\ell - 1] := \mathcal{R}(\mathbf{f}[\ell]); \quad (\text{cf. (2.15)}) \\ \quad \mathbf{f}[\ell - 1] := \mathbf{f}[\ell - 1] + \mathbf{d}[\ell - 1]; \\ \quad \mathbf{f}[\ell] := \mathbf{f}[\ell] - \mathcal{P}(\mathbf{d}[\ell - 1]) \quad (\text{cf. (2.14)}) \\ \text{end;} \end{array}}$$

yields the representation (3.4). Note that  $f^\ell$  is split orthogonally into  $f^\ell = P_{\ell-1} f^\ell + (I - P_{\ell-1}) f^\ell$ . The part  $P_{\ell-1} f^\ell$  is realised by the data  $\mathcal{R}(\mathbf{f}[\ell])$  on level  $\ell - 1$ .

For simplicity, we have fixed the polynomial degree by  $p$ .

### 3.4 Justification of the Approximation

In §3 we have replaced  $P_\lambda \mathcal{K} P_\ell$  by  $P_{\min\{\lambda, \ell\}} \mathcal{K} P_{\min\{\lambda, \ell\}}$ . In the following we describe a situation, where this replacement (for  $\lambda < \ell$ ) make sense. We recall that in this setting the source function  $f$  and the convolution  $u$  from (1.1) are represented in the same grid system. In general, however, we have to use another adapted grid for  $u$ , which might be very different from the  $f$ -grid as the second Example 3.4 will show. As in §3.3 we assume that the replacement of  $P_\lambda \mathcal{K} P_\ell$  by  $P_\lambda \mathcal{K} P_\lambda$  for  $\lambda = \ell - 1$  happens only for  $x \in B_\lambda$  with  $\text{dist}(x, B_\ell) \geq h_\lambda$  (using the minimal value  $m = 1$ ). Note that for  $\lambda < \ell - 1$  this distance conditions follows from (2.9).

**Example 3.3** We assume that  $f$  satisfies (i)  $\text{supp}(f)$  has diameter  $\mathcal{O}(1)$ , (ii)  $f \in C^1$  with the Lipschitz condition (iii):

$$|\nabla f(x) - \nabla f(y)| \leq L |\nabla f(x)| \|x - y\|. \quad (3.5)$$

The characteristics of the grid are: (a) The size is  $\mathcal{O}(1)$  according to (i), (b) the polynomial degree  $p = 0$  is chosen, (c) for a fixed position  $x$  the grid is refined until the approximation  $\tilde{f} \in S$  satisfies  $\|f - \tilde{f}\|_\infty \leq \varepsilon$  for a given  $\varepsilon > 0$ .

Assumption (i) concerns the size of  $\text{supp}(f)$ . Of course, the image  $u = \mathcal{K}f$  needs a larger support for approximation, but there may be reasons to approximate  $u$  only in the  $f$ -grid (one reason is the scalar product (1.2) involving a function with the corresponding support).

Assumption (ii) allows pointwise error estimates for the choice  $p = 0$  (see (b)).

The main difficulty in this analysis is the formulation of the variation of smoothness. If the smoothness (here expressed by the size of  $\nabla f$ ) is similar everywhere, we need only *one* uniform grid and the replacement of  $P_\lambda \mathcal{K} P_\ell$  by  $P_\lambda \mathcal{K} P_\lambda$  does not happen. Different grid sizes occur due to a variation of smoothness. Condition (3.5) is an attempt to model the variation by a relative Lipschitz condition.

Remark 2.5a led to a unique representation of  $f = \sum_\ell f_\ell$ . Here, we use the representation (3.4). The contributions  $f_\ell$  are defined by  $P_\lambda f = \sum_{\ell \leq \lambda} f_\ell$ , i.e.,  $f_\ell := (P_\ell - P_{\ell-1}) f$ . Together with  $p = 0$ , this describes the Haar wavelet representation. For simplicity, we first consider a 1D-grid and therein an interval  $I_\nu^{\ell+1}$  (cf. (2.2)). The coefficient  $f_\nu^{\ell+1}$  in  $f^{\ell+1} := \sum_j f_j^{\ell+1} \Phi_{j,0}^{\ell+1}$  (the  $\beta$ -indices are not needed since  $\beta = 0$  because of  $p = 0$ ) is defined by  $\langle f^{\ell+1}, \Phi_{\nu,0}^{\ell+1} \rangle$ . Let  $\nu$  be even. While  $\Phi_{\nu,0}^{\ell+1} + \Phi_{\nu+1,0}^{\ell+1}$  belongs to the range of the projection  $P_\ell$ ,  $\Phi_{\nu,0}^{\ell+1} - \Phi_{\nu+1,0}^{\ell+1}$  is orthogonal. Hence,  $f_\nu^{\ell+1} = -f_{\nu+1}^{\ell+1}$  and

$$f_\nu^{\ell+1} = \frac{1}{2} \langle f, \Phi_{\nu,0}^{\ell+1} - \Phi_{\nu+1,0}^{\ell+1} \rangle$$

holds. Since  $\Phi_{\nu,0}^{\ell+1}$  has the value  $2^{(\ell+1)/2} = h_{\ell+1}^{-1/2}$  in  $I_\nu^{\ell+1}$ , there is a  $\xi \in I_\nu^{\ell+1} \cup I_{\nu+1}^{\ell+1} = I_{\nu/2}^\ell$  with

$$f_\nu^{\ell+1} = \frac{h_{\ell+1}^{1+1/2}}{2} f'(\xi).$$

The projection error  $\delta f_\ell := f - P_\ell f$  is the infinite sum  $\sum_{\lambda=\ell+1}^\infty \sum_j f_j^\lambda \Phi_{j,0}^\lambda$ . At a fixed point  $y$  the error is  $\delta f_\ell(y) = \sum_{\lambda=\ell+1}^\infty f_{\nu(\lambda,y)}^\lambda \Phi_{\nu(\lambda,y),0}^\lambda$ , where  $\nu = \nu(\ell, y)$  is the index with  $x_0 \in I_{\nu(\lambda,x_0)}^\lambda$ . As  $\|\Phi_{\nu(\lambda,y),0}^\lambda\|_\infty = h_\lambda^{-1/2}$ , we have

$$|\delta f_\ell(y)| \leq \frac{1}{2} \sum_{\lambda=\ell+1}^\infty h_{\ell+1} \|f'\|_{\infty, I_{\nu/2}^\ell} = h_{\ell+1} \|f'\|_{\infty, I_{\nu/2}^\ell} \quad (y \in I_{\nu/2}^\ell).$$

Up to a factor 2, the leading term of  $\delta f_\ell$  is the contribution  $f_\nu^{\ell+1} \Phi_{\nu,0}^{\ell+1}$  of level  $\ell+1$ . Replacing the argument  $\xi \in I_{\nu/2}^\ell$  by  $y$  we write simply

$$|\delta f_\ell(y)| \lesssim h_\ell |f'(y)|.$$

When an operator with kernel  $k(x, y)$  is applied to  $f_\nu^{\ell+1} (\Phi_{\nu,0}^{\ell+1} - \Phi_{\nu+1,0}^{\ell+1})$ , the result is  $f_\nu^{\ell+1} h_{\ell+1} \frac{\partial}{\partial y} k(x, \tilde{y})$  with  $\tilde{y} \in I_{\nu/2}^\ell$ . Hence

$$\left| \int_{I_{\nu/2}^\ell} k(x, y) \delta f_\ell(y) dy \right| \leq \|f'\|_{\infty, I_{\nu/2}^\ell} h_\ell^2 \left| \int_{I_{\nu/2}^\ell} \frac{\partial}{\partial y} k(x, \tilde{y}) dy \right| \lesssim h_\ell^2 \left| \int_{I_{\nu/2}^\ell} f'(y) \frac{\partial}{\partial y} k(x, y) dy \right| \quad (3.6)$$

Now we return to the  $d$ -dimensional case. The same argument shows

$$|\delta f_\ell(y)| \lesssim h_\ell \|\nabla f\|_{\infty, \mathbf{I}_{\nu/2}^\ell}.$$

(3.6) becomes

$$\left| \int_{\mathbf{I}_{\nu/2}^\ell} \frac{\delta f_\ell(y) dy}{\|x - y\|} \right| \lesssim h_\ell^2 \int_{\mathbf{I}_{\nu/2}^\ell} \frac{|\nabla f(y)| dy}{\|x - y\|^2}. \quad (3.7)$$

The function  $\delta f(x)$  is defined by  $\delta f_\ell(x)$  with  $\ell$  such that  $x \in B_\ell \setminus B_{\ell+1}$ .

Now we assume that refinement is done such that  $\|\delta f\|_\infty \leq \varepsilon$  (assumption (c) of Example 3.3). Therefore, an error of  $u = \mathcal{K}f$  of the size  $\int_{B_0} \frac{\varepsilon dy}{\|x-y\|}$  is acceptable. Let  $x \in B_\lambda \setminus B_{\lambda+1}$  and  $y \in B_\ell$ , where  $\ell > \lambda$ . Replacing  $P_\lambda \mathcal{K} P_\ell$  by  $P_\lambda \mathcal{K} P_\lambda$  means to replace  $\delta f_\ell$  in  $B_\ell$  by  $\delta f_\lambda$ . Following (3.7),  $\delta f_\lambda$  leads to the error contribution  $h_\lambda^2 \int_{B_\ell} \frac{|\nabla f(y)| dy}{\|x-y\|^2}$  from  $B_\ell$ . The Lipschitz condition (3.5) yields

$$h_\lambda^2 \frac{|\nabla f(y)|}{\|x-y\|^2} \leq h_\lambda^2 \frac{|\nabla f(x)|}{\|x-y\|^2} + L h_\lambda^2 \frac{|\nabla f(x)|}{\|x-y\|}.$$

Since the replacement of  $P_\lambda \mathcal{K} P_\ell$  by  $P_\lambda \mathcal{K} P_\lambda$  is only made if  $\|x-y\| \geq h_\lambda$  (cf. §3.3),  $h_\lambda^2 / \|x-y\|^2 \leq h_\lambda / \|x-y\|$  holds. Together we have

$$h_\lambda^2 \frac{|\nabla f(y)|}{\|x-y\|^2} \leq h_\lambda \frac{|\nabla f(x)|}{\|x-y\|} (1 + L h_\lambda).$$

Since  $\|\delta f\|_\infty \leq \varepsilon$  and  $x \in B_\lambda \setminus B_{\lambda+1}$  is assumed,  $h_\lambda |\nabla f(x)| \lesssim \varepsilon$  follows. Hence the error contribution from  $B_\ell$  is of acceptable size:

$$h_\lambda^2 \int_{B_\ell} \frac{|\nabla f(y)| dy}{\|x-y\|^2} \leq (1 + L h_\lambda) \int_{B_\ell} \frac{h_\lambda |\nabla f(x)|}{\|x-y\|} dy \lesssim \int_{B_\ell} \frac{\varepsilon dy}{\|x-y\|}.$$

**Example 3.4** Let  $\ell^* \in \mathbb{N}$  be fixed and set  $f := \Phi_{\mathbf{0},\mathbf{0}}^{\ell^*}$ . Since  $\text{supp } f = \mathbf{I}_{\mathbf{0}}^{\ell^*}$ , the grid for the representation of  $f$  requires only one interval. Obviously, the function  $f$  is not smooth, but its (non-)smoothness is not expressed by (omitted) contributions  $f^\ell$  in  $f = \sum_\ell f^\ell$  for  $\ell > \ell^*$ . The image  $u = \mathcal{K}f$  requires its own adapted grid by two reasons. First,  $u(x)$  behaves as  $\mathcal{O}(1/\|x\|)$  as  $\|x\| \rightarrow \infty$  and needs a large grid (which can be easily managed by choosing a sufficiently negative  $\underline{L}$ ). Second, the discontinuity of  $f$  on  $\partial \mathbf{I}_{\mathbf{0}}^{\ell^*}$  requires a refinement in the neighbourhood of  $\mathbf{I}_{\mathbf{0}}^{\ell^*}$ .

We add the remark that we should not compute  $u$  from the latter example if the scalar product  $\langle g, u \rangle$  is desired, since this value can better be computed via  $\langle \mathcal{K}g, f \rangle = \langle \mathcal{K}g, \Phi_{\mathbf{0},\mathbf{0}}^{\ell^*} \rangle$ .

## 4 Evaluation of the convolution

### 4.1 Convolution at level $\ell$

Due to the approximation made in §3.1, the coefficients (2.16) are only needed for the case  $\ell' = \ell$ . Since  $\Phi_{\mathbf{i},\alpha}^\ell(x) = \Phi_{\mathbf{0},\alpha}^\ell(x - \mathbf{i}h_\ell)$ , substitution of the integration variables shows that the integrals

$$N_{\mathbf{i}-\mathbf{j},\alpha,\beta}^\ell := \iint \frac{\Phi_{\mathbf{i},\alpha}^\ell(x) \Phi_{\mathbf{j},\beta}^\ell(y)}{\|x-y\|} dx dy = \iint \frac{\Phi_{\mathbf{i}-\mathbf{j},\alpha}^\ell(x) \Phi_{\mathbf{0},\beta}^\ell(y)}{\|x-y\|} dx dy \quad (4.1)$$

depend only on the difference  $\mathbf{i} - \mathbf{j}$ .

**Remark 4.1** Let  $f^\ell$  be as in (2.11). The  $L^2$ -orthogonal projection of  $F(x) := \int \frac{f^\ell(y)}{\|x-y\|} dy$  onto  $\mathcal{S}_\ell$  yields

$$P_\ell F = P_\ell \mathcal{K} f^\ell = \sum_{\mathbf{i} \in \mathbb{Z}^d} \sum_{\mathbf{0} \leq \alpha, \beta \leq p\mathbf{1}} \left( \sum_{\mathbf{j} \in \mathbb{Z}^d} N_{\mathbf{i}-\mathbf{j},\alpha,\beta}^\ell f_{\mathbf{j},\beta}^\ell \right) \Phi_{\mathbf{i},\alpha}^\ell.$$

Set

$$F_{\mathbf{i},\alpha}^\ell := \sum_{\mathbf{0} \leq \beta \leq p\mathbf{1}} \sum_{\mathbf{j} \in \mathbb{Z}^d} N_{\mathbf{i}-\mathbf{j},\alpha,\beta}^\ell f_{\mathbf{j},\beta}^\ell. \quad (4.2)$$

Besides the  $\beta$ -summation it is a discrete convolution and can be computed by fast Fourier Transform (FFT), provided that the quantities  $N_{\mathbf{k},\alpha,\beta}^\ell$  from (4.1) are known (this will be the subject of §4.2).  $F_{\mathbf{i},\alpha}^\ell$  are the coefficients of  $P_\ell F = \sum_{\mathbf{i} \in \mathbb{Z}^d} \sum_{\mathbf{0} \leq \alpha \leq p\mathbf{1}} F_{\mathbf{i},\alpha}^\ell \Phi_{\mathbf{i},\alpha}^\ell$ .

