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The Efficient Computation of Certain Determinants Arising in the Treatment of Schrödinger's Equations

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Abstract

The solution of Schrödinger's equation leads to a high number N of independent variables. Furthermore, the restriction to (anti)symmetric functions implies some complications. We propose a sparse-grid approximation which leads to a set of non-orthogonal basis. Due to the antisymmetry, scalar products are expressed by sums of $N \times N$-determinants. Because of the sparsity of the sparse-grid approximation, these determinants can be reduced from $N \times N$ to a much smaller size $K \times K$. The sums over all permutations reduce to the quantities $\det_K(\alpha_1, \ldots, \alpha_K) := \sum_{1 \le i_1, i_2, \ldots, i_K \le N} \det\left(a^{(\alpha_\beta)}_{i_\alpha, i_\beta}\right)_{\alpha,\beta=1,\ldots,K}$ to be determined, where $a^{(\alpha_\beta)}_{i,j}$ are certain one-dimensional scalar products involving (sparse-grid) basis functions φ_{α_β}. We propose a method to evaluate this expression such that the asymptotics of the computational cost with respect to N is $O(N^3)$ for fixed K, while the storage requirements increase only with the factor N^2. Furthermore, we describe a parallel version (N processors) with full speed up.

AMS Subject Classifications: 65F40, 81-08.

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1. Introduction

The background of our considerations is the numerical treatment of *Schrödinger's equation* characterised by the operator H,

$$H\Phi := -\frac{1}{2}\sum_{i=1}^{N} \triangle_{x_i}\Phi + \sum_{1\le i<j\le N} \frac{\Phi}{|x_i - x_j|} - \sum_{\substack{1\le i\le A \\ 1\le j\le N}} \frac{Q_i\Phi}{|\xi_i - x_j|} + \sum_{1\le i<j\le A} \frac{Q_i Q_j \Phi}{|\xi_i - \xi_j|}. \quad (1.1)$$

Here, $\xi_i \in \mathbb{R}^3, 1 \le i \le A$, are the fixed positions of A nuclei with charges $Q_i \in \mathbb{N}$. The eigenfunction Φ, one is looking for, is a function in $\mathbb{R}^{3N}$, where N is the number of electrons. Because of the *Pauli principle*, the eigenfunctions have to be found in the space of *antisymmetric* functions, i.e.,

$$\Phi(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_N) = -\Phi(x_1, \ldots, x_j, \ldots, x_i, \ldots, x_N) \quad \text{for all } i \ne j. \quad (1.2)$$

Therefore, the particular characteristics of this problem are

1. the high number of independent variables,

2. the subspace of antisymmetric functions.

Readers interested in the quantum mechanics background are referred to the books [12], [13], [4] and the review articles [9], [11]. Symmetry properties of the wave function are discussed in [10].

The standard discretisation technique in quantum chemistry uses basis functions of Gauß type (cf. [8]). The Gaussian basis functions have a number of elegant properties. On the other hand, there are severe disadvantages due to the global support and the missing flexibility in local adaptation. In this paper, we allow the use of finite elements and are therefore faced with other difficulties discussed below.

Concerning Topic 1 from above, we propose to use sparse grids. It turns out that sparse grids are even much cheaper when used for symmetric or antisymmetric functions (see §2.2).

The computational subspace of the Galerkin method will be of the form $f_{sym} * \Phi_{anti}$, where Φ_{anti} is a fixed antisymmetric function, while f_{sym} varies in a symmetrised sparse-grid space. Hence, f_{sym} is spanned by $S\varphi$, where S is the symmetrisation operator explained in Subsection 2 and φ is a product $\prod_{i=1}^{N} \varphi_i(x_i)$ of sparse-grid basis functions φ_i. It is characteristic for Schrödinger's equation that already the computation of the entries of the Galerkin matrix is nontrivial. In this paper we do not discuss the terms arising from the middle sums in (1.1), but concentrate on the simple scalar product

$$\langle S\varphi^I * \Phi_{anti}, S\varphi^{II} * \Phi_{anti} \rangle_{L^2(\mathbb{R}^{3N})} \tag{1.3}$$

arising from the Gram matrix (mass matrix) in the eigenvalue problem. Here we mention that the first term $\sum_{i=1}^{N} \triangle_{x_i} \Phi$ leads to a similar expression (cf. Lemma 2.11). Concerning the underlying product form $f_{sym} * \Phi_{anti}$ we refer to [1].

The difficulty in computing (1.3) is twofold:

(a) Since the symmetrisation operator S involves all permutations, a large sum of single expressions is obtained.

(b) Each single expression is an $N \times N$-determinant.

The precise definition of the problem to be solved is given in Subsection 3.1. The dimension of the symmetric sparse-grid space with L levels is shown to be $O(b^L)$. Therefore, the number of matrix entries is $O(b^{2L})$. The overall computational cost amounts to $O(N^3 b^{2L})$ (see Subsection 4.3), while the parallel version with N processors leads to $O(N^2 b^{2L})$ (see Subsection 4.5). The storage amount is $O(N^2 b^{2L})$ and can be perfectly distributed in the parallel case.

The next Section starts with the notation of symmetric and antisymmetric functions. In the following Subsection §2.2 we discuss the sparse-grid space used in our case. In §2.4 we describe the scalar products of simple product functions. Products of symmetric and antisymmetric functions together with their scalar products are discussed in §2.5.

2. Notations

2.1. Symmetric and Antisymmetric Functions

Let P_N be the set of permutations of $\{1, \ldots, N\}$. A permutation $\sigma \in P_N$ can also viewed as an operator on $L^2(X^N)$ defined by

$$\sigma : f(x_1, \ldots, x_N) \mapsto f(x_{\sigma(1)}, \ldots, x_{\sigma(N)}) =: (\sigma f)(x_1, \ldots, x_N) \quad \text{for } \sigma \in P_N.$$

Here, X is a measurable set (for Schrödinger's equation, $X = \mathbb{R}^3$ is of particular interest) and $L^2(X^N)$ is the set of measurable and square-integrable functions defined on X^N.