**Remark 4.2** The sequence  $(f_{\mathbf{j},\beta}^\ell)_{\mathbf{j} \in \mathbb{Z}^d}$  has a finite support, since  $f_{\mathbf{j},\beta}^\ell = 0$  as soon as  $\mathbf{j}h_\ell$  is outside of the refinement box  $B_\ell$ . Let  $N := \#\{\mathbf{j} : \mathbf{j}h_\ell \in B_\ell\}$  be the data size. The sequence  $(N_{\mathbf{i},\alpha,\beta}^\ell)_{\mathbf{i} \in \mathbb{Z}^d}$  has unbounded support, which implies that also  $(F_{\mathbf{i},\alpha}^\ell)_{\mathbf{i} \in \mathbb{Z}^d}$  has unbounded support. But since we are only interested in the finite part  $\{F_{\mathbf{i},\alpha}^\ell : \mathbf{j}h_\ell \in B_\ell\}$ , one can truncate the support of  $(N_{\mathbf{i},\alpha,\beta}^\ell)_{\mathbf{i} \in \mathbb{Z}^d}$  so that the data size is  $\mathcal{O}(N)$  while the discrete convolution yields the same values  $\{F_{\mathbf{i},\alpha}^\ell : \mathbf{j}h_\ell \in B_\ell\}$ . Applying fast Fourier transform, the discrete convolution (4.2) requires  $\mathcal{O}(Np^d \log N)$  arithmetical operations.

## 4.2 Computation of $N_{\mathbf{i},\alpha,\beta}^\ell$

### 4.2.1 Properties

First we describe some helpful properties of  $N_{\mathbf{i},\alpha,\beta}^\ell$ . Its dependence on  $\ell$  is given by a factor. Since  $\Phi_{\mathbf{i},\alpha}^\ell(x) = 2^{\ell d/2} \Phi_{\mathbf{i},\alpha}^0(2^\ell x)$ , we have

$$\begin{aligned} N_{\mathbf{i},\alpha,\beta}^\ell &= \iint \frac{\Phi_{\mathbf{i},\alpha}^\ell(x) \Phi_{\mathbf{0},\beta}^\ell(y)}{\|x - y\|} dx dy = 2^{\ell d} \iint \frac{\Phi_{\mathbf{i},\alpha}^0(2^\ell x) \Phi_{\mathbf{0},\beta}^0(2^\ell y)}{\|x - y\|} dx dy \\ &= 2^{\ell d} 2^\ell \iint \frac{\Phi_{\mathbf{i},\alpha}^0(2^\ell x) \Phi_{\mathbf{0},\beta}^0(2^\ell y)}{\|2^\ell x - 2^\ell y\|} dx dy = 2^{\ell(1-d)} \iint \frac{\Phi_{\mathbf{i},\alpha}^0(x') \Phi_{\mathbf{0},\beta}^0(y')}{\|x' - y'\|} dx' dy' \\ &= 2^{\ell(1-d)} N_{\mathbf{i},\alpha,\beta}^0. \end{aligned} \tag{4.3}$$

Hence, it is sufficient to determine  $N_{\mathbf{i},\alpha,\beta}^0$  only for the level  $\ell = 0$  (or any other fixed level). For a fixed range of the indices  $\mathbf{i}, \alpha, \beta$  these data can be calculated once for all.

Furthermore, various symmetries may be exploited.

**Remark 4.3 (permutation)** Let  $\pi$  be a permutation of  $\{1, \dots, d\}$ . Then

$$N_{\mathbf{i},\alpha,\beta}^0 = N_{\pi(\mathbf{i}),\pi(\alpha),\pi(\beta)}^0,$$

where  $\pi(\mathbf{i}) := (i_{\pi(1)}, \dots, i_{\pi(d)})$  ( $\pi(\alpha)$  and  $\pi(\beta)$  analogously).

**Remark 4.4 (mirror symmetry)** Let  $\delta \in \{1, \dots, d\}$ . Then

$$N_{\mathbf{i},\alpha,\beta}^0 = (-1)^{\alpha_\delta + \beta_\delta} N_{\mathbf{i}',\alpha,\beta}^0 \quad \text{with } \mathbf{i}' := (i_1, \dots, i_{\delta-1}, -i_\delta, i_{\delta+1}, \dots, i_d).$$

*Proof.* Use the substitutions  $x'_\delta := 1 - x_\delta$ ,  $y'_\delta := 1 - y_\delta$  and  $\Phi_{0,\alpha}^0(1 - x) = (-1)^\alpha \Phi_{0,\alpha}^0(x)$ . ■

**Remark 4.5 ( $\alpha, \beta$  symmetry)** Given  $\alpha, \beta \geq \mathbf{0}$ , we define the multi-indices with interchanged components at position  $\delta \in \{1, \dots, d\}$  by  $\alpha' := (\alpha_1, \dots, \alpha_{\delta-1}, \beta_\delta, \alpha_{\delta+1}, \dots, \alpha_d)$  and  $\beta' := (\beta_1, \dots, \beta_{\delta-1}, \alpha_\delta, \beta_{\delta+1}, \dots, \beta_d)$ . Then

$$N_{\mathbf{i},\alpha,\beta}^0 = (-1)^{\alpha_\delta + \beta_\delta} N_{\mathbf{i},\alpha',\beta'}^0.$$

*Proof.* Note that<sup>7</sup>

$$N_{\mathbf{i},\alpha,\beta}^0 = \int_0^1 \int_0^1 k(x'_\delta - y_\delta) \Phi_{0,\alpha_\delta}^0(x'_\delta) \Phi_{0,\beta_\delta}^0(y_\delta) dx_\delta dy_\delta \tag{4.4}$$

with the kernel

$$k(x_\delta - y_\delta - i_\delta) := \int \dots \int \frac{\Phi_{\mathbf{i},\alpha}^\ell(x) \Phi_{\mathbf{0},\beta}^\ell(y)}{\|x - y\|} dx_1 \dots dx_{\delta-1} dx_{\delta+1} \dots dx_d dy_1 \dots dy_{\delta-1} dy_{\delta+1} \dots dy_d,$$

where the integration is performed over all variables except  $x_\delta$  and  $y_\delta$ . Note that the shift by  $-i_\delta$  on the left-hand side allows to replace  $\Phi_{i_\delta,\alpha_\delta}^0(x_\delta)$  in (4.4) by  $\Phi_{0,\alpha_\delta}^0(x'_\delta)$  with  $x'_\delta = x_\delta - i_\delta$ . We substitute the variables

<sup>7</sup>The given proof is more general than needed for this remark. Later, however, we need the symmetry for general kernels  $k(\cdot)$ .

in (4.4) by  $x'_\delta = \frac{1}{2} + x$ ,  $y_\delta = \frac{1}{2} + y$ . Symmetry of  $\Phi_{0,\alpha}^0$  yields

$$\begin{aligned} N_{\mathbf{i},\alpha,\beta}^0 &= \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} k(x-y) \Phi_{0,\alpha_\delta}^0\left(\frac{1}{2}+x\right) \Phi_{0,\beta_\delta}^0\left(\frac{1}{2}+y\right) dx dy \\ &= (-1)^{\alpha_\delta+\beta_\delta} \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} k(x-y) \Phi_{0,\alpha_\delta}^0\left(\frac{1}{2}-x\right) \Phi_{0,\beta_\delta}^0\left(\frac{1}{2}-y\right) dx dy. \end{aligned}$$

Substitution  $x' = \frac{1}{2} - x$ ,  $y' = \frac{1}{2} - y$  together with  $x - y = y' - x'$  yields

$$N_{\mathbf{i},\alpha,\beta}^0 = (-1)^{\alpha_\delta+\beta_\delta} \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} k(y' - x') \Phi_{0,\alpha_\delta}^0(x') \Phi_{0,\beta_\delta}^0(y') dx' dy'.$$

Interchanging the symbols  $x', y'$  shows  $N_{\mathbf{i},\alpha,\beta}^0 = (-1)^{\alpha_\delta+\beta_\delta} \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} k(x' - y') \Phi_{0,\beta_\delta}^0(x') \Phi_{0,\alpha_\delta}^0(y') dx' dy' = (-1)^{\alpha_\delta+\beta_\delta} N_{\mathbf{i},\alpha',\beta'}^0$ . ■

**Conclusion 4.6** *If  $N_{\mathbf{i},\alpha,\beta}^0$  are known for indices  $\mathbf{i}$  with  $0 \leq i_1 \leq i_2 \leq \dots \leq i_d$  and  $\alpha \leq \beta$ , all other  $N_{\mathbf{i},\alpha,\beta}^0$  can be determined by means of the previous Remarks.*

#### 4.2.2 Exact computation

At least for  $d \leq 3$ , the integrals (4.1) can be determined exactly from the (symbolic) integration described in [6]. For instance, for  $N_{\mathbf{0},\mathbf{0},\mathbf{0}}^0$  one gets the (exact) result

$$\int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 \int_0^1 \frac{dx dy}{\|x - y\|} = \frac{2}{5} + \frac{2}{5} * \sqrt{2} - \frac{4}{5} * \sqrt{3} - 2 * \ln(2) + 2 * \ln(1 + \sqrt{2}) + 4 * \ln(1 + \sqrt{3}) - \frac{2}{3} * \pi,$$

i.e.,  $N_{\mathbf{0},\mathbf{0},\mathbf{0}}^0 \approx 1.882$ .

But instead of the exact computation we propose an easy but good approximation. For this purpose we first discuss the so-called far field case, where integrands without singularity are discussed. Having these results, it turns out that the singular cases can be treated quite easily without any further numerical approximation.

#### 4.2.3 Far field computation ( $\|\mathbf{i}\|_\infty \geq 2$ )

If  $\|\mathbf{i}\|_\infty \geq 2$ , the integration in  $N_{\mathbf{i},\alpha,\beta}^0 := \iint \frac{\Phi_{\mathbf{i},\alpha}^0(x) \Phi_{\mathbf{0},\beta}^0(y)}{\|x - y\|} dx dy$  can be reduced to the product  $\mathbf{I}_1^0 \times \mathbf{I}_0^0$  of the supports  $\mathbf{I}_1^0$  and  $\mathbf{I}_0^0$ . Since these cubes have a distance  $\geq \|\mathbf{i}\|_\infty - 1 \geq 1$  and therefore  $\|x - y\| \geq \|x - y\|_\infty \geq 1$ , the integrand is an analytic function without singularity.

As shown in Appendix A.3, the data  $N_{\mathbf{i},\alpha,\beta}^0$  can be derived from the quantities

$$\int_0^1 \dots \int_0^1 \frac{\Phi_{\mathbf{0},\alpha}^0(y)}{\|\mathbf{j} - y\|} dy \tag{4.5}$$

for  $\mathbf{j}$  with  $\mathbf{i} \leq \mathbf{j} \leq \mathbf{i} + \mathbf{1}$  by means of simple recursions. Note that  $\|\mathbf{j} - y\| \geq \|\mathbf{j} - \mathbf{1}\| \geq \|\mathbf{i} - \mathbf{1}\| \geq \|\mathbf{i} - \mathbf{1}\|_\infty \geq 1$ .

For fixed  $\mathbf{j}$  the integration in (4.5) is to be performed in the  $d$ -dimensional cube  $[\mathbf{j} - \mathbf{1}, \mathbf{j}] = \prod_{\delta=1}^d [j_\delta - 1, j_\delta]$ . Consider the function  $F_{\mathbf{j}}(y) := 1/\|\mathbf{j} - y\|$  in  $[0, 1]^d$ . Since  $F_{\mathbf{j}}$  is analytic in all directions  $y_\delta$ , it has a power series representation  $F_{\mathbf{j}}(y) = \sum_{\nu \geq \mathbf{0}} \alpha_\nu y^\nu$ . The basis of the monomials  $y^\nu = \prod_{\delta=1}^d y_\delta^{\nu_\delta}$  can be replaced by the Legendre polynomials  $\Phi_{\mathbf{0},\beta}^0(y)$ , i.e.,

$$F_{\mathbf{j}}(y) = \sum_{\beta \geq \mathbf{0}} k_{\mathbf{j},\beta} \Phi_{\mathbf{0},\beta}^0(y).$$

**Remark 4.7** *By the orthonormality of the  $\Phi_{\mathbf{0},\alpha}^0$  the coefficients  $k_{\mathbf{j},\beta}$  in the representation from above are equal to the integrals (4.5).*

The analyticity of  $F_{\mathbf{j}}(y)$  can be quantified by means of bounds of the derivatives. More precisely,  $F_{\mathbf{j}}(y) = 1/\|\mathbf{j} - y\|$  is asymptotically smooth<sup>8</sup>, in particular the bounds

$$\left| \left( \frac{\partial}{\partial y_\delta} \right)^k \frac{1}{\|\mathbf{j} - y\|} \right| \leq \frac{(1 + \mathcal{O}(k)) k!}{\|\mathbf{j} - y\|^{k+1}} \leq \frac{(1 + \mathcal{O}(k)) k!}{(\|\mathbf{j}\|_\infty - 1)^{k+1}} \leq (1 + \mathcal{O}(k)) k! \quad (4.6)$$

hold for all  $k \in \mathbb{N}_0$  and all  $y \in \mathbf{I}_0^0 = [0, 1]^d$ .

Two obvious numerical approaches can be applied.