Definition 2.1. *$f \in L^2(X^N)$ is called symmetric (notation: $f \in L^2_{sym}(X^N)$), if $f = \sigma f$ for all $\sigma \in P_N$. $f \in L^2(X^N)$ is called antisymmetric (notation: $f \in L^2_{anti}(X^N)$), if $f = \operatorname{sign}(\sigma) * \sigma f$ for all $\sigma \in P_N$.*

The following operators produce symmetric and antisymmetric functions, respectively:

$$S := \sum_{\sigma \in P_N} \sigma, \quad A := \sum_{\sigma \in P_N} \operatorname{sign}(\sigma) * \sigma. \tag{2.1}$$

Scaling by the number $N! = \operatorname{card}(P_N)$ of permutations, one obtains

$$S' := \frac{1}{N!} \sum_{\sigma \in P_N} \sigma, \quad A' := \frac{1}{N!} \sum_{\sigma \in P_N} \operatorname{sign}(\sigma) * \sigma. \tag{2.2}$$

Remark 2.2. *$S' = S'^2$ is a projection onto the subspace $L^2_{sym}(X^N)$ and $A' = A'^2$ is a projection onto the subspace $L^2_{anti}(X^N)$.*

2.2. Sparse Grids

2.2.1. Basic Spaces

Let $\{V_\ell\}_{\ell \in \mathbb{N}_0}$ be a hierarchy of finite dimensional and nested subspaces defined on X (not X^N). In the case of Schrödinger's equation and conforming discretisations, the discretisation is based on a subspace of $H^1(X)$, where $H^1(X)$ is the usual Sobolev space (cf. [6, Chapter 6.2]). Since the functions from V_ℓ will be multiplied by an H^1-function (cf. (1.3)), we require

$$V_0 \subset V_1 \subset \cdots \subset V_{\ell-1} \subset V_\ell \subset \cdots \subset C^1(X). \tag{2.3}$$

We assume that the dimension of V_ℓ increases by a fixed factor. For simplicity, we write

$$\dim V_\ell = b^\ell \tag{2.4}$$

($b = 8$ corresponds to halving the grid size in[1] $X = \mathbb{R}^3$). The following considerations remain true if we replace (2.4) by $\dim V_\ell \le b^\ell$, allowing local refinement. The coarsest space V_0 (with dimension 1) is spanned by the constant function only:

$$V_0 = \operatorname{span}\{1\}. \tag{2.5}$$

2.2.2. Sparse Grids in X^N

Let a level number $L \in \mathbb{N}$ be given, where

$$L \ll N$$

is assumed. The sparse-grid space V_L^{sg} associated with L is

$$V_L^{sg} := \operatorname{span}\left\{ V_{\ell_1} \times V_{\ell_2} \times \cdots \times V_{\ell_N} : \ell_i \in \mathbb{N}_0 \text{ with } \sum_{i=1}^{N} \ell_i = L \right\}.$$

The dimension of $V_{\ell_1} \times V_{\ell_2} \times \cdots \times V_{\ell_N}$ is

$$\dim V_{\ell_1} \cdot \dim V_{\ell_2} \cdots \dim V_{\ell_N} = b^{\ell_1} \cdots b^{\ell_N} = b^{\sum_{i=1}^{N} \ell_i} = b^L.$$

The number of N-tuples $(\ell_1, \dots, \ell_N) \in \mathbb{N}_0^N$ with $\sum_{i=1}^{N} \ell_i = L$ amounts to $\binom{N}{L} = O(N^L)$ for $L \ll N$.

Remark 2.3. *Under the assumption* (2.4), *the sparse-grid dimension is bounded by* $\dim V_L^{sg} \le O(b^L N^L)$.

Since $L = O(\log b^L)$ is only the logarithm of the space dimension $\dim V_L = b^L$, the bound behaves much better than $(\dim V_L)^N$ is the full-grid case, but for large N, the number N^L becomes dangerous.

Concerning literature about sparse-grids, we refer to [14] and [2]. Higher order approximations are discussed in [3].

2.2.3. Sparse Grids for Symmetric Functions in X^N

In the following, we consider a sparse-grid space consisting only of symmetric functions. For this purpose, we make use of the symmetrisation S:

[1] Using sparse grids also in $\mathbb{R}^3$ leads to $b = 2$, while N is to be replaced by $3N$. However, notice that the later mentioned antisymmetry does not hold for the variables in $X = \mathbb{R}^3$.

$$V_L^{symm,sg} := SV_L^{sg} = \operatorname{span}\left\{S(V_{\ell_1} \times V_{\ell_2} \times \cdots \times V_{\ell_N}) : \ell_i \in \mathbb{N}_0 \text{ with } \sum_{i=1}^{N} \ell_i = L\right\}.$$

Since after symmetrisation $V_{\ell_1} \times \cdots \times V_{\ell_i} \times \cdots \times V_{\ell_j} \times \cdots \times V_{\ell_N}$ and $V_{\ell_1} \times \cdots \times V_{\ell_j} \times \cdots \times V_{\ell_i} \times \cdots \times V_{\ell_N}$ lead to identical spaces, the ordering of the level numbers ℓ_i is irrelevant. Without loss of generality, one may order the N-tuples $(\ell_1, \ldots, \ell_N)$ by $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_N$. Hence,

$$V_L^{symm,sg} = \operatorname{span}\left\{S(V_{\ell_1} \times V_{\ell_2} \times \cdots \times V_{\ell_N}) : \ell_i \in \mathbb{N}_0 \text{ with } \sum_{i=1}^{N} \ell_i = L \text{ and } \ell_1 \geq \ell_2 \geq \cdots \geq \ell_N\right\}.$$

The number of N-tuples $(\ell_1, \ldots, \ell_N)$ with this properties is bounded by a constant c_L for all N, as explained below. This together with $\dim V_L^{symm,sg} \leq \sum_{\text{all admissible } N\text{-tuples } (\ell_1,\ldots,\ell_N)} \dim(V_{\ell_1} \times V_{\ell_2} \times \cdots \times V_{\ell_N})$ yields

Remark 2.4. *The symmetric sparse-grid space satisfies* $\dim V_L^{symm,sg} \leq c_L b^L$.

This remark shows that the symmetric sparse-grid functions are optimal for large N. The same holds for antisymmetric functions, since $\dim V_L^{antisymm,sg} < \dim V_L^{symm,sg}$. Here, $V_L^{antisymm,sg}$ is defined as AV_L^{sg} (A from (2.1)).

The constant c_L can be determined as follows. Let $\eta(\ell, L)$ be the number of all sequences $\ell_1 \geq \ell_2 \geq \cdots$ such that $\sum \ell_i = L$ and $\ell_1 \leq \ell$. The induction with respect to L starts with $\eta(\ell, 0) = 1$ (only the zero sequence exists). The recursive definition of η is

$$\eta(\ell, L) = \sum_{k=1}^{\ell} \eta(k, L-k).$$

The right-hand side corresponds to the fact that a sequence starting with $\ell_1 = k$ can be followed by any of the $\eta(k, L-k)$ sequences $\ell_2 \geq \cdots$ with sum $L-k$ and $\ell_2 \leq k$. For *any* N we have

$$\operatorname{card}\left\{\ell_1 \geq \ell_2 \geq \cdots \geq \ell_N \text{ with } \sum_{i=1}^{N} \ell_i = L\right\} \leq \eta(L, L).$$

The bounds $\eta(L, L)$ are given in the table below. The function $\eta(\ell, L)$ is known in number theory as the *partition function* $p_\ell(L)$. Concerning $\eta(L, L)$, the asymptotic behaviour[2]

[2] I thank my colleague Prof. Dr. A. Srivastav (Kiel) for providing this information.

$$\eta(L,L) = \left(\frac{1}{4\sqrt{3}} + o(1)\right)\frac{\exp\left(\pi\sqrt{2L/3}\right)}{L}$$

is described in [7].

However, the estimates by means of $\eta(L,L)$ are too pessimistic. If it happens that $\ell_1 \geq \ell_2 \geq \cdots \geq \ell_N$ contains k identical members $\ell := \ell_{i+1} = \ell_{i+2} = \cdots = \ell_{i+k}$, $\dim S(V_\ell^k)$ is overestimated by $\dim V_\ell^k = (\dim V_\ell)^k$. The exact bound is $\dim S(V_\ell^k) = \mathrm{card}\{(i_1, i_2, \ldots, i_k) \in \{1, \ldots, \dim V_\ell\}^k : i_1 \leq i_2 \leq \cdots \leq i_k\}$, which is approximately $(\dim V_\ell)^k/k!$. Therefore, we should count the equal (non-zero) members in the sequence and divide by their faculty:

$$w(\ell_1 \geq \ell_2 \geq \cdots \geq \ell_N) := \prod_{\alpha=1}^{L} \frac{1}{k_\alpha!}, \text{ where } k_\alpha = \mathrm{card}\{i : \ell_i = \alpha\}.$$

Instead of $\eta(L,L)$, we get the weighted cardinality

$$\eta_w(L) := \sum_{\text{all admissible } N\text{-tuples } (\ell_1,\ldots,\ell_N)} w(\ell_1 \geq \ell_2 \geq \cdots \geq \ell_N) \leq \eta(L,L).$$

The number $c_L * b^L$ can also be interpreted as follows. Let J_ℓ be the indices of the basis functions in V_ℓ (disjoint for different levels ℓ) and set $J := \bigcup_{\ell=0}^{L} J_\ell$. The basis in $V_L^{symm,sg}$ is given by $S(\prod_{i=1}^{N} \varphi_{\alpha_i}(x_i))$ where the indices $\alpha_i \in J$ form a subset of those indices with the side conditions $\sum_{i=1}^{N} level(\alpha_i) = L$ and $level(\alpha_1) \geq level(\alpha_2) \geq \cdots \geq level(\alpha_N)$. Further restrictions hold if equal levels $\ell_{i+1} = \cdots = \ell_{i+k}$ appear. Here, $level(\alpha) = \ell$ is defined by $\alpha \in J_\ell$. The result is stated in the next remark.

Remark 2.5. *The dimension of $V_L^{symm,sg}$ is bounded by the numbers listed in Table 1.*

2.3. Separable Functions

The standard ansatz for function in $L^2(X^N)$ are linear combinations of products of the form $f(x_1, \ldots, x_N) := \prod \varphi_i(x_i) := \varphi_1(x_1) * \cdots * \varphi_N(x_N)$, where the basis functions φ_i belong to any of the spaces V_ℓ. Symmetrisation yields

$$f_{sym} = Sf = \sum_{\sigma \in P_N} \prod_{i=1}^{N} \varphi_i(x_{\sigma(i)}) = \sum_{\sigma \in P_N} \prod_{i=1}^{N} \varphi_{\sigma(i)}(x_i).$$

Table 1. Bounds for the constant c_L in $\dim V_L^{symm,sg} \leq c_L * b^L$

L	1	2	3	4	5	6	7	8	9	10	20	30
$\eta(L,L)$	1	2	3	5	7	11	15	22	30	42	627	5604
$\eta_w(L)$	1	1.5	2.167	3.042	4.175	5.626	7.467	9.781	12.67	16.24	134.7	746.4

Similarly, the antisymmetrisation yields

$$\Phi = Af = \sum_{\sigma \in P_N} \text{sign}(\sigma) * \prod_{i=1}^{N} \varphi_i(x_{\sigma(i)}) = \sum_{\sigma \in P_N} \text{sign}(\sigma) * \prod_{i=1}^{N} \varphi_{\sigma(i)}(x_i).$$