**Method A** (tensor-product interpolation of the function  $F_{\mathbf{j}}(y) := 1/\|\mathbf{j} - y\|$  in  $\mathbf{I}_0^0$ ): For this purpose,  $p + 1$  points  $0 \leq \zeta_0 < \zeta_1 < \dots < \zeta_p \leq 1$  are chosen. The one-dimensional interpolation in  $x_\delta$ -direction uses the interpolation points  $j_\delta - \zeta_k$ . The resulting interpolation polynomial  $Q_p(x, y)$  of partial degree  $\leq p$  satisfies the error estimate

$$\|F_{\mathbf{j}} - Q_p\|_{\infty, \mathbf{I}_0^0} \leq \frac{C}{(p+1)!} \max_\delta \left\| \frac{\partial^{p+1}}{\partial y_\delta^{p+1}} F_{\mathbf{j}} \right\|_{\infty, \mathbf{I}_0^0}, \quad (4.7)$$

where  $C = C(p, d)$  depends on the choice of interpolation points. A good choice are the zeros of the Chebyshev polynomial  $T_{p+1}$  (transformed onto  $[0, 1]$ ). In this case,

$$C(p, d) = 4^{-p-1} \sum_{\delta=0}^{d-1} \left( 1 + \frac{2}{\pi} \log(p+1) \right)^\delta \quad (4.8)$$

is an upper bound in (4.7). Together with the estimate (4.6), we get

$$\|F_{\mathbf{j}} - Q_p\|_{\infty, \mathbf{I}_0^0} \leq C(p, d) \frac{1 + \mathcal{O}(p+1)}{(\|\mathbf{j}\|_\infty - 1)^{p+2}} \lesssim \mathcal{O}([4(\|\mathbf{j}\|_\infty - 1)]^{-p-2}), \quad (4.9)$$

where the last expression ignores the  $\log(p+1)$  contribution. In the worst case  $\|\mathbf{j}\|_\infty = 2$ , the exponential convergence is like  $\mathcal{O}(4^{-p})$ .

The polynomial  $Q_p$  (restricted to  $\mathbf{I}_0^0$ ) can be rewritten in the form  $Q_p(y) = \sum_\alpha q_\alpha \Phi_{0,\alpha}^0(y)$ . As in Remark 4.7 we obtain

$$\int_0^1 \dots \int_0^1 \frac{\Phi_{0,\alpha}^0(y)}{\|\mathbf{j} - y\|} dy \approx q_\alpha. \quad (4.10)$$

**Remark 4.8** The error (4.9) corresponds to the quantities at level 0. For a general level  $\ell$ , the factor  $4^{-(p+1)}$  in (4.8) becomes  $(4/h_\ell)^{-(p+1)}$ . Hence, the error estimate (4.9) has to be replaced by

$$\mathcal{O} \left( \left[ \frac{4}{h_\ell} (\|\mathbf{j}\|_\infty - 1) \right]^{-p-2} \right). \quad (4.11)$$

**Remark 4.9** There are two possibilities to improve the error.

a) One can interpolate  $F_{\mathbf{j}}$  by a polynomial  $Q_{p'}$  of higher degree  $p' > p$  and form  $Q_{p'}(x, y) = \sum_\alpha q_\alpha \Phi_{0,\alpha}^0(y)$  including functions  $\Phi_{0,\alpha}^0$  with  $p < |\alpha| \leq p'$ . The result in (4.10) uses only the coefficients with  $|\alpha| \leq p$ .

b) One can restrict the computation of  $N_{\mathbf{i},\alpha,\beta}^0$  to those coefficients with  $\|\mathbf{i}\|_\infty \geq 1 + N$  for some fixed  $N > 1$ . Then the exponential convergence in (4.11) is improved:  $\mathcal{O}((\frac{4N}{h_\ell})^{-p-2})$ . As we will see in Remark 4.11, the coefficients  $N_{\mathbf{i},\alpha,\beta}^0$ ,  $\|\mathbf{i}\|_\infty < 1 + N$ , can be computed exactly from those with  $\|\mathbf{i}\|_\infty \geq 1 + N$ .

**Method B:** Perform the tensor-product Gauss quadrature with at least  $p + 1$  nodal points. Again, one gets error estimates involving the derivatives bounded in (4.6).

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<sup>8</sup>This fact is used in multipole methods (cf. [4]) or the more general panel clustering method (cf. [12]).

#### 4.2.4 Near field computation

The near field case is defined by  $\|\mathbf{i}\|_\infty \leq 1$ . If  $\|\mathbf{i}\|_\infty = 1$ , the singular case  $x = y$  occurs for  $x \in \partial\mathbf{I}_1^0$  and  $y \in \partial\mathbf{I}_0^0$ , whereas for  $\|\mathbf{i}\|_\infty = 0$  (i.e.,  $\mathbf{i} = 0$ )  $x = y$  occurs also for inner points. Interpolations or standard quadratures cannot be accurate in the presence of singularities. Nevertheless, the computation of  $N_{\mathbf{i},\alpha,\beta}^0$  for  $\|\mathbf{i}\|_\infty \leq 1$  turns out to be an easy task, provided that the far field coefficients from above are already determined.

The method of choice is the “hierarchical quadrature” described in [2]. First, we remark that only  $d+1$  cases  $\mathbf{i} = (0, \dots, 0)$ ,  $(0, \dots, 0, 1)$ ,  $(0, \dots, 0, 1, 1), \dots, (0, 1, \dots, 1)$ ,  $(1, \dots, 1)$  are to be treated (cf. Conclusion 4.6). A summary of the hierarchical quadrature method is given in the following remark.

**Remark 4.10** *a) Let the exact values  $N_{\mathbf{i},\alpha,\beta}^0$  be given for  $2 \leq \|\mathbf{i}\|_\infty \leq 3$ . Then  $N_{\mathbf{i},\alpha,\beta}^0$  for  $\|\mathbf{i}\|_\infty \leq 1$  can be computed by simple algebraic operations without any quadrature error.*

*b) If the input values  $N_{\mathbf{i},\alpha,\beta}^0$ ,  $2 \leq \|\mathbf{i}\|_\infty \leq 3$ , contain approximation errors, these are of course transferred to  $N_{\mathbf{i},\alpha,\beta}^0$ ,  $\|\mathbf{i}\|_\infty \leq 1$ , but no further error is introduced.*

We start with the case  $\mathbf{i} = \mathbf{1}$ . The cubes  $\mathbf{I}_0^0$  and  $\mathbf{I}_1^0$  touch at the corner point  $(1, \dots, 1) \in \mathbb{R}^d$ . Both cubes are written as unions of cubes of the half mesh size  $h_1$ :

$$\mathbf{I}_0^0 = \bigcup_{\mathbf{0} \leq \mathbf{k} \leq \mathbf{1}} \mathbf{I}_{\mathbf{k}}^1, \quad \mathbf{I}_1^0 = \bigcup_{\mathbf{0} \leq \mathbf{k} \leq \mathbf{1}} \mathbf{I}_{\mathbf{2}+\mathbf{k}}^1.$$

Further, we use the identity

$$\Phi_{\nu,\alpha}^0 = \sum_{\mathbf{0} \leq \mathbf{k} \leq \mathbf{1}} \sum_{\varkappa \leq \alpha} \xi_{\alpha,\varkappa,\mathbf{k}} \Phi_{\mathbf{2}\nu+\mathbf{k},\varkappa}^1 \quad \text{with } \xi_{\alpha,\varkappa,\mathbf{k}} := (-1)^{\langle \varkappa+\alpha, \mathbf{1}-\mathbf{k} \rangle} \xi_{\alpha,\varkappa}$$

from Lemma 2.2. This leads to

$$\begin{aligned} N_{\mathbf{1},\alpha,\beta}^0 &= \sum_{\mathbf{0} \leq \mathbf{k} \leq \mathbf{1}} \sum_{\mathbf{0} \leq \mathbf{k}' \leq \mathbf{1}} \sum_{\varkappa \leq \alpha} \sum_{\varkappa' \leq \beta} \xi_{\alpha,\varkappa,\mathbf{k}} \xi_{\beta,\varkappa',\mathbf{k}'} \iint \frac{\Phi_{\mathbf{2}+\mathbf{k},\varkappa}^1(x) \Phi_{\mathbf{k}',\varkappa'}^1(y)}{\|x-y\|} dx dy \\ &= \sum_{\mathbf{0} \leq \mathbf{k} \leq \mathbf{1}} \sum_{\mathbf{0} \leq \mathbf{k}' \leq \mathbf{1}} \sum_{\varkappa \leq \alpha} \sum_{\varkappa' \leq \beta} \xi_{\alpha,\varkappa,\mathbf{k}} \xi_{\beta,\varkappa',\mathbf{k}'} N_{\mathbf{2}+\mathbf{k}-\mathbf{k}',\varkappa,\varkappa'}^1 \stackrel{(4.3)}{=} \\ &= 2^{1-d} \sum_{\mathbf{0} \leq \mathbf{k} \leq \mathbf{1}} \sum_{\mathbf{0} \leq \mathbf{k}' \leq \mathbf{1}} \sum_{\varkappa \leq \alpha} \sum_{\varkappa' \leq \beta} \xi_{\alpha,\varkappa,\mathbf{k}} \xi_{\beta,\varkappa',\mathbf{k}'} N_{\mathbf{2}+\mathbf{k}-\mathbf{k}',\varkappa,\varkappa'}^0. \end{aligned} \tag{4.12}$$

All coefficients  $N_{\mathbf{2}+\mathbf{k}-\mathbf{k}',\varkappa,\varkappa'}^0$  are known (i.e.,  $\|\mathbf{2}+\mathbf{k}-\mathbf{k}'\|_\infty > 1$ ) except  $N_{\mathbf{1},\varkappa,\varkappa'}^0$  which results from  $\mathbf{k} = \mathbf{0}$  and  $\mathbf{k}' = \mathbf{1}$ . We obtain the equation

$$\begin{aligned} N_{\mathbf{1},\alpha,\beta}^0 &= 2^{1-d} \sum_{\varkappa \leq \alpha} \sum_{\varkappa' \leq \beta} \xi_{\alpha,\varkappa,\mathbf{0}} \xi_{\beta,\varkappa',\mathbf{1}} N_{\mathbf{1},\varkappa,\varkappa'}^0 + R_{\mathbf{1},\alpha,\beta}^0 \quad \text{with} \\ R_{\mathbf{1},\alpha,\beta}^0 &:= 2^{1-d} \sum_{\substack{\mathbf{0} \leq \mathbf{k} \leq \mathbf{1} \\ \mathbf{k}' - \mathbf{k} \neq \mathbf{1}}} \sum_{\mathbf{0} \leq \mathbf{k}' \leq \mathbf{1}} \sum_{\varkappa \leq \alpha} \sum_{\varkappa' \leq \beta} \xi_{\alpha,\varkappa,\mathbf{k}} \xi_{\beta,\varkappa',\mathbf{k}'} N_{\mathbf{2}+\mathbf{k}-\mathbf{k}',\varkappa,\varkappa'}^0. \end{aligned}$$

The  $R_{\mathbf{1},\alpha,\beta}^0$  are known quantities on the right-hand side. The equation from above is a linear system for the  $p^{2d}$  components  $N_{\mathbf{1},\alpha,\beta}^0$  ( $\alpha, \beta \in \{0, \dots, p\}^d$ ). Fortunately, this systems is staggered because of the inequalities



$\varkappa \leq \alpha$ ,  $\varkappa' \leq \beta$ . Its explicit solution is given in the form<sup>9</sup>

$$\begin{aligned}
N_{\mathbf{1}, \mathbf{0}, \mathbf{0}}^0 &= \frac{R_{\mathbf{1}, \mathbf{0}, \mathbf{0}}^0}{1 - 2^{1-d} \xi_{\mathbf{0}, \mathbf{0}, \mathbf{0}} \xi_{\mathbf{0}, \mathbf{0}, \mathbf{1}}}, \\
N_{\mathbf{1}, (1, 0, \dots, 0), \mathbf{0}}^0 &= \frac{R_{\mathbf{1}, (1, 0, \dots, 0), \mathbf{0}}^0 + 2^{1-d} \xi_{(1, 0, \dots, 0), \mathbf{0}, \mathbf{0}} \xi_{\mathbf{0}, \mathbf{0}, \mathbf{1}} N_{\mathbf{1}, \mathbf{0}, \mathbf{0}}^0}{1 - 2^{1-d} \xi_{(1, 0, \dots, 0), (1, 0, \dots, 0), \mathbf{0}} \xi_{\mathbf{0}, \mathbf{0}, \mathbf{1}}}, \\
&\vdots \\
N_{\mathbf{1}, \alpha, \beta}^0 &= \frac{R_{\mathbf{1}, \alpha, \beta}^0 + 2^{1-d} \sum_{\varkappa \leq \alpha, \varkappa' \leq \beta, \varkappa + \varkappa' \neq \alpha + \beta} \xi_{\alpha, \varkappa, \mathbf{0}} \xi_{\beta, \varkappa', \mathbf{1}} N_{\mathbf{1}, \varkappa, \varkappa'}^0}{1 - 2^{1-d} \xi_{\alpha, \alpha, \mathbf{0}} \xi_{\beta, \beta, \mathbf{1}}}, \\
&\vdots
\end{aligned}$$

The sequence of computations follows the increasing values of  $|\alpha| + |\beta| = \alpha_1 + \dots + \alpha_d + \beta_1 + \dots + \beta_d$ .