The latter is also called the *Slater determinant*

$$\Phi = \det \begin{bmatrix} \varphi_1(x_1) & \varphi_2(x_1) & \dots & \varphi_N(x_1) \\ \varphi_1(x_2) & \varphi_2(x_2) & \dots & \varphi_N(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_1(x_N) & \varphi_2(x_N) & \dots & \varphi_N(x_N) \end{bmatrix}. \tag{2.6}$$

2.4. Scalar Products

The L^2-scalar product on X^N is denoted by $\langle \cdot, \cdot \rangle_N$:

$$\langle f, g \rangle_N := \int_{X^N} f(x_1, \dots, x_N) \overline{g(x_1, \dots, x_N)} dx_1 \dots dx_N.$$

An obvious result is stated in

Remark 2.6. *$A = A^*$ is selfadjoint, i.e., $\langle Af, g \rangle_N = \langle f, Ag \rangle_N$ for all $f, g \in L^2(X^N)$.*

Product functions $\varphi = \prod_{i=1}^N \varphi_i(x_i)$ and $\psi = \prod_{i=1}^N \psi_i(x_i)$ satisfy $\langle \varphi, \psi \rangle_N = \prod_{i=1}^N \langle \varphi_i, \psi_i \rangle_1$, enabling a reduction to *one-dimensional* integrals. In the case of $A\varphi$ and $A\psi$, one obtains a determinant of one-dimensional expressions.

Lemma 2.7. *Let $\varphi = \prod_{i=1}^N \varphi_i(x_i)$ and $\psi = \prod_{i=1}^N \psi_i(x_i)$. Then*

$$\langle A\varphi, A\psi \rangle_N = N! \det(\langle \varphi_i, \psi_j \rangle_1)_{i,j=1,\dots,N}. \tag{2.7}$$

The proof can be performed by induction over N using the induction hypothesis

$$\langle \varphi, A\psi \rangle_N = \det(\langle \varphi_i, \psi_j \rangle_1)_{i,j=1,\dots,N}. \tag{2.8}$$

Corollary 2.8. *If the function systems $\{\varphi_i\}$ and $\{\psi_i\}$ are biorthonormal (i.e., $\langle \varphi_i, \psi_j \rangle_1 = \delta_{ij}$), we have $\langle A\varphi, A\psi \rangle_N = N!$. The function systems are in particular biorthonormal, if $\varphi_i = \psi_i$ is an orthonormal system.*

2.5. Composition of Symmetric and Antisymmetric Functions

Lemma 2.9. *a) If $f \in L^2_{sym}(X^N)$ and $g \in L^2_{anti}(X^N)$ then $fg \in L^1_{anti}(X^N)$.*

b) Let $f \in L^2(X^N)$ *and* $g = A'g \in L^2_{anti}(X^N)$. *Then* $A'(fg) = (S'f)g$ *is the antisymmetrised product.*

c) Let $f \in L^2_{sym}(X^N)$ *and* $g \in L^2(X^N)$. *Then* $A'(fg) = f(A'g)$ *is the antisymmetrised product.*

In the following, we shall deal with antisymmetric functions of the form

$$(S\varphi) * (A\psi) \quad \text{with } \varphi = \prod_{i=1}^{N} \varphi_i(x_i) \text{ and } \psi = \prod_{i=1}^{N} \psi_i(x_i).$$

Below the scalar product $\langle (S\varphi) * (A\psi), A\hat{\psi} \rangle_N$ with φ, ψ as above and $\hat{\psi} = \prod_{i=1}^{N} \hat{\psi}_i(x_i)$ will be characterised. Due to $A = N!A'$ and the projection property of A', one obtains

$$\left\langle (S\varphi) * (A\psi), A\hat{\psi} \right\rangle_N = N! \left\langle (S\varphi) * (A\psi), \hat{\psi} \right\rangle_N.$$

By definition of S,

$$\begin{aligned} \left\langle (S\varphi) * (A\psi), \hat{\psi} \right\rangle_N &= N! \sum_{\sigma \in P_N} \left\langle \prod_{i=1}^{N} \varphi_{\sigma(i)}(x_i) * (A\psi), \prod_{j=1}^{N} \hat{\psi}_j(x_j) \right\rangle_N \\ &= N! \sum_{\sigma \in P_N} \left\langle A\psi, \prod_{j=1}^{N} \Big(\varphi_{\sigma(j)}(x_j) * \hat{\psi}_j(x_j) \Big) \right\rangle_N \end{aligned}$$

holds. Since the scalar products are of the form (2.8), it follows that

$$\left\langle (S\varphi) * (A\psi), A\hat{\psi} \right\rangle_N = N! \sum_{\sigma \in P_N} \det\Big(\left\langle \psi_i, \varphi_{\sigma(j)} * \hat{\psi}_j \right\rangle_1 \Big)_{i,j=1,\ldots,N}.$$

Similarly, $\langle (S\varphi) * (A\psi), (S\hat{\varphi}) * (A\hat{\psi}) \rangle_N = N! \langle (S\varphi) * (A\psi), (S\hat{\varphi}) * \hat{\psi} \rangle_N$ is treated (cf. Lemma 2.9c). Using $\langle (S\varphi) * (A\psi), (S\hat{\varphi}) * \hat{\psi} \rangle_N = \sum_{\sigma \in P_N} \sum_{\tau \in P_N} \langle A\psi, \prod_{j=1}^{N} (\varphi_{\sigma(j)}(x_j) * \hat{\varphi}_{\tau(j)}(x_j) * \hat{\psi}_j(x_j)) \rangle_N$, one proves

Lemma 2.10. $\langle (S\varphi) * (A\psi), (S\hat{\varphi}) * (A\hat{\psi}) \rangle_N = N! \sum_{\sigma \in P_N} \sum_{\tau \in P_N} \det(\langle \psi_i, \varphi_{\sigma(j)} * \hat{\varphi}_{\tau(j)} * \hat{\psi}_j \rangle_1)_{i,j=1,\ldots,N}$.

Finally, we mention the bilinear form associated with the first term $-\sum_{i=1}^{N} \triangle_{x_i}$ of Schrödinger's operator.

Lemma 2.11. *Define* $\nabla^{(i,j)} (1 \le i, j \le N)$ *as the identity for* $i \ne j$ *while* $\nabla^{(i,i)} := \nabla$ *is the gradient. Then*

$$\sum_{i=1}^{N}\left\langle \nabla_{x_i}(S\varphi) * (A\psi), \nabla_{x_i}(S\hat{\varphi}) * (A\hat{\psi})\right\rangle_N$$
$$= N! \sum_{\sigma\in P_N}\sum_{\tau\in P_N}\sum_{i=1}^{N} \det\left(\left\langle \nabla^{(i,\ell)}(\varphi_{\sigma(\ell)} * \psi_k), \nabla^{(i,\ell)}\left(\hat{\varphi}_{\tau(\ell)} * \hat{\psi}_\ell\right)\right\rangle_1\right)_{k,\ell=1,\dots,N}. \quad (2.9)$$

3. Description of the Problem

3.1. Definition of the Linear Space

We assume that the following data are given:

1. An orthonormal system $\{\phi_1, \dots, \phi_N\} \subset L^2(X)$.

Then

$$\Phi := A\prod_{i=1}^{N}\phi_i(x_i) \quad (3.1)$$

denotes the antisymmetric function generated by $\{\phi_1, \dots, \phi_N\}$. In the case of Schrödinger's equations, a good approximation is given by the solution $\{\phi_1, \dots, \phi_N\}$ of the Hartree-Fock equation (cf. [12]).

2. A family $\{\varphi_\alpha \in L^2(X) : \alpha \in J_\ell\}$ of basis functions of V_ℓ for $0 \le \ell \le L$ (cf. (2.3)).

Usually, the index sets J_ℓ are disjoint; however, in the case of a hierarchical basis $J_{\ell-1} \subset J_\ell$ holds. The basis functions may be of standard finite element type, but one may also think about wavelet basis functions. The union of all (disjoint) index sets is

$$J := \bigcup_{\ell=0}^{L} J_\ell. \quad (3.2)$$

Since Φ will be only a rough approximation of the first eigenfunction of (1.1), we are looking for better approximations contained in the linear space[3]

$$V_L^\Phi := \{f * \Phi : f \in V_L^{symm,sg}\}. \quad (3.3)$$

Obviously, the dimension of this space equals $\dim V_L^{symm,sg}$, which is characterised in Remark 2.4.

In the case of Schrödinger's equation, a typical correction of Φ may be a factor f, where $f(x_1, x_2) = f(|x_1 - x_2|)$ is a function of only two variables due to the interaction of two electrons. The direct approximation of f by $f = \sum a_\alpha\varphi_\alpha$ as a

[3] Instead of one product, one may also introduce the space $V_L^{\Phi_1,\dots,\Phi_M} := \{\sum_{\mu=1}^{M} f_\mu * \Phi_\mu : f_\mu \in V_L^{symm,sg}\}$ based on M different antisymmetric functions (3.1).

function of $x_1 - x_2$ leads to the difficulty that scalar products in $L^2(X^N)$ involving $(Sf) * \Phi$ cannot be reduced to one-dimensional scalar products $\langle \cdot, \cdot \rangle_1$. Therefore, $f(x_1, x_2) = f(|x_1 - x_2|)$ will be approximated by

$$f(x_1, x_2) = S \sum_{\alpha,\beta \in J_\ell} f_{\alpha,\beta} * \varphi_\alpha(x_1) * \varphi_\beta(x_2) + \text{remainder}. \tag{3.4}$$

Since $\varphi_\alpha, \varphi_\beta \in V_\ell$, the sum in (3.4) belongs to the sparse-grid space V_L^{sg} with $L := 2\ell$ (formally we may add the factors $\varphi_0(x_3) = \cdots = \varphi_0(x_N) := 1 \in V_0$; cf. (2.5)). This argument gives an idea how large L should be: The level $\ell = L/2$ should be sufficiently high to yield a small enough remainder in (3.4).

3.2. Galerkin Coefficients

Using the Galerkin method in the space V_L^Φ, already for the Gram matrix (and similarly for the bilinear form corresponding to the Laplace operator) scalar products of the form

$$I_{\alpha\beta;\gamma\delta} := \left\langle S(\varphi_\alpha(x_1) * \varphi_\beta(x_2)) * \Phi, S(\varphi_\gamma(x_1) * \varphi_\delta(x_2)) * \Phi \right\rangle_N \tag{3.5}$$

appear, where the index pairs (α, β) and (γ, δ) correspond to different terms from (3.4). Products of two basis functions as in (3.4) are only particular examples of sparse-grid basis functions. Next, we consider the general case.

3.2.1. General Case

In general, scalar products of the form

$$I := I_{\alpha_1 \ldots \alpha_k; \beta_1 \ldots \beta_\ell} := \left\langle S\left(\prod_{i=1}^{k} \varphi_{\alpha_i}(x_i)\right) * \Phi, S\left(\prod_{j=1}^{\ell} \varphi_{\beta_j}(x_j)\right) * \Phi \right\rangle_N \tag{3.6}$$

occur, where $1 \le k, \ell \le N$. The subscripts $\alpha_i, \beta_j \in J$ are arbitrary indices from J, which are not necessarily different and may belong to different levels. Due to Lemma 2.10,

$$I_{\alpha_1 \ldots \alpha_k; \beta_1 \ldots \beta_\ell} = N! \sum_{\sigma,\tau \in P_N} \det\left(\left\langle \phi_i, \hat{\varphi}_{\sigma(j)} * \check{\varphi}_{\tau(j)} * \phi_j \right\rangle_1\right)_{i,j=1,\ldots,N} \tag{3.7}$$

holds, where

$$\hat{\varphi}_i := \begin{Bmatrix} \varphi_{\alpha_i} & \text{for } 1 \le i \le k \\ 1 & \text{for } k < i \le N \end{Bmatrix}, \quad \check{\varphi}_j := \begin{Bmatrix} \varphi_{\beta_j} & \text{for } 1 \le i \le \ell \\ 1 & \text{for } \ell < i \le N \end{Bmatrix}. \tag{3.8}$$

3.2.2. The Case $k = \ell = 1$

For the convenience of the reader, we discuss the simplest case $k = \ell = 1$ before the general problem is presented in §3.2.3.