Having determined  $N_{\mathbf{i}, \alpha, \beta}^0$  for  $\mathbf{i} = \mathbf{1}$ , we consider the next case  $\mathbf{i} = (0, 1, \dots, 1)$ . The cubes  $\mathbf{I}_{\mathbf{0}}^0$  and  $\mathbf{I}_{\mathbf{i}}^0$  touch in the edge  $x_1 \in [0, 1]$ ,  $x_2 = \dots = x_d = 1$ . The same procedure as above yields

$$N_{\mathbf{i}, \alpha, \beta}^0 = 2^{1-d} \sum_{\mathbf{0} \leq \mathbf{k} \leq \mathbf{1}} \sum_{\mathbf{0} \leq \mathbf{k}' \leq \mathbf{1}} \sum_{\varkappa \leq \alpha} \sum_{\varkappa' \leq \beta} \xi_{\alpha, \varkappa, \mathbf{k}} \xi_{\beta, \varkappa', \mathbf{k}'} N_{2\mathbf{i} + \mathbf{k} - \mathbf{k}', \varkappa, \varkappa'}^0.$$

Coefficients  $N_{2\mathbf{i} + \mathbf{k} - \mathbf{k}', \varkappa, \varkappa'}^0$  with  $\|2\mathbf{i} + \mathbf{k} - \mathbf{k}'\|_{\infty} \leq 1$  arise for the pairs  $(\mathbf{k}, \mathbf{k}')$  from the following table:

	$\mathbf{k}$	$\mathbf{k}'$	$\Rightarrow$	$2\mathbf{i} + \mathbf{k} - \mathbf{k}'$
a)	$(0, 0, \dots, 0)$	$(1, 1, \dots, 1)$		$(-1, 1, \dots, 1)$
b)	$(1, 0, \dots, 0)$	$(1, 1, \dots, 1)$		$(0, 1, \dots, 1)$
c)	$(0, 0, \dots, 0)$	$(0, 1, \dots, 1)$		$(0, 1, \dots, 1)$
d)	$(1, 0, \dots, 0)$	$(0, 1, \dots, 1)$		$(1, 1, \dots, 1)$

By Remark 4.4, case a) reduces to case d). But for  $2\mathbf{i} + \mathbf{k} - \mathbf{k}' = \mathbf{1}$ , the values of  $N_{\mathbf{1}, \varkappa, \varkappa'}^0$  are already determined in the previous step. In the cases b) and c) the same index  $(0, 1, \dots, 1)$  appears. Hence,

$$N_{\mathbf{i}, \alpha, \beta}^0 = 2^{1-d} \sum_{\mathbf{k}, \mathbf{k}': \begin{cases} 0 \leq k_1 = k'_1 \leq 1, & \text{for } \delta = 1 \\ 0 = k_{\delta} < k'_{\delta} = 1 & \text{for } \delta \geq 2 \end{cases}} \sum_{\varkappa \leq \alpha} \sum_{\varkappa' \leq \beta} \xi_{\alpha, \varkappa, \mathbf{k}} \xi_{\beta, \varkappa', \mathbf{k}'} N_{2\mathbf{i} + \mathbf{k} - \mathbf{k}', \varkappa, \varkappa'}^0 + R_{\mathbf{i}, \alpha, \beta}^0,$$

where  $R_{\mathbf{i}, \alpha, \beta}^0$  contains only known terms. Again, we can make use of a staggered system of equations starting with

$$N_{(0, 1, \dots, 1), \mathbf{0}, \mathbf{0}}^0 = \frac{R_{(0, 1, \dots, 1), \mathbf{0}, \mathbf{0}}^0}{1 - 2^{1-d} (\xi_{\mathbf{0}, \mathbf{0}, \mathbf{0}} \xi_{\mathbf{0}, \mathbf{0}, (0, 1, \dots, 1)} + \xi_{\mathbf{0}, \mathbf{0}, (1, 0, \dots, 0)} \xi_{\mathbf{0}, \mathbf{0}, \mathbf{1}})}.$$

Similarly, we proceed with  $\mathbf{i} = (0, 0, 1, \dots, 1)$ ,  $(0, 0, 0, 1, \dots, 1)$ ,  $\dots$ ,  $\mathbf{0} = (0, \dots, 0)$ .

Remark 4.10 can be generalised so that also the quantities  $N_{\mathbf{i}, \alpha, \beta}^0$  are computable from  $N_{\mathbf{i}', \alpha, \beta}^0$  with larger  $\mathbf{i}'$ .

**Remark 4.11** *The same procedure as above allows to compute all  $N_{\mathbf{i}, \alpha, \beta}^0$  with fixed  $\|\mathbf{i}\|_{\infty}$  from  $N_{\mathbf{i}', \alpha', \beta'}^0$  with  $\|\mathbf{i}'\|_{\infty} \in \{2\|\mathbf{i}\|_{\infty}, 2\|\mathbf{i}\|_{\infty} + 1\}$ .*

## 5 Tensor product approximations

### 5.1 Preliminaries

In Remark 4.2 we have mentioned the almost linear complexity  $\mathcal{O}(N \log N)$ . The difficulty is that  $N$  is large for dimensions  $d \geq 3$ . If, e.g.,  $B_{\ell} = [-1, 1]^d$ , the number of grid points is  $N = n^d$ , where  $n = 2/h_{\ell} = 2^{1+\ell}$ .

<sup>9</sup>Because of Remark 4.3 not all combinations of  $\alpha, \beta$  need to be determined. It suffices to consider  $\alpha_1 \leq \alpha_2 \leq \dots \leq \alpha_d$ .

In the following we want to change the exponent  $d$  into a factor  $d$ , i.e., we aim at a complexity proportional to  $dn \log(n)$ .

To introduce the next steps, we assume that the function  $f$  has the product form

$$f(x) = f_1(x_1) \cdot f_2(x_2) \cdot \dots \cdot f_d(x_d). \quad (5.1)$$

If the kernel function had the form

$$k(x) = k_1(x_1) \cdot k_2(x_2) \cdot \dots \cdot k_d(x_d), \quad (5.2)$$

the convolution

$$\begin{aligned} (k * f)(x) &= \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} k(x-y) f(y) dy \\ &= \left( \int_{\mathbb{R}} \int_{\mathbb{R}} k_1(x_1 - y_1) f_1(y_1) dy_1 \right) \cdot \dots \cdot \left( \int_{\mathbb{R}} \int_{\mathbb{R}} k_d(x_d - y_d) f_d(y_d) dy_d \right) \\ &= (k_1 * f_1)(x_1) \cdot (k_2 * f_2)(x_2) \cdot \dots \cdot (k_d * f_d)(x_d) \end{aligned}$$

could be reduced to  $d$  one-dimensional convolutions.

Of course, the Newton potential is not of the form (5.2). Furthermore, we will not use the ansatz (5.1) for  $f$ , since factors  $f_j$  belonging to (one-dimensional) locally refined subspaces (2.10) of  $L^2(\mathbb{R})$  lead to an anisotropic grid (see Figure 5.1).

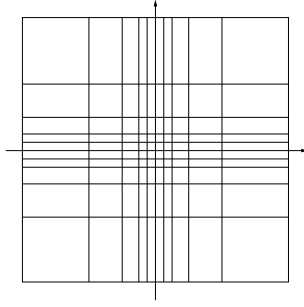


Figure 5.1: Tensor product grid

Instead we assume that  $f$  is a sum of products (5.1) with support in  $B_\ell$  and all factors belonging to the univariate ansatz space  $S_\ell^{(1)}$  corresponding to the identical step size  $h_\ell$ .

The precise notations are as follows.

$$\begin{aligned} S_\ell^{(1)} &:= \text{span} \left\{ \Phi_{\nu, \alpha}^\ell : \nu \in \mathbb{Z}, 0 \leq \alpha \leq p \right\} \subset L^2(\mathbb{R}) \quad (\text{one-dimensional domain } \mathbb{R}), \\ S_\ell &:= \text{span} \left\{ \Phi_{\nu, \alpha}^\ell : \nu \in \mathbb{Z}^d, \alpha \in \{0, \dots, p\}^d \right\} \quad (d\text{-dimensional domain } \mathbb{R}^d \text{ as in (2.6)}), \\ S &:= \text{span} \left\{ u : u \in S_\ell \text{ and } \text{supp}(u) \subset B_\ell \text{ for some } \underline{L} \leq \ell \leq \overline{L} \right\}. \end{aligned} \quad (5.3)$$

The representation of  $f$  is

$$f = \sum_{\ell=\underline{L}}^{\overline{L}} \sum_{\nu=1}^{k_\ell} f_{\ell, \nu} \quad \text{with} \quad \begin{cases} f_{\ell, \nu}(x_1, \dots, x_d) = f_{\ell, \nu}^{(1)}(x_1) \cdot \dots \cdot f_{\ell, \nu}^{(d)}(x_d), & f_{\ell, \nu}^{(\delta)} \in S_\ell^{(1)}, \\ \text{supp}(f_{\ell, \nu}) \subset B_\ell, \end{cases} \quad (5.4)$$

where the box  $B_\ell$  is defined as follows. For each variable  $x_\delta$  ( $1 \leq \delta \leq d$ ) we define intervals (one-dimensional boxes)  $\dots \supset B_{\ell-1, \delta} \supset B_{\ell, \delta} \supset \dots$  as in (2.8). Then

$$B_\ell := B_{\ell, 1} \times \dots \times B_{\ell, d}$$

defines the  $d$ -dimensional box used in (5.4).

Since  $S_\ell$  is equal to the  $d$ -fold tensor space  $\bigotimes_{\delta=1}^d S_\ell^{(1)}$ , we have  $f_{\ell,\nu} \in S_\ell$  as well as  $f^\ell := \sum_\nu f_{\ell,\nu} \in S_\ell$  with  $\text{supp}(f^\ell) \subset B_\ell$ . Hence, we have again a decomposition of  $f$  into  $f = \sum_{\ell=\underline{L}}^{\underline{T}} f^\ell$  with  $f^\ell \in S_\ell$  with  $\text{supp}(f^\ell) \subset B_\ell$ . The additional property is that  $f_\ell$  should be representable by a hopefully small number of terms  $f_{\ell,\nu}$  in product form (5.4).

The tensor-product representation can be justified, e.g., for analytic functions (cf. [10], [11]). But it is even more important that functions appearing in the density function theory like the spatial orbital functions or the electron density of molecules allow an approximation by tensor-product representations up to chemical accuracy. Details including examples for  $\text{CH}_4$ ,  $\text{C}_2\text{H}_6$ ,  $\text{C}_2\text{H}_2$ ,  $\text{CH}_3\text{OH}$  can be found in [13] and [14]. Note that just in electronic structure calculations (e.g., two-electron integrals) convolutions with the Newton potential ( $d = 3$ ) arise.

In the following we consider one term  $f_{\ell,\nu}$ , i.e., we assume that  $f = f_{\ell,\nu}$  is given in the form (5.4) and want to obtain the (approximation of the) image  $u = \mathcal{K}f$  in the same form. For that purpose we have to approximate the convolution in tensor form.

## 5.2 Tensor-product approximation of the Newton potential

Although the Newton potential is not of the form (5.2), it can be approximated in essential parts by sums of products (5.2). For this purpose we make use of the approximation of the function  $1/\sqrt{t}$  by exponential sums  $\sum_{\nu=1}^k \omega_\nu \exp(-\vartheta_\nu t)$ .

**Remark 5.1** *a) Let  $R > 1$  (including  $R = \infty$ ).  $E_{k,R}(t) := \sum_{\nu=1}^k \omega_\nu \exp(-\vartheta_\nu t)$  is called an exponential sum. Its difference from  $1/\sqrt{t}$  in  $[1, R]$  with respect to the maximum norm is denoted by*

$$\eta := \left\| \frac{1}{\sqrt{t}} - \sum_{\nu=1}^k \omega_\nu \exp(-\vartheta_\nu t) \right\|_{\infty, [1, R]}. \quad (5.5)$$

*b) Let  $[A, B] \subset (0, \infty]$  with  $B/A = R$  ( $R$  from Part a)). The function*

$$E_{k,[A,B]}(t) := \sum_{\nu=1}^k \omega_{\nu,[A,B]} \exp(-\vartheta_{\nu,[A,B]} t) \quad \text{with} \\ \omega_{\nu,[A,B]} := \sqrt{A} \omega_\nu \quad \text{and} \quad \vartheta_{\nu,[A,B]} := A \vartheta_\nu \quad (\omega_\nu, \vartheta_\nu \text{ from Part a)})$$

*approximates  $1/\sqrt{t}$  in  $[A, B]$  with the accuracy*

$$\eta_{[A,B]} = \left\| \frac{1}{\sqrt{t}} - \sum_{\nu=1}^k \omega_{\nu,[A,B]} \exp(-\vartheta_{\nu,[A,B]} t) \right\|_{\infty, [A,B]} = \frac{1}{\sqrt{A}} \eta \quad (\eta \text{ from (5.5)}).$$

*Vice versa, an approximation in  $[A, B]$  can be transformed into an approximation in  $[1, R]$ .*

The previous remark allows to restrict the approximation to intervals of the form  $[1, R]$ .

**Remark 5.2** *a) The best approximation  $E_{k,R}^*$  is the exponential sum  $E_{k,R}$  with the smallest error (5.5), which is then denoted by  $\eta_{k,R}^*$ .*

*b) Best approximations in  $[1, R]$  and  $[A, B]$  can be related as described in Remark 5.1.*

*c) The coefficients  $\omega_\nu, \vartheta_\nu$  of  $E_{k,R}^*$  are positive.*

*d) For fixed finite  $R$ , the error  $\eta_{k,R}^*$  decays like  $\mathcal{O}(\exp(-ck))$  with  $c = c(R) > 0$ , while for  $R = \infty$ , still  $\eta_{k,R}^* = \mathcal{O}(\exp(-c\sqrt{k}))$  holds.*

Substitution of  $t$  by  $\|x - y\|^2$  yields

$$\frac{1}{\|x - y\|} \approx E_{k,R}^* \left( \|x - y\|^2 \right) = \sum_{\nu=1}^k \omega_\nu \exp \left( -\vartheta_\nu \|x - y\|^2 \right) \\ = \sum_{\nu=1}^k \omega_\nu \prod_{\delta=1}^d \exp \left( -\vartheta_\nu (x_\delta - y_\delta)^2 \right). \quad (5.6)$$

**Remark 5.3** a) If  $1 \leq \|x - y\| \leq \sqrt{R}$ , the right-hand side in (5.6) is a sum of products (5.2) and approximates the Newton potential  $1/\|x - y\|$ . The maximum norm of the difference of both sides from (5.6) for  $x, y$  with  $1 \leq \|x - y\| \leq \sqrt{R}$  is described by  $\eta_{k,R}^*$  from Remark 5.2a.

b) If  $h_\ell \leq \|x - y\| \leq \sqrt{R}h_\ell$ , one uses the approximation

$$\frac{1}{\|x - y\|} = \frac{h_\ell}{\|(x - y)/h_\ell\|} \approx \sum_{\nu=1}^k h_\ell \omega_\nu \prod_{\delta=1}^d \exp\left(-\frac{\vartheta_\nu}{h_\ell^2} (x_\delta - y_\delta)^2\right).$$

Consider the grid from §2.3. If the far field is defined by  $\|\mathbf{i}\|_\infty \geq 2$  as in §4.2.3, the minimal Euclidean distance  $\|x - y\|$  is the corresponding step size  $h_\ell$ . The maximal distance depends on the choice of  $B_\ell$ . The smallest choice of  $B_\ell$  according to Remark 2.4 yields  $\|x - y\| \leq 4\sqrt{d}h_\ell$ . This leads to the bound  $R = 16d$ . The largest possible bound is of course  $R = \infty$ . With suitably defined  $R$  and  $k$  depending on the required accuracy, we choose<sup>10</sup> the exponential sum  $E_{k,R}^*$  as approximation of  $1/\|x - y\|$ . For  $\|\mathbf{i}\|_\infty \geq 2$ , the  $N^\ell$ -coefficients are approximated by

$$\begin{aligned} N_{\mathbf{i},\alpha,\beta}^\ell &= \iint \frac{\Phi_{\mathbf{i},\alpha}^\ell(x) \Phi_{\mathbf{0},\beta}^\ell(y)}{\|x - y\|} dx dy \\ &\approx E_{\mathbf{i},\alpha,\beta}^\ell := h_\ell \iint E_{k,R}^*(\|x - y\|^2/h_\ell^2) \Phi_{\mathbf{i},\alpha}^\ell(x) \Phi_{\mathbf{0},\beta}^\ell(y) dx dy = \sum_{\nu=1}^k h_\ell \omega_\nu \prod_{\delta=1}^d E_{i_\delta,\alpha_\delta,\beta_\delta}^{\ell,\nu} \end{aligned}$$

with new coefficients

$$E_{\mathbf{i},\alpha,\beta}^{\ell,\nu} := \int_{\mathbb{R}} \int_{\mathbb{R}} \exp\left(-\frac{\vartheta_\nu}{h_\ell^2} (x - y)^2\right) \Phi_{\mathbf{i},\alpha}^\ell(x) \Phi_{\mathbf{0},\beta}^\ell(y) dx dy \quad (1 \leq \nu \leq k, i \in \mathbb{Z}, 0 \leq \alpha, \beta \leq p). \quad (5.7)$$

**Remark 5.4** a) We define  $E_{\mathbf{i},\alpha,\beta}^\ell$  for all  $\mathbf{i} \in \mathbb{Z}^d$  and  $\mathbf{0} \leq \alpha, \beta \leq p\mathbf{1}$ , not only for  $\|\mathbf{i}\|_\infty \geq 2$ . The error  $N_{\mathbf{i},\alpha,\beta}^\ell - E_{\mathbf{i},\alpha,\beta}^\ell$ , however, is by definition only sufficiently small for  $\|\mathbf{i}\|_\infty \geq 2$ . For  $\|\mathbf{i}\|_\infty \leq 1$ , an additional correction  $\delta N_{\mathbf{i},\alpha,\beta}^\ell := N_{\mathbf{i},\alpha,\beta}^\ell - E_{\mathbf{i},\alpha,\beta}^\ell$  is necessary. A tensor representation of  $\delta N_{\mathbf{i},\alpha,\beta}^\ell$  is mentioned in §5.3.

b) The identity  $\Phi_{\mathbf{i},\alpha}^\ell(x) = h_\ell^{-1/2} \Phi_{\mathbf{0},\alpha}^0(x/h_\ell - i)$  allows to express  $E_{\mathbf{i},\alpha,\beta}^{\ell,\nu}$  by means of  $E_{\mathbf{i},\alpha,\beta}^{0,\nu}$  (i.e.,  $\ell = 0$ ):

$$E_{\mathbf{i},\alpha,\beta}^{\ell,\nu} = h_\ell E_{\mathbf{i},\alpha,\beta}^{0,\nu} = h_\ell \int_{\mathbb{R}} \int_{\mathbb{R}} \exp\left(-\vartheta_\nu (x - y + i)^2\right) \Phi_{\mathbf{0},\alpha}^0(x) \Phi_{\mathbf{0},\beta}^0(y) dx dy.$$

For the computation of the entries  $E_{\mathbf{i},\alpha,\beta}^{0,\nu}$ , one can apply the methods described in §A.2 with

$$k(t) := \exp\left(-\vartheta_\nu (t + i)^2\right).$$

Note that the considerations of §A.2 belong to a fixed value of  $i \in \mathbb{Z}$ . Indicating this dependence by  $k = k^{(i)}$ , we observe  $k_{\alpha,+}^{(i)} = k_{\alpha,-}^{(i-1)}$  for the quantities from (A.2).

### 5.3 Convolution with the Newton potential in the regular grid

We consider one term  $f_{\ell,\nu}(x_1, \dots, x_d) = f_{\ell,\nu}^{(1)}(x_1) \cdot \dots \cdot f_{\ell,\nu}^{(d)}(x_d)$  of (5.4) and write it simply as

$$f(x_1, \dots, x_d) = f^{(1)}(x_1) \cdot \dots \cdot f^{(d)}(x_d)$$

without subscripts. The representation of the factors with respect to the basis is

$$f^{(\delta)} = \sum_{j \in \mathbb{Z}} f_{j,\beta}^{(\delta)} \Phi_{j,\beta}^\ell \in S_\ell^{(1)}$$

implying

$$f = \sum_{\mathbf{j} \in \mathbb{Z}^d} f_{\mathbf{j},\beta} \Phi_{\mathbf{j},\beta}^\ell \in S_\ell \quad \text{with} \quad f_{\mathbf{j},\beta} := \prod_{\delta=1}^d f_{j_\delta,\beta_\delta}^{(\delta)}. \quad (5.8)$$

<sup>10</sup>Concerning coefficients and accuracies for different  $k$  and  $R$  see [7] and the mentioned web page.

The projected convolution of the Newton potential with  $f = \sum_{\mathbf{j} \in \mathbb{Z}^d} f_{\mathbf{j},\beta} \Phi_{\mathbf{j},\beta}^\ell \in S_\ell$  results in

$$u_\ell(x) = \sum_{\mathbf{i} \in \mathbb{Z}^d} u_{\mathbf{i},\alpha} \Phi_{\mathbf{i},\alpha}^\ell \quad \text{with } u_{\mathbf{i},\alpha} := \sum_{\mathbf{j} \in \mathbb{Z}^d} \sum_{\beta} N_{\mathbf{i}-\mathbf{j},\alpha,\beta}^\ell f_{\mathbf{j},\beta}.$$

The previous Subsection §5.2 shows that there are approximations  $\tilde{N}_{\mathbf{i},\alpha,\beta}^\ell$  to  $N_{\mathbf{i},\alpha,\beta}^\ell$  of the form

$$\tilde{N}_{\mathbf{i},\alpha,\beta}^\ell = E_{\mathbf{i},\alpha,\beta}^\ell + \delta N_{\mathbf{i},\alpha,\beta}^\ell, \quad (5.9)$$

where  $\delta N_{\mathbf{i},\alpha,\beta}^\ell = 0$  for  $\|\mathbf{i}\|_\infty \geq 2$ . We approximate  $u_{\mathbf{i},\alpha}$  by

$$\begin{aligned} u_{\mathbf{i},\alpha} &\approx \tilde{u}_{\mathbf{i},\alpha} := \sum_{\mathbf{j} \in \mathbb{Z}^d} \sum_{\beta} \tilde{N}_{\mathbf{i}-\mathbf{j},\alpha,\beta}^\ell f_{\mathbf{j},\beta} = \sum_{\mathbf{j} \in \mathbb{Z}^d} \sum_{\beta} E_{\mathbf{i}-\mathbf{j},\alpha,\beta}^\ell f_{\mathbf{j},\beta} + \sum_{\mathbf{j}: \|\mathbf{i}-\mathbf{j}\|_\infty \leq 1} \sum_{\beta} \delta N_{\mathbf{i}-\mathbf{j},\alpha,\beta}^\ell f_{\mathbf{j},\beta} \\ &= \sum_{\nu=1}^k \omega_\nu \prod_{\delta=1}^d \sum_{\beta_\delta=0}^p \sum_{j_\delta \in \mathbb{Z}} E_{i_\delta-j_\delta, \alpha_\delta, \beta_\delta}^{\ell, \nu} f_{j_\delta, \beta_\delta}^{(\delta)} + \sum_{\mathbf{j}: \|\mathbf{i}-\mathbf{j}\|_\infty \leq 1} \sum_{\beta} \delta N_{\mathbf{i}-\mathbf{j},\alpha,\beta}^\ell f_{\mathbf{j},\beta}. \end{aligned}$$

The first sum involving  $E_{i_\delta-j_\delta, \alpha_\delta, \beta_\delta}^{\ell, \nu} f_{j_\delta, \beta_\delta}^{(\delta)}$  reduces the discrete  $d$ -dimensional convolution to  $d$  one-dimensional discrete convolutions. The second term involves only  $3^d$  terms w.r.t. the  $\mathbf{j}$ -summation. To see that each term has again a tensor structure, rewrite  $\delta N_{\mathbf{i},\alpha,\beta}^\ell$  for all  $\mathbf{i} \in \mathbb{Z}^d$  as  $\sum_{\|\mathbf{m}\|_\infty \leq 1} \delta N_{\mathbf{i},\alpha,\beta}^{\ell, \mathbf{m}}$  with  $\delta N_{\mathbf{i},\alpha,\beta}^{\ell, \mathbf{m}} = \delta N_{\mathbf{m},\alpha,\beta}^\ell \prod_{\delta=1}^d \delta_{i_\delta-m_\delta}$  involving a product of Kronecker deltas. Hence, the tensor rank of  $\delta N_{\mathbf{i},\alpha,\beta}^\ell$  (for fixed  $\alpha, \beta$ ) is at most  $3^d$ . In fact, the tensor rank is much smaller as explained next.

For  $d = 2$ , the data  $\delta N_{\mathbf{i},\alpha,\beta}^\ell$  which are nonzero only for  $\|\mathbf{i}\|_\infty \leq 1$  can be visualised by a stencil of the form

$$\delta N_{\mathbf{i},\alpha,\beta}^\ell = \begin{pmatrix} D & B & D \\ C & A & C \\ D & B & D \end{pmatrix}$$

with coefficients  $A, B, C$  depending on  $\alpha, \beta$  (concerning difference stencils see [5, (4.2.12)]). Here we have exploited the symmetry properties of  $N_{\mathbf{i},\alpha,\beta}^\ell$  (see Remark 4.5). For this example we assume even sums  $\alpha_\delta + \beta_\delta$  of polynomial degrees, otherwise the signs must be changed. The stencil can be written as a sum of two simple tensor products:

$$\begin{aligned} &\begin{pmatrix} BC/A & B & BC/A \\ C & A & C \\ BC/A & B & BC/A \end{pmatrix} + \begin{pmatrix} D - BC/A & 0 & D - BC/A \\ 0 & 0 & 0 \\ D - BC/A & 0 & D - BC/A \end{pmatrix} \\ &= \begin{pmatrix} C & A & C \end{pmatrix} \begin{pmatrix} B/A \\ 1 \\ B/A \end{pmatrix} + \begin{pmatrix} D - BC/A & 0 & D - BC/A \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}. \end{aligned}$$

Hence, the tensor rank is 2 instead of  $3^d = 9$ . A smaller rank than 2 is not possible unless  $AD = BC$ .

We remark that because of the symmetry, it is sufficient to consider only a  $2 \times 2$  stencil:  $\begin{pmatrix} B & D \\ A & C \end{pmatrix} =$

$$\begin{pmatrix} B/A \\ 1 \end{pmatrix} \otimes \begin{pmatrix} C \\ A \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} D - BC/A \\ 0 \end{pmatrix}$$

For the practically important case of  $d = 3$ , representations by rank 3 are possible. Without loss of generality we assume again symmetry:  $\delta N_{\mathbf{i},\alpha,\beta}^\ell = \delta N_{\mathbf{i}',\alpha,\beta}^\ell$  for  $i_\mu = \pm i'_\mu$  for  $\mu = 1, 2, 3$ . As just mentioned we can restrict  $\mathbf{i}$  to  $\{0, 1\}^3$ . The stencil notation for a tensor in  $\bigotimes_{\nu=1}^3 \mathbb{R}^2$  is  $\left[ \begin{array}{cc|cc} B & D & F & H \\ A & C & E & G \end{array} \right]$  where these

coefficients correspond to the indices  $\left[ \begin{array}{cc|cc} (1, 0, 0) & (1, 1, 0) & (1, 0, 1) & (1, 1, 1) \\ (0, 0, 0) & (0, 1, 0) & (0, 0, 1) & (0, 1, 1) \end{array} \right]$ . One verifies that

$$\begin{aligned} &\left[ \begin{array}{cc|cc} B & D & F & H \\ A & C & E & G \end{array} \right] = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} G - CF/B \\ E - AF/B \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} + \\ &\begin{pmatrix} B/A \\ 1 \end{pmatrix} \otimes \begin{pmatrix} C \\ A \end{pmatrix} \otimes \begin{pmatrix} F/B \\ 1 \end{pmatrix} + \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} D - BC/A \\ 0 \end{pmatrix} \otimes \begin{pmatrix} AH - CF \\ AD - BC \\ 1 \end{pmatrix}. \end{aligned}$$

This representation of tensor rank 3 requires that  $A, B, AD - BC$  do not vanish. However, the representation is not unique. If one or more quantities of  $A, B, AD - BC$  are zero, other representations of tensor rank 3 exist. While this rank-3 representation is easy to verify, this is harder for the following representation of rank 2:

$$\left[ \begin{array}{cc|cc} B & D & F & H \\ A & C & E & G \end{array} \right] = \alpha \begin{pmatrix} a_1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} a_2 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} a_3 \\ 1 \end{pmatrix} + \beta \begin{pmatrix} b_1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} b_2 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} b_3 \\ 1 \end{pmatrix}.$$

The parameters  $\alpha, \beta, a_\nu, b_\nu$  ( $\nu = 1, 2, 3$ ) can be determined as follows:

$$\begin{aligned} a_1 &= \frac{1}{2} \frac{DE - AH - BG + CF + W}{CE - AG}, & b_1 &= \frac{1}{2} \frac{DE - AH - BG + CF - W}{CE - AG}, \\ a_2 &= \frac{1}{2} \frac{DE - AH + BG - CF + W}{BE - AF}, & b_2 &= \frac{1}{2} \frac{DE - AH + BG - CF - W}{BE - AF} \end{aligned}$$

with

$$W = \sqrt{2(AD - BC)(FG - HE) + 2(BE - AF)(CH - GD) + (CF - DE)^2 + (AH - BG)^2}.$$

The further parameters are

$$\beta = \frac{C - a_2 A}{b_2 - a_2} = \frac{B - a_1 A}{b_1 - a_1}, \quad b_3 = \frac{G - a_2 E}{\beta(b_2 - a_2)} = \frac{F - a_1 E}{\beta(b_1 - a_1)}, \quad \alpha = A - \beta, \quad a_3 = (E - \beta b_3) / \alpha$$

(the second equality sign for the first two expressions holds due to the definition of  $a_1, a_2, b_1, b_2$ ). This representation requires the conditions  $EB - AF \neq 0, CE - AG \neq 0, a_1 \neq b_1, a_2 \neq b_2, \alpha \neq 0, \beta \neq 0$ . In the case of a imaginary root  $W$ , this approach may be less advantageous.