For $k = \ell = 1, \hat{\varphi}_1 = \varphi_\alpha$ $(\alpha = \alpha_1)$ and $\check{\varphi}_1 = \varphi_\beta$ $(\beta = \beta_1)$ holds, while $\hat{\varphi}_j = \check{\varphi}_j = 1$ for $j > 1$. The factors $\hat{\varphi}_{\sigma(j)} * \check{\varphi}_{\tau(j)}$ in (3.7) take one of the following four values:

$$\hat{\varphi}_{\sigma(j)} * \check{\varphi}_{\tau(j)} = \begin{cases} \varphi_\alpha\varphi_\beta & \text{for } \sigma(j) = \tau(j) = 1, \\ \varphi_\alpha & \text{for } \sigma(j) = 1, \tau(j) \neq 1, \\ \varphi_\beta & \text{for } \tau(j) = 1, \sigma(j) \neq 1, \\ 1 & \text{otherwise.} \end{cases}$$

This shows that the only interesting fact about the permutation σ is the value $\sigma^{-1}(1)$. The set P_N of permutations can be decomposed into

$$P_N = P_N^{(1)} \cup P_N^{(2)} \cup \cdots \cup P_N^{(N)}, \quad \text{where } P_N^{(v)} := \{\sigma \in P_N : \sigma(v) = 1\}.$$

Remark 3.1. $\#P_N^{(v)} = (N-1)!$ *for* $1 \leq v \leq N$.

The double sum $\sum_{\sigma,\tau\in P_N}$ in (3.7) can be rewritten as $\sum_{v,\mu=1}^N \sum_{\sigma\in P_N^{(v)}} \sum_{\tau\in P_N^{(\mu)}}$. First we consider the case $v = \mu$. Using Remark 3.1, we conclude that

$$I' := N! \sum_{v=1}^N \sum_{\sigma,\tau\in P_N^{(v)}} \det\left(\left\langle \phi_i, \begin{Bmatrix} \varphi_\alpha\varphi_\beta & \text{for } j = v \\ 1 & \text{for } j \neq v \end{Bmatrix} * \phi_j \right\rangle_1\right)_{i,j=1,\ldots,N}$$
$$= N!(N-1)!^2 \sum_{v=1}^N \det\left(\left\langle \phi_i, \begin{Bmatrix} \varphi_\alpha\varphi_\beta & \text{for } j = v \\ 1 & \text{for } j \neq v \end{Bmatrix} * \phi_j \right\rangle_1\right)_{i,j=1,\ldots,N}.$$

Since the system $\{\phi_1, \ldots, \phi_N\} \subset L^2(X)$ is assumed to be orthonormal, the scalar products are $\langle\cdots\rangle_1 = \delta_{ij}$ for $j \neq v$, so that

$$I' = N!(N-1)!^2 \sum_{v=1}^N \det\left(\begin{Bmatrix} \langle\phi_i, \varphi_\alpha\varphi_\beta * \phi_j\rangle_1 & \text{for } j = v \\ \delta_{ij} & \text{for } j \neq v \end{Bmatrix}_{i,j=1,\ldots,N}\right)$$

(δ_{ij}: Kronecker symbol). For fixed v, the $N \times N$-matrix $(\cdots)$ is the identity matrix in which the vth column is replaced by $(\langle\phi_i, \varphi_\alpha\varphi_\beta * \phi_v\rangle_1)_{i=1,\ldots,N}$. Expanding the determinant with respect to this column (or elimination of the column entries for $i \neq v$ by means of the ith column (=unit vector)) yields $\det(\cdots) = \langle\phi_v, \varphi_\alpha\varphi_\beta * \phi_v\rangle_1$; hence,

$$I' = N!(N-1)!^2 \sum_{v=1}^N \langle\phi_v, \varphi_\alpha\varphi_\beta * \phi_v\rangle_1. \tag{3.9}$$

Remark 3.2. *The evaluation of I' requires the computation of N one-dimensional scalar products. The summation needs $O(N)$ operations. If $\varphi_\alpha, \varphi_\beta$ are basis functions with disjoint support, $I' = 0$ holds.*

Finally, we consider the remaining case $\nu \neq \mu$. Then

$$I'' := N! \sum_{\nu=1}^{N} \sum_{\mu\in\{1,\dots,N\}\backslash\nu} \sum_{\sigma\in P_N^{(\nu)}} \sum_{\tau\in P_N^{(\mu)}} \det\left(\left\langle \phi_i, \begin{Bmatrix} \varphi_\alpha & \text{for } j=\nu \\ \varphi_\beta & \text{for } j=\mu \\ 1 & \text{otherwise} \end{Bmatrix} * \phi_j \right\rangle_1\right)_{i,j=1,\dots,N}$$

$$= N!(N-1)!^2 \sum_{\nu} \sum_{\mu\neq\nu} \det\left(\left\langle \phi_i, \begin{Bmatrix} \varphi_\alpha & \text{for } j=\nu \\ \varphi_\beta & \text{for } j=\mu \\ 1 & \text{otherwise} \end{Bmatrix} * \phi_j \right\rangle_1\right)_{i,j=1,\dots,N}$$

$$= N!(N-1)!^2 \sum_{\nu} \sum_{\mu\neq\nu} \det\begin{pmatrix} \langle \phi_i, \varphi_\alpha * \phi_\nu\rangle_1 & \text{for } j=\nu \\ \langle \phi_i, \varphi_\beta * \phi_\mu\rangle_1 & \text{for } j=\mu \\ \delta_{ij} & \text{otherwise} \end{pmatrix}_{i,j=1,\dots,N}.$$