For general  $d$  the minimal possible rank is not known to the author, but estimates are possible. The worse rank is  $2^{d-1}$ . A bound from the other side will be discussed next. A general tensor in  $\bigotimes_{\nu=1}^d \mathbb{R}^2$  contains  $2^d$  free parameters. An ansatz of tensor rank  $r$  is

$$\sum_{\rho=1}^r \alpha_\rho \bigotimes_{\nu=1}^d \begin{pmatrix} a_{\nu,\rho} \\ 1 \end{pmatrix}$$

with  $r(d+1)$  free parameters. Obviously,  $r(d+1) \geq 2^d$  must hold<sup>11</sup>. This inequality is satisfied for  $r = d$  as long as  $d \leq 4$ . According to this consideration  $r \geq 2^d / (d+1)$  forms a lower bound of the rank, which would imply an exponential cost as  $d \rightarrow \infty$ . However, the assumption that the tensor contains  $2^d$  free parameters holds only for unlimited polynomial degree  $p$  (more precisely, if  $p > d$ ). For instance,  $p = 0$  implies  $\alpha = \beta = \mathbf{0}$  and therefore  $\delta N_{\mathbf{i}, \mathbf{0}, \mathbf{0}}^\ell = \delta N_{\mathbf{i}', \mathbf{0}, \mathbf{0}}^\ell$  for all permutations  $\mathbf{i}' \in \{0, 1\}^d$  of  $\mathbf{i}$ . In this case the number of free parameters is only  $d+1$ . These parameters are  $b_\mu := \delta N_{\mathbf{i}, \mathbf{0}, \mathbf{0}}^\ell$  for all  $\mathbf{i}$  with  $|\mathbf{i}| = i_1 + i_2 + \dots + i_d = \mu$  ( $0 \leq \mu \leq d$ ). They define a subspace  $V_d \subset \bigotimes_{\nu=1}^{d+1} \mathbb{R}^2$  of dimension  $d+1$ . A possible representation of rank  $d+1$  is

$$(\delta N_{\mathbf{i}, \mathbf{0}, \mathbf{0}}^\ell)_{\mathbf{i} \in \{0, 1\}^d} = \sum_{\rho=1}^{d+1} \alpha_\rho \bigotimes_{\nu=1}^d \begin{pmatrix} a_\rho \\ 1 \end{pmatrix}.$$

This leads to the equations  $\sum_{\rho=1}^{d+1} \alpha_\rho a_\rho^\mu = b_\mu$  ( $0 \leq \mu \leq d$ ). Since  $(a_\rho^\mu)$  is the transposed of the Vandermonde matrix, we may fix any distinct values of  $a_\rho$  and can solve the system for  $\alpha_\rho$ . One may even look for representations of rank  $\leq d$ .

In the general case of a maximal polynomial  $p$ , we consider the pair sets  $\{(\alpha, \beta), (\beta, \alpha)\}$  with  $0 \leq \alpha, \beta \leq p$ . There are  $P := (p+1)(p+2)/2$  pair sets, which we denote by  $\pi_1, \dots, \pi_P$ . Given  $\delta N_{\mathbf{i}, \alpha, \beta}^\ell$  with  $\alpha, \beta \in \{0, \dots, p\}$ , we may order the coordinates such that  $(\alpha_\nu, \beta_\nu) \in \pi_j$  for  $\sum_{\mu=1}^{j-1} m_\mu + 1 \leq \nu \leq \sum_{\mu=1}^j m_\mu$  where  $m_\mu$  are suitable integers with  $\sum_{\mu=1}^P m_\mu = d$ . The tensor space  $\bigotimes_{\nu=1}^d \mathbb{R}^2$  is isomorphic to  $\bigotimes_{\mu=1}^P (\bigotimes_{\nu=1}^{m_\mu} \mathbb{R}^2)$ .

<sup>11</sup>Note that for  $d = 3$  the smallest  $r$  satisfying this inequality (i.e.,  $r = 2$ ) is indeed an attainable rank as shown above.

Now  $\bigotimes_{\nu=1}^{m_\mu} \mathbb{R}^2$  can be restricted to the respective subspace  $V_{m_\mu}$ , i.e.,  $(\delta N_{\mathbf{i},\alpha,\beta}^\ell)_{\mathbf{i} \in \{0,1\}^d} \in \bigotimes_{\mu=1}^P V_{m_\mu}$ . A representation of  $(\delta N_{\mathbf{i},\alpha,\beta}^\ell)_{\mathbf{i} \in \{0,1\}^d}$  by

$$(\delta N_{\mathbf{i},\alpha,\beta}^\ell)_{\mathbf{i} \in \{0,1\}^d} = \sum_{\rho=1}^r \bigotimes_{\mu=1}^P v_{\mu,\rho} \quad \text{with} \quad v_{\mu,\rho} \in V_{m_\mu}$$

is always possible for  $r \geq \min_{\sigma=1}^P \prod_{\substack{\mu=1 \\ \mu \neq \sigma}}^P \dim V_{m_\mu} = \min_{\sigma=1}^P \prod_{\substack{\mu=1 \\ \mu \neq \sigma}}^P (m_\mu + 1)$ . Maximising the right-hand side over all  $m_\mu$  subject to  $\sum_{\mu=1}^P m_\mu = d$  shows that the rank  $r := \left\lceil \left(\frac{d}{P} + 1\right)^{P-1} \right\rceil$  is always attainable which is only polynomial in  $d$ , not exponential as  $d \rightarrow \infty$ . Again, it must be emphasised that this  $r$  may be a very pessimistic bound. For the determination of the minimal rank (in particular under approximation aspects) see [3].

**Conclusion 5.5** *For fixed  $\alpha, \beta$ , the tensor  $\tilde{N}_{\mathbf{i},\alpha,\beta}^\ell$  from (5.9) can be represented as a sum of  $k' = k + r$  terms of the tensor product form  $\prod_{\delta=1}^d v_{i_\delta,\alpha,\beta}^{(\nu,\delta)}$ , i.e.,*

$$\tilde{N}_{\mathbf{i},\alpha,\beta}^\ell = \sum_{\nu=1}^{k'} \prod_{\delta=1}^d v_{i_\delta,\alpha,\beta}^{(\nu,\delta)},$$

where  $r$  is the rank needed for  $(\delta N_{\mathbf{i},\alpha,\beta}^\ell)_{\mathbf{i} \in \{0,1\}^d}$ . Therefore a convolution of  $\tilde{N}_{\mathbf{i},\alpha,\beta}^\ell$  with  $f_{\mathbf{j},\beta}$  from (5.8) reduces to  $k'd$  one-dimensional convolutions:

$$\sum_{\mathbf{j} \in \mathbb{Z}^d} \tilde{N}_{\mathbf{i}-\mathbf{j},\alpha,\beta}^\ell f_{\mathbf{j},\beta} = \sum_{\nu=1}^{k'} \prod_{\delta=1}^d \sum_{j_\delta \in \mathbb{Z}} v_{i_\delta-j_\delta,\alpha,\beta}^{(\nu,\delta)} f_{j_\delta,\beta}^{(\delta)}. \quad (5.10)$$

**Remark 5.6** *The function  $f(x) = f^{(1)}(x_1) \cdots f^{(d)}(x_d)$  has tensor rank 1. If  $f$  consists of a sum involving  $r$  terms of this form (tensor rank  $r$ ), the result of the convolution consists of an increased number of tensor products. In order to reduce this number, one should apply methods which reduce the tensor rank (at the cost of an additional error; cf. Espig [3]).*

## 5.4 Algorithm

In principle, the algorithm is the same as in (3.2), where  $f = \sum_\ell f^\ell$ . Here we have  $f^\ell = \sum_{\nu=1}^{k_\ell} f_{\ell,\nu}$  according to (5.4) and therefore Algorithm (3.2) must be interpreted in a particular way.

- Line 4 in (3.2):  $u|_{B_\ell} := u|_{B_\ell} + (P_\ell \mathcal{K} P_\ell f^\ell)|_{B_\ell}$ ;

$P_\ell \mathcal{K} P_\ell$  is replaced by the tensor product approximation with the coefficients  $\tilde{N}_{\mathbf{i},\alpha,\beta}^\ell$ . For each term  $f_{\ell,\nu}$  the convolution follows (5.10). Note that only the result in  $B_\ell$  is to be computed (the part outside  $B_\ell$  is done in later steps of the  $\ell$ -loop at Line 5).

- Line 6:  $F := F + f^\ell$ ;

Since also  $F$  is organised as a sum of tensor products, this addition is not performed. Instead the list of tensor products increases by the  $k_\ell$  terms  $f^\ell = \sum_{\nu=1}^{k_\ell} f_{\ell,\nu}$ . Here one may try to reduce the number of terms according to Remark 5.6.

- Line 3:  $F := P_\ell F$ ;

By induction  $F \in S_{\ell+1}$  holds:  $F = \sum_{\nu=1}^{k_{\ell+1,F}} F_{\ell+1,\nu}$ , where each  $F_{\ell+1,\nu}$  is of product form (cf. (5.4)). Then the projection  $P_\ell$  can be performed for each direction separately:

$$(P_\ell F_{\ell+1,\nu})(x_1, \dots, x_d) = \left(P_\ell^{(1)} F_{\ell+1,\nu}^{(1)}\right)(x_1) \cdots \left(P_\ell^{(1)} F_{\ell+1,\nu}^{(d)}\right)(x_d),$$

where  $P_\ell^{(1)}$  is the one-dimensional prolongation, i.e., the orthogonal projection onto  $S_\ell^{(1)}$  (cf. (5.3)). The corresponding coefficients are the result of the restriction (2.15) for  $d = 1$ . Note that number of terms is not changing:  $k_{\ell,F} = k_{\ell+1,F}$  in  $P_\ell F = \sum_{\nu=1}^{k_{\ell,F}} F_{\ell,\nu}$  with  $F_{\ell,\nu} = P_\ell F_{\ell+1,\nu}$ .

- Line 5:  $u|_{B_\ell \setminus B_{\ell+1}} := (P_\ell \mathcal{K} P_\ell F)|_{B_\ell \setminus B_{\ell+1}}$ ;

Consider one term  $F_{\ell,\nu}$  of  $F = \sum_{\nu=1}^{k_{\ell,F}} F_{\ell,\nu}$ . First  $P_\ell \mathcal{K} P_\ell F_{\ell,\nu}$  is determined as in Line 4 with support in  $B_\ell$ . Let  $u_{\ell,\mu}(x_1, \dots, x_d) = u_{\ell,\mu}^{(1)}(x_1) \cdot \dots \cdot u_{\ell,\mu}^{(d)}(x_d)$  by one of the tensor products of the result. The characteristic function of  $B_{\ell+1}$  is again a product  $\chi_{1,\ell+1} \cdot \dots \cdot \chi_{d,\ell+1}$ . Obviously,  $\check{u}_{\ell,\mu}(x_1, \dots, x_d) := \prod_{\delta=1}^d u_{\ell,\mu}^{(\delta)}(x_\delta) \chi_{\delta,\ell+1}$  equals  $u_{\ell,\mu}|_{B_{\ell+1}}$ . Therefore,

$$u_{\ell,\mu} - \check{u}_{\ell,\mu} = u_{\ell,\mu}|_{B_\ell \setminus B_{\ell+1}}.$$

Note that this approach doubles the tensor rank. If the tensor rank reduction according to Remark 5.6 is intended, two versions are possible: 1)  $\check{u}_{\ell,\mu}$  can be treated as a term of level  $\ell$  with support in  $B_\ell$ , 2) since  $\text{supp}(\check{u}_{\ell,\mu}) \subset B_{\ell+1}$ ,  $\check{u}_{\ell,\mu}$  can be prolonged to level  $\ell + 1$ . Depending on this choice, the rank reduction is done among all contributions of either level  $\ell$  or level  $\ell + 1$ .

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## A Additional comments

### A.1 Example of a tensor approximation of the Newton potential

As an example we consider the boxes  $B_\ell = 2h_\ell [-1, 1]$  of Example 2.4. The Euclidean distance of  $x \in \text{supp}(\Phi_{\mathbf{i},\alpha}^\ell) \subset \overline{B}_\ell$  from  $y \in \text{supp}(\Phi_{\mathbf{j},\beta}^\ell) \subset \overline{B}_\ell$  with  $\|\mathbf{i} - \mathbf{j}\|_\infty \geq 2$  (far field case) is at least  $h_\ell$  and at most  $4h_\ell\sqrt{d}$  (depending on the spatial dimension  $d$ ). This implies that the approximation (5.5) is needed in the interval  $[1, R]$  with  $R = 4\sqrt{d}$ . For the 3D-case this is  $R = 4\sqrt{3} = 6.9282\dots$ . Different choices of the number  $k$  of terms yield the following approximation errors  $\eta$ :

$k$	1	2	3	4	5	6	7	8	9
$\eta$	7.09E-2	3.58E-3	1.82E-4	9.26E-6	4.72E-7	2.41E-8	1.23E-9	6.26E-11	3.19E-12

For the cases  $k = 3$  and  $k = 9$ , the corresponding coefficients  $\omega_\nu, \vartheta_\nu$  of (5.5) are given below:

$\nu$	$\omega_\nu$	$\vartheta_\nu$
1	0.560124245592825410	0.059931283387658894
2	0.670756602248168953	0.607882152449899544
3	1.008349653847160430	2.242794652929559598

$\nu$	$\omega_\nu$	$\vartheta_\nu$
1	0.324283398516544698	0.0205875663651470187
2	0.330125262978802426	0.187499336444026598
3	0.342586070199041368	0.533720636686782973
4	0.363363837823695047	1.087171421568844598
5	0.395369588643770928	1.898629677561829318
6	0.443303043137218010	3.055937748084754945
7	0.515470983731095820	4.711989509641412826
8	0.631816622474811241	7.152604614505099386
9	0.875684785527278758	11.055681349670407167

In [7] and the web page given therein one finds the data for further choices of  $R$  and  $k$ .