The latter matrix is the identity matrix in which the νth column is replaced by $(\langle \phi_i, \varphi_\alpha * \phi_\nu\rangle_1)_{i=1,\dots,N}$ and the μth column by $(\langle \phi_i, \varphi_\beta * \phi_\mu\rangle_1)_{i=1,\dots,N}$. Elimination by the jth columns ($j \notin \{\nu,\mu\}$) reduces the determinant to the 2×2-determinant

$$\det\begin{pmatrix} \langle \phi_\nu, \varphi_\alpha * \phi_\nu\rangle_1 & \langle \phi_\nu, \varphi_\beta * \phi_\mu\rangle_1 \\ \langle \phi_\mu, \varphi_\alpha * \phi_\nu\rangle_1 & \langle \phi_\mu, \varphi_\beta * \phi_\mu\rangle_1 \end{pmatrix}, \tag{3.10}$$

if $\nu < \mu$. In the case $\nu > \mu$, the indices ν, μ are to be interchanged, but the determinant remains invariant. Finally, the following remark enables a simplification.

Remark 3.3. *Since for $\nu = \mu$ the determinant* (3.10) *contains identical rows, it vanishes and the summation $\sum_\nu \sum_{\mu\neq\nu}$ may be changed into $\sum_{\nu,\mu=1}^N$.*

Hence, the part I'' takes the form

$$I'' = N!(N-1)!^2 \sum_{\nu,\mu=1}^{N} \det\begin{pmatrix} \langle \phi_\nu, \varphi_\alpha * \phi_\nu\rangle_1 & \langle \phi_\nu, \varphi_\beta * \phi_\mu\rangle_1 \\ \langle \phi_\mu, \varphi_\alpha * \phi_\nu\rangle_1 & \langle \phi_\mu, \varphi_\beta * \phi_\mu\rangle_1 \end{pmatrix}. \tag{3.11}$$

Remark 3.4. *The evaluation of I'' requires the computation of $2N^2$ one-dimensional scalar products $\langle \phi_\nu, \varphi_\alpha * \phi_\mu\rangle_1$, $\langle \phi_\nu, \varphi_\beta * \phi_\mu\rangle_1$, $1 \le \nu, \mu \le N$. The summation needs $O(N^2)$ operations.*

Together with the results about I' we obtain the following remark.

Remark 3.5. *In the case of $k = \ell = 1$, the computation of $I_{\alpha;\beta}$ requires the computation of $O(N^2)$ one-dimensional scalar products of the form $\langle \phi_\nu, \varphi * \phi_\mu\rangle_1$ with $\varphi = \varphi_\alpha, \varphi_\beta, \varphi_\alpha * \varphi_\beta$ and further $O(N^2)$ additions. The underlying representation of $I_{\alpha;\beta}$ is*

$$I_{\alpha;\beta} = N!(N-1)!^2 \left(\sum_{\nu=1}^{N} \langle \phi_\nu, \varphi_\alpha \varphi_\beta * \phi_\nu\rangle_1 + \sum_{\nu,\mu=1}^{N} \det\begin{pmatrix} \langle \phi_\nu, \varphi_\alpha * \phi_\nu\rangle_1 & \langle \phi_\nu, \varphi_\beta * \phi_\mu\rangle_1 \\ \langle \phi_\mu, \varphi_\alpha * \phi_\nu\rangle_1 & \langle \phi_\mu, \varphi_\beta * \phi_\mu\rangle_1 \end{pmatrix} \right).$$

In the general case of $k > 1$ or $\ell > 1$, we are not able to obtain an $O(N^2)$ bound for the computational cost. Instead we shall describe an $O(N^3)$-algorithm in §4.

3.2.3. Representation of the Scalar Product in the General Case

Let $\hat{\varphi}_j, \check{\varphi}_j$ as in (3.8). In the general case, the factor in (3.7) for fixed $\sigma, \tau \in P_N$ takes one of the following values:

$$\hat{\varphi}_{\sigma(j)} * \check{\varphi}_{\tau(j)} = \begin{cases} \varphi_{\alpha_{\sigma(j)}} \varphi_{\beta_{\tau(j)}} & \text{for} 1 \le \sigma(j) \le k, 1 \le \tau(j) \le \ell, \\ \varphi_{\alpha_{\sigma(j)}} & \text{for } 1 \le \sigma(j) \le k, \tau(j) > \ell, \\ \varphi_{\beta_{\tau(j)}} & \text{for } \sigma(j) > k, 1 \le \tau(j) \le \ell, \\ 1 & \text{for } \sigma(j) > k, \tau(j) > \ell. \end{cases} \tag{3.12}$$

Here, the important part of the permutation σ is the k-tuple

$$T_I := \sigma^{-1}(1, \ldots, k) := (\sigma^{-1}(1), \ldots, \sigma^{-1}(k)), \tag{3.13}$$

while $T_{II} := \tau^{-1}(1, \ldots, \ell)$ contains the essential properties of τ. Correspondingly, we define the subsets

$$P_N(T_I; k) := \{\sigma \in P_N : \sigma(T_I) = (1, \ldots, k)\},$$
$$P_N(T_{II}; \ell) := \{\tau \in P_N : \tau(T_{II}) = (1, \ldots, \ell)\}$$

of P_N for all k-tuples $T_I \subset \{1, \ldots, N\}^k$ and all ℓ-tuples $T_{II} \subset \{1, \ldots, N\}^\ell$. The summation $\sum_{\sigma \in P_N} \sum_{\tau \in P_N}$ can be replaced by $\sum_{T_I} \sum_{T_{II}} \sum_{\sigma \in P_N(T_I;k)} \sum_{\tau \in P_N(T_{II};\ell)}$, where the first two sums run over all tuples defined above.