If one wants to approximate the Newton potential on the half-infinite interval  $1 \leq \|x - y\| < \infty$  the accuracies  $\eta$  for varying  $k$  are as follows:

$k$	1	2	3	4	5	6	7	8	9
$\eta$	1.40E-1	4.09E-2	1.56E-2	6.83E-3	3.30E-3	1.70E-3	9.25E-4	5.24E-4	3.07E-4

### A.2 Galerkin matrix entries for convolution kernels (1D case)

In the following,  $k : [-1, 1] \rightarrow \mathbb{R}$  is a general differentiable kernel function. We want to determine the values

$$k_{\alpha,\beta} := \int_0^1 \int_0^1 k(x-y) \Phi_{0,\alpha}^0(x) \Phi_{0,\beta}^0(y) dx dy, \quad (\text{A.1})$$

where  $\Phi_{0,\alpha}^0$  and  $\Phi_{0,\beta}^0$  are the one-dimensional Legendre polynomials with support in  $[0, 1]$ . Note that  $x - y$  varies in  $[-1, 1]$ . We introduce the quantities

$$\begin{aligned} k_{\alpha,+} &:= \int_0^1 k(x-1) \Phi_{0,\alpha}^0(x) dx, & k_{+,\beta} &:= \int_0^1 k(1-y) \Phi_{0,\beta}^0(y) dy, \\ k_{\alpha,-} &:= \int_0^1 k(x) \Phi_{0,\alpha}^0(x) dx, & k_{-,\beta} &:= \int_0^1 k(-y) \Phi_{0,\beta}^0(y) dy, \end{aligned} \quad (\text{A.2})$$

which use point evaluations of  $x$  or  $y$  at the upper or lower end point of  $[0, 1]$ . The calculation of  $k_{\pm,\beta}$  can be reduced to that of  $k_{\alpha,\pm}$  because of the next remark.

**Remark A.1** *The symmetry properties of  $\Phi_{0,\alpha}^0$  imply*

$$k_{\alpha,-} = (-1)^\alpha k_{+,\alpha}, \quad k_{\alpha,+} = (-1)^\alpha k_{-,\alpha}. \quad (\text{A.3})$$

**Step 1.** First the quantities  $k_{\alpha,\pm}$  are to be computed. For instance, the function  $k$  can be interpolated in  $[0, 1]$  by a polynomial which then is reformulated by means of the transformed Legendre polynomial  $\Phi_{0,\alpha}^0$ .

**Step 2.** We define

$$k'_{\alpha,0} := \int_0^1 \int_0^1 k(x-y) \frac{d}{dx} \Phi_{0,\alpha}^0(x) dx dy \quad (\alpha \geq 0).$$

**Lemma A.2** *The values of  $k'_{\alpha,0}$  are explicitly given by the quantities  $k_{\alpha,\pm}$  and  $k_{\pm,\beta}$  from Step 1:*

$$\begin{aligned} k'_{0,0} &= 0, & \text{for } \alpha = 0, \\ k'_{\alpha,0} &= \sqrt{2\alpha+1} (k_{+,0} - (-1)^\alpha k_{-,0}) + k_{\alpha,+} - k_{\alpha,-} & \text{for } \alpha \geq 1. \end{aligned} \quad (\text{A.4})$$

*Proof.* Partial integration yields

$$k'_{\alpha,0} = \int_0^1 k(x-y) \Phi_{0,\alpha}^0(x) \Big|_{x=0}^{x=1} dy - \int_0^1 \int_0^1 \frac{dk(x-y)}{dx} \Phi_{0,\alpha}^0(x) dx dy.$$

Since

$$\Phi_{0,\alpha}^0(1) = \sqrt{2\alpha+1}, \quad \Phi_{0,\alpha}^0(0) = (-1)^\alpha \sqrt{2\alpha+1}, \quad (\text{A.5})$$

the first term equals  $\sqrt{2\alpha+1} (k_{+,0} - (-1)^\alpha k_{-,0})$ . For the second term use  $\frac{d}{dx} k(x-y) = -\frac{d}{dy} k(x-y)$  and

$$\int_0^1 \int_0^1 \frac{d}{dy} k(x-y) \Phi_{0,\alpha}^0(x) dx dy = \int_0^1 k(x-y) \Big|_{y=0}^{y=1} \Phi_{0,\alpha}^0(x) dx = k_{\alpha,+} - k_{\alpha,-}.$$

■

**Step 3.** Next, we compute the quantities  $k_{\alpha,0}$ .

**Lemma A.3** *Let  $\alpha \geq 0$ . The coefficients  $k_{\alpha,0}$  can be determined from the recursion formula*

$$k_{\alpha,0} = \begin{cases} \frac{1}{2\sqrt{3}} k'_{1,0} & \text{for } \alpha = 0, \\ \frac{1}{2\sqrt{(2\alpha+1)(2\alpha+3)}} k'_{\alpha+1,0} - \frac{1}{2\sqrt{(2\alpha-1)(2\alpha+1)}} k'_{\alpha-1,0} & \text{for } \alpha \geq 1. \end{cases}$$

*Proof.* a) By definition (using  $\Phi_{0,0}^0 = 1$  in  $[0, 1]$ )

$$k_{\alpha,0} = \int_0^1 \int_0^1 k(x-y) \Phi_{0,\alpha}^0(x) \Phi_{0,0}^0(y) dx dy = \int_0^1 \int_0^1 k(x-y) \Phi_{0,\alpha}^0(x) dx dy \quad (\text{A.6})$$

holds.

b) Case  $\alpha = 0$ . The explicit values  $\Phi_{0,0}^0(x) = 1$  and  $\Phi_{0,1}^0(x) = 2\sqrt{3}(x - 1/2)$  show

$$\Phi_{0,0}^0 = \frac{1}{2\sqrt{3}} \frac{d}{dx} \Phi_{0,1}^0 \quad (0 < x < 1).$$

Replacing  $\Phi_{0,\alpha}^0$  in (A.6) by this expression yields  $k'_{1,0}/(2\sqrt{3})$ .

c) Case  $\alpha \geq 1$ . The antiderivative of  $\Phi_{0,\alpha}^0$  equals

$$\int_0^x \Phi_{0,\alpha}^0(t) dt = \frac{\Phi_{0,\alpha+1}^0(x)}{2\sqrt{(2\alpha+1)(2\alpha+3)}} - \frac{\Phi_{0,\alpha-1}^0(x)}{2\sqrt{(2\alpha-1)(2\alpha+1)}} \quad (\alpha \geq 1, 0 < x < 1) \quad (\text{A.7})$$

(cf. [9]). Differentiation yields

$$\Phi_{0,\alpha}^0 = \frac{\frac{d}{dx} \Phi_{0,\alpha+1}^0}{2\sqrt{(2\alpha+1)(2\alpha+3)}} - \frac{\frac{d}{dx} \Phi_{0,\alpha-1}^0}{2\sqrt{(2\alpha-1)(2\alpha+1)}} \quad (\alpha \geq 1, 0 < x < 1). \quad (\text{A.8})$$

Inserting the latter identity into (A.6) yields the statement. ■

**Step 4.** Now we consider the case of  $k_{\alpha,\beta}$  with general  $\alpha, \beta$ .

**Remark A.4** The symmetry properties of  $\Phi_{0,\alpha}^0, \Phi_{0,\beta}^0$  imply  $k_{\alpha,\beta} = (-1)^{\alpha+\beta} k_{\beta,\alpha}$  for  $\alpha, \beta \in \mathbb{N}$ .

*Proof.* The proof of Remark 4.5 is already formulated for a general kernel  $k(x-y)$ . ■

By the previous remark,  $k_{\alpha,\beta}$  is already known from Step 3 if either  $\alpha = 0$  or  $\beta = 0$ . Hence, we restrict the considerations to  $\alpha, \beta \geq 1$ . The next lemma yields a recursion with respect to the first index  $\alpha$ .

**Lemma A.5** For  $\alpha, \beta \geq 1$  the quantities  $k_{\alpha,\beta}$  satisfy the recursion

$$k_{\alpha,\beta} = \begin{cases} \frac{\sqrt{2\alpha+1}}{\sqrt{2\alpha-3}} k_{\alpha-2,\beta} + \frac{\sqrt{(2\alpha-1)(2\alpha+1)}}{\sqrt{(2\beta-1)(2\beta+1)}} k_{\alpha-1,\beta-1} - \frac{\sqrt{(2\alpha-1)(2\alpha+1)}}{\sqrt{(2\beta+1)(2\beta+3)}} k_{\alpha-1,\beta+1} & \text{for } \alpha \geq 2 \\ \frac{\sqrt{3}}{\sqrt{(2\beta-1)(2\beta+1)}} \left( k_{0,\beta-1} - \frac{k_{+, \beta-1} + k_{-, \beta-1}}{2} \right) - \frac{\sqrt{3}}{\sqrt{(2\beta+1)(2\beta+3)}} \left( k_{0,\beta+1} - \frac{k_{+, \beta+1} + k_{-, \beta+1}}{2} \right) & \text{for } \alpha = 1. \end{cases}$$

*Proof.* First we assume  $\alpha \geq 2$  and consider the linear combination

$$\begin{aligned} & \frac{k_{\alpha,\beta}}{2\sqrt{(2\alpha-1)(2\alpha+1)}} - \frac{k_{\alpha-2,\beta}}{2\sqrt{(2\alpha-3)(2\alpha-1)}} \\ &= \int_0^1 \int_0^1 k(x-y) \left( \frac{\Phi_{0,\alpha}^0(x)}{2\sqrt{(2\alpha-1)(2\alpha+1)}} - \frac{\Phi_{0,\alpha-2}^0(x)}{2\sqrt{(2\alpha-3)(2\alpha-1)}} \right) \Phi_{0,\beta}^0(y) dx dy \stackrel{(A.7)}{=} \\ &= \int_0^1 \int_0^1 k(x-y) \left( \int_0^x \Phi_{0,\alpha-1}^0(t) dt \right) \Phi_{0,\beta}^0(y) dx dy \stackrel{(A.8)}{=} \\ &= \int_0^1 \int_0^1 k(x-y) \left( \int_0^x \Phi_{0,\alpha-1}^0(t) dt \right) \frac{d}{dy} \left( \frac{\Phi_{0,\beta+1}^0(y)}{2\sqrt{(2\beta+1)(2\beta+3)}} - \frac{\Phi_{0,\beta-1}^0(y)}{2\sqrt{(2\beta-1)(2\beta+1)}} \right) dx dy. \end{aligned}$$

The partial integration with respect to  $y$  does not produce boundary terms since

$$\frac{1}{2\sqrt{(2\beta+1)(2\beta+3)}} \Phi_{0,\beta+1}^0(y) = \frac{1}{2\sqrt{(2\beta-1)(2\beta+1)}} \Phi_{0,\beta-1}^0(y) \quad \text{for } y \in \{0, 1\}.$$

The same statement holds for the boundary values of  $\int_0^x \Phi_{0,\alpha-1}^0(t) dt$  at  $x \in \{0, 1\}$ . Hence,

$$\begin{aligned} & \frac{1}{2\sqrt{(2\alpha-1)(2\alpha+1)}} k_{\alpha,\beta} - \frac{1}{2\sqrt{(2\alpha-3)(2\alpha-1)}} k_{\alpha-2,\beta} \\ &= - \int_0^1 \int_0^1 \frac{dk(x-y)}{dy} \left( \int_0^x \Phi_{0,\alpha-1}^0(t) dt \right) \left( \frac{\Phi_{0,\beta+1}^0(y)}{2\sqrt{(2\beta+1)(2\beta+3)}} - \frac{\Phi_{0,\beta-1}^0(y)}{2\sqrt{(2\beta-1)(2\beta+1)}} \right) dx dy \\ &= \int_0^1 \int_0^1 \frac{dk(x-y)}{dx} \left( \int_0^x \Phi_{0,\alpha-1}^0(t) dt \right) \left( \frac{\Phi_{0,\beta+1}^0(y)}{2\sqrt{(2\beta+1)(2\beta+3)}} - \frac{\Phi_{0,\beta-1}^0(y)}{2\sqrt{(2\beta-1)(2\beta+1)}} \right) dx dy \\ &= - \int_0^1 \int_0^1 k(x-y) \Phi_{0,\alpha-1}^0(x) \left( \frac{\Phi_{0,\beta+1}^0(y)}{2\sqrt{(2\beta+1)(2\beta+3)}} - \frac{\Phi_{0,\beta-1}^0(y)}{2\sqrt{(2\beta-1)(2\beta+1)}} \right) dx dy \\ &= \frac{1}{2\sqrt{(2\beta-1)(2\beta+1)}} k_{\alpha-1,\beta-1} - \frac{1}{2\sqrt{(2\beta+1)(2\beta+3)}} k_{\alpha-1,\beta+1} \end{aligned}$$

proves the statement for  $\alpha \geq 2$ .

For  $\alpha = 1$  we repeat the argument from above with the modification that  $2\sqrt{3} \int_{1/2}^x \Phi_{0,0}^0(t) dt = \Phi_{0,1}^0(x)$  :

$$\begin{aligned}
k_{1,\beta} &= 2\sqrt{3} \int_0^1 \int_0^1 k(x-y) \left( \int_{1/2}^x \Phi_{0,0}^0(t) dt \right) \Phi_{0,\beta}^0(y) dx dy \\
&= 2\sqrt{3} \int_0^1 \int_0^1 k(x-y) \left( \int_{1/2}^x \Phi_{0,0}^0(t) dt \right) \frac{d}{dy} \left( \frac{\Phi_{0,\beta+1}^0(y)}{2\sqrt{(2\beta+1)(2\beta+3)}} - \frac{\Phi_{0,\beta-1}^0(y)}{2\sqrt{(2\beta-1)(2\beta+1)}} \right) dx dy \\
&= 2\sqrt{3} \int_0^1 \int_0^1 \frac{dk(x-y)}{dx} \left( \int_{1/2}^x \Phi_{0,0}^0(t) dt \right) \left( \frac{\Phi_{0,\beta+1}^0(y)}{2\sqrt{(2\beta+1)(2\beta+3)}} - \frac{\Phi_{0,\beta-1}^0(y)}{2\sqrt{(2\beta-1)(2\beta+1)}} \right) dx dy \\
&= 2\sqrt{3} \int_0^1 k(x-y) \left( \int_{1/2}^x \Phi_{0,0}^0(t) dt \right) \Big|_{x=0}^{x=1} \left( \frac{\Phi_{0,\beta+1}^0(y)}{2\sqrt{(2\beta+1)(2\beta+3)}} - \frac{\Phi_{0,\beta-1}^0(y)}{2\sqrt{(2\beta-1)(2\beta+1)}} \right) dx dy \\
&\quad - 2\sqrt{3} \int_0^1 \int_0^1 k(x-y) \Phi_{0,0}^0(x) \left( \frac{\Phi_{0,\beta+1}^0(y)}{2\sqrt{(2\beta+1)(2\beta+3)}} - \frac{\Phi_{0,\beta-1}^0(y)}{2\sqrt{(2\beta-1)(2\beta+1)}} \right) dx dy \\
&= \frac{\sqrt{3}}{2\sqrt{(2\beta+1)(2\beta+3)}} (k_{+,\beta+1} + k_{-,\beta+1}) - \frac{\sqrt{3}}{2\sqrt{(2\beta-1)(2\beta+1)}} (k_{+,\beta-1} + k_{-,\beta-1}) \\
&\quad - \frac{\sqrt{3}}{\sqrt{(2\beta+1)(2\beta+3)}} k_{0,\beta+1} + \frac{\sqrt{3}}{\sqrt{(2\beta-1)(2\beta+1)}} k_{0,\beta-1}.
\end{aligned}$$

■

### A.3 Galerkin matrix entries in the multi-dimensional case

Now we consider a general differentiable kernel function  $K(z)$  in  $[-1, 1]^d$  and want to determine the Galerkin matrix entries

$$K_{\alpha,\beta} := \iint K(x-y) \Phi_{0,\alpha}^0(x) \Phi_{0,\beta}^0(y) dx dy \quad \text{for } \alpha, \beta \in \mathbb{N}_0^d.$$

The application we have in mind is

$$K(x-y) := 1/\|x-y+\mathbf{i}\| \quad \text{for } \mathbf{i} \in \mathbb{Z}^d, \quad \|\mathbf{i}\|_\infty \geq 2, \quad (\text{A.9})$$

where  $K_{\alpha,\beta} = N_{\mathbf{i},\alpha,\beta}^0$  (cf. (4.3)).

When we fix an index  $i \in \{1, \dots, d\}$  and fix values  $x_{i'}, y_{i'}$  for  $i' \neq i$  or apply certain functionals (integrations) to  $x_{i'}, y_{i'}$ , we arrive at

$$k(x_i - y_i) := K(x - y) \quad (x_i, y_i \in \mathbb{R}).$$

Renaming  $x_i, y_i$  by  $x, y$ , we can again apply the considerations of §A.2.

In the  $d$ -dimensional case, the quantities  $K_{\alpha,\beta}$  depend on multi-indices  $\alpha, \beta \in \mathbb{N}_0^d$ . We recall that  $\Phi_{0,\alpha}^0(x) = \prod_{j=1}^d \Phi_{0,\alpha_j}^0(x_j)$  with  $\alpha_j \geq 0$ . We extend the range of  $\alpha_j$  to  $\mathbb{N}_0 \cup \{-1, -2\}$  and use  $\alpha_j = -1$  instead of “+” and  $\alpha_j = -2$  instead of “-” in (A.2). Another interpretation is that  $\Phi_{0,\alpha_j}^0$  for  $\alpha_j \in \{-1, -2\}$  is the Dirac functional at  $2 + \alpha_j$ . With this replacement the definition in (A.2) (one-dimensional case) becomes

$$k_{\alpha,+} = \int_0^1 k(x-1) \Phi_{0,\alpha}^0(x) dx = \int_0^1 \int_0^1 k(x-y) \Phi_{0,\alpha}^0(x) \Phi_{0,-1}^0(y) dx dy.$$

Next we introduce the function

$$\mu(\alpha, j, m) := (\alpha_1, \dots, \alpha_{j-1}, m, \alpha_{j+1}, \dots, \alpha_d),$$

which replaces the  $j$ th component of the multi-index  $\alpha$  by the integer  $m$ .

With these notations the recursion from Lemmata A.3 and A.5 can be generalised to the  $d$ -dimensional case:

**Lemma A.6** a) For some  $j \in \{1, \dots, d\}$  let  $\alpha_j \geq 0$  and  $\beta_j = 0$ . Then

$$K_{\alpha, \beta} = \begin{cases} \frac{1}{2\sqrt{3}} K_{\mu(\alpha, j, 1), \beta}^{(j)} & \text{for } \alpha_j = 0, \\ \frac{1}{2\sqrt{(2\alpha_j+1)(2\alpha_j+3)}} K_{\mu(\alpha, j, \alpha_j+1), \beta}^{(j)} - \frac{1}{2\sqrt{(2\alpha_j-1)(2\alpha_j+1)}} K_{\mu(\alpha, j, \alpha_j-1), \beta}^{(j)} & \text{for } \alpha_j \geq 1, \end{cases}$$

where the quantities on the right-hand side are

$$K_{\alpha, \beta}^{(j)} := \begin{cases} 0 & \text{for } \alpha_j = 0, \beta_j = 0, \\ \left\{ \begin{aligned} &\sqrt{2\alpha_j+1} (K_{\mu(\alpha, j, -1), \beta} - (-1)^{\alpha_j} K_{\mu(\alpha, j, -2), \beta}) \\ &+ K_{\alpha, \mu(\beta, j, -1)} - K_{\alpha, \mu(\beta, j, -2)} \end{aligned} \right\} & \text{for } \alpha_j \geq 1, \beta_j = 0. \end{cases}$$

b) For  $\alpha_j \geq 1$  and  $\beta_j \geq 1$  we have

$$K_{\alpha, \beta} = \begin{cases} \left\{ \begin{aligned} &\frac{\sqrt{2\alpha_j+1}}{\sqrt{2\alpha_j-3}} K_{\mu(\alpha, j, \alpha_j-2), \beta} + \frac{\sqrt{(2\alpha_j-1)(2\alpha_j+1)}}{\sqrt{(2\beta_j-1)(2\beta_j+1)}} K_{\mu(\alpha, j, \alpha_j-1), \mu(\beta, j, \beta_j-1)} \\ &- \frac{\sqrt{(2\alpha_j-1)(2\alpha_j+1)}}{\sqrt{(2\beta_j+1)(2\beta_j+3)}} K_{\mu(\alpha, j, \alpha_j-1), \mu(\beta, j, \beta_j+1)} \end{aligned} \right\} & \text{for } \alpha_j \geq 2, \\ \left\{ \begin{aligned} &\frac{\sqrt{3}}{\sqrt{(2\beta_j-1)(2\beta_j+1)}} \left( K_{\mu(\alpha, j, 0), \mu(\beta, j, \beta_j-1)} - \frac{K_{\mu(\alpha, j, -1), \mu(\beta, j, \beta_j-1)} + K_{\mu(\alpha, j, -2), \mu(\beta, j, \beta_j-1)}}{2} \right) \\ &- \frac{\sqrt{3}}{\sqrt{(2\beta_j+1)(2\beta_j+3)}} \left( K_{\mu(\alpha, j, 0), \mu(\beta, j, \beta_j+1)} - \frac{K_{\mu(\alpha, j, -1), \mu(\beta, j, \beta_j+1)} + K_{\mu(\alpha, j, -2), \mu(\beta, j, \beta_j+1)}}{2} \right) \end{aligned} \right\} & \text{for } \alpha_j = 1. \end{cases}$$

The concrete calculation can be performed in 3 steps.

**Step 1** Evaluate  $K_{\alpha, \beta}$  and  $K_{\beta, \alpha}$  for all  $\alpha_j = -1, -2$  and  $0 \leq \beta_j \leq 2p+1$  ( $1 \leq j \leq d$ ).

**Step 2** The recursions of Lemma A.6 are applied in alphabetic order:

```

1  for  $j := 1$  to  $d$  do
2    for all  $\beta \in [-2, p]^{j-1} \times \{0\} \times [-2, -1]^{d-j}$  do
3      begin for all  $\alpha$  with  $\alpha_1, \dots, \alpha_{j-1}, \alpha_{j+1}, \dots, \alpha_d \in [-2, p]$  do
4        begin for  $\alpha_j := 0$  to  $2p$  evaluate  $K_{\alpha, \beta}$  by Lemma A.6a;           {note that  $\beta_j = 0$ }
5        for  $\beta_j := 1$  to  $p$  do for  $\alpha_j := \beta_j$  to  $2p - \beta_j$  do evaluate  $K_{\alpha, \beta}$  by Lemma A.6b
6      end end;

```

*Ad Step 1:* Step 1 makes use the symmetry relations (A.3). In the main application, the quantities  $K_{\alpha, \beta} := N_{\mathbf{i}, \alpha, \beta}^0 = \iint \frac{\Phi_{\mathbf{i}, \alpha}^0(x) \Phi_{\mathbf{i}, \beta}^0(y)}{\|x-y\|} dx dy$  are introduced for a fixed multi-index  $\mathbf{i}$  (cf. (A.9)). The relation of  $\mathbf{i}$  and  $\alpha$  in Step 1 is discussed in the next remark.

**Remark A.7** Let  $\alpha \in \{-1, -2\}^d$ . Then

$$N_{\mathbf{i}, \alpha, \beta}^0 = N_{\mathbf{i}+\alpha+1, -1, \beta}^0.$$

**Conclusion A.8** In Step 1, it suffices to consider the case  $\alpha = -1$  (i.e.,  $\alpha_\delta = -1$  for all  $\delta$ ). If  $N_{\mathbf{i}, \alpha, \beta}^0$  is needed for all  $\mathbf{i}_a \leq \mathbf{i} \leq \mathbf{i}_b$  and all  $\alpha \in \{-1, -2\}^d$ , one has to compute  $N_{\mathbf{i}', -1, \beta}^0$  for all  $\mathbf{i}_a - \mathbf{1} \leq \mathbf{i}' \leq \mathbf{i}_b$ .

*Ad Step 2:* The two loops in the lines 1,2 of the algorithm run through all  $\beta$  with at least one component  $\beta_j = 0$  in a particular order. For  $j = 1$  the set  $[-2, p]^{j-1} \times \{0\} \times [-2, -1]^{d-j}$  equals  $\{0\} \times [-2, -1]^{d-1}$ .

The loops in the lines 3,4 organise the multi-indices  $\alpha$  with increasing component  $\alpha_j$ . Note that never both  $\alpha_\delta$  and  $\beta_\delta$  are negative, i.e., if  $\beta_\delta \in [-2, -1]$  in line 2, then  $\alpha_\delta \in [0, p]$  in line 3.

In line 4,  $\beta_j = 0$  holds. Therefore, Lemma A.6a is applicable. Note that the computation of  $K_{\alpha, \beta}$  requires, e.g.,  $K_{\mu(\alpha, j, -2), \beta}$  and  $K_{\mu(\alpha, j, \alpha_j+1), \mu(\beta, j, -1)}$ , which are already determined by the loop.

In line 5, the recursion of Lemma A.6b is performed. Only the case  $\beta_j \leq \alpha_j$  is considered. For  $\beta_j > \alpha_j$  use the symmetry identity from Remark 4.5. Although we are only interested in the coefficients for  $\alpha_j, \beta_j \leq p$ , the double loop in line 5 yields results even for  $\alpha_j > p$ . This is necessary, since, e.g., the case  $\alpha_j = \beta_j = p$  requires coefficients for  $\alpha_j = p+1$  and  $\beta_j = p-1$  (cf. Lemma A.6b).

After terminating the computations for a certain value  $j$  of the loop in line 1, we keep all values  $K_{\alpha, \beta}$  for

$$\begin{aligned} &\alpha_\delta, \beta_\delta \in [-2, p] \text{ and not both } \alpha_\delta, \beta_\delta \text{ negative} && \text{for } 1 \leq \delta \leq j, \\ &(\alpha_\delta, \beta_\delta) \in [0, p] \times [-2, -1] && \text{for } j+1 \leq \delta \leq d. \end{aligned}$$

#### A.4 Coefficients $\xi_{\varkappa,\alpha}$

In Lemma 2.1 we need the coefficients  $\xi_{\varkappa,\alpha}$  for  $0 \leq \varkappa \leq p$ ,  $0 \leq \alpha \leq \varkappa$ . As derived in [9], these values are obtainable by the following algorithm:

```

 $\xi_{0,0} := 1/\sqrt{2};$ 
for  $q := 1$  to  $2p$  do for  $n := 0$  to  $q$  do
begin  $m := q - n;$ 
  if  $n < m$  then  $\xi_{n,m} := 0$  else
    begin  $\xi_{n,m} := \frac{a_{n-1}}{2} (\xi_{n-1,m+1}/a_m + \xi_{n-1,m});$ 
      if  $m > 0$  then  $\xi_{n,m} := \xi_{n,m} + \frac{a_{n-1}}{2} \frac{b_m}{a_m} \xi_{n-1,m-1};$ 
      if  $n \geq 2$  then  $\xi_{n,m} := \xi_{n,m} - b_{n-1} \xi_{n-2,m}$ 
    end
  end
end end;
```

where  $a_n = \frac{\sqrt{2n+3}\sqrt{2n+1}}{n+1}$  and  $b_n = \frac{\sqrt{2n+3}}{\sqrt{2n-1}} \frac{n}{n+1}$  are the factors in the recursion formula  $\Phi_{i,n+1}^\ell(x) = a_n(-1 - 2i + 2x/h_\ell) \Phi_{i,n}^\ell(x) - b_n \Phi_{i,n-1}^\ell(x)$  of the Legendre basis functions.