While T_I and T_{II} describe tuples (for which the ordering of the components is essential), the corresponding sets are denoted by $M(T_I)$ and $M(T_{II})$:

$$M(T_I) := \{i_\nu : \nu = 1, \ldots, k\} \quad \text{for } T_I = (i_1, \ldots, i_k).$$

For a complete description, we have to consider all possible intersections of $M(T_I)$ and $M(T_{II})$. The dimension of the arising determinants is the largest when $M(T_I) \cap M(T_{II}) = \emptyset$. Therefore, we first discuss this case.

Case of $M(T_I) \cap M(T_{II}) = \emptyset$. Under the condition $M(T_I) \cap M(T_{II}) = \emptyset$, the first case in (3.12) cannot appear, while the second (third) one occurs for $j \in M(T_I) (j \in M(T_{II}))$. The fourth case holds for $j \notin M(T_I) \cup M(T_{II})$. For fixed T_I, T_{II}, we define the (pairwise different) indices

$$j[1], \ldots, j[k], j[k+1], \ldots, j[k+\ell]$$

by concatenating the k-tuple T_I and the ℓ-tuple T_{II}. Hence, the $j[\cdot]$-values are defined by

$$j[\kappa] = \begin{cases} \sigma^{-1}(\kappa) & \text{for } 1 \le \kappa \le k \\ \tau^{-1}(\kappa - k) & \text{for } k+1 \le \kappa \le k+\ell \end{cases}$$

(cf. (3.13)). Again, the determinant in (3.7) is the identity matrix in which all columns corresponding to the indices $j[\kappa], 1 \le \kappa \le k+\ell$, are replaced by

$$\left(\left\langle \phi_i, \omega_\kappa * \phi_{j[\kappa]} \right\rangle_1\right)_{i=1,\dots,N} \quad \text{with } \omega_\kappa = \varphi_{\gamma[\kappa]},$$

$$\gamma[\kappa] := \begin{cases} \alpha_\kappa & \text{for} 1 \le \kappa \le k \\ \beta_{\kappa-k} & \text{for } k+1 \le \kappa \le k+\ell' \end{cases} \tag{3.14}$$

where the properties $\sigma(j[\kappa]) = \kappa$ and $\tau(j[\kappa]) = \kappa - k$ are used.

As in §3.2.2, the $N \times N$-determinant can be reduced to the format $(k+\ell) \times (k+\ell)$:

$$\det\left(\left\langle \phi_{j[\lambda]}, \omega_\kappa * \phi_{j[\kappa]} \right\rangle_1\right)_{\lambda,\kappa=1,\dots,k+\ell}. \tag{3.15}$$

Note that all information about the basis functions $S(\prod_{i=1}^k \varphi_{\alpha_i}(x_i))$ and $S(\prod_{j=1}^\ell \varphi_{\beta_j}(x_j))$ (cf. (3.6)) is expressed by the factors ω_κ $(\kappa = 1, \dots, k+\ell)$.

Remark 3.6. *The ordering of* $j[1], \dots, j[k], j[k+1], \dots, j[k+\ell]$ *or the order in which the indices* λ, κ *in* (3.15) *take the values* $1, \dots, k+\ell$ *is arbitrary, since a simultaneous permutation of the rows and columns does not change the determinant.*

The summation $\sum_{T_I} \sum_{T_{II}} \sum_{\sigma \in P_N(T_I;k)} \sum_{\tau \in P_N(T_{II};\ell)}$ can be replaced by

$$(N-k)!(N-\ell)! \sum_{(j[1],j[2],\dots,j[k+\ell])},$$

where the summation is performed over all pairwise different $(\ell+k)$-tuples $(j[1], j[2], \dots, j[k+\ell]) \in \{1, \dots, N\}^{k+\ell}$. For fixed $T_I = (j[1], \dots, j[k])$, the determinant does not depend on $\sigma \in P_N(T_I;k)$; hence, the summation over $\sigma \in P_N(T_I;k)$ can be replaced by the factor $(N-k)! = \#P_N(T_I;k)$. Analogously, the $P_N(T_{II};\ell)$-summation yields the factor $(N-\ell)! = \#P_N(T_{II};\ell)$.

As in Remark 3.3, we observe that the determinant (3.15) vanishes if $(j[1], j[2], \dots, j[k+\ell])$ contains at least two equal entries. This allows us to include also tuples which are not pairwise different and proves the first part of the following lemma.

Lemma 3.7. *a) Let* ω_κ *be defined as in* (3.14). *The part of* $I_{\alpha_1 \dots \alpha_k; \beta_1 \dots \beta_\ell}$ *corresponding to* $M(T_I) \cap M(T_{II}) = \emptyset$ *(i.e., the sum* (3.7) *taken over all* $\sigma, \tau \in P_N$ *with* $\sigma^{-1}(\varkappa) \neq \tau^{-1}(\lambda)$ *for all* $\varkappa \in \{1, \dots, k\}$, $\lambda \in \{1, \dots, \ell\}$) *is of the form*

$$N!(N-k)!(N-\ell)! \sum_{j[1],j[2],\dots,j[k+\ell]=1}^{N} \det\Big(\Big\langle \phi_{j[\lambda]}, \omega_\kappa * \phi_{j[\kappa]} \Big\rangle_1\Big)_{\lambda,\kappa=1,\dots,k+\ell}. \tag{3.16}$$

b) Denote the sum $\sum_{j[1],j[2],\dots,j[k+\ell]=1}^{N} \det(\cdots)$ *in* (3.16) *by* $D_{k+\ell}(\omega_1,\dots,\omega_{k+\ell})$. *Then* $D_{k+\ell}$ *is a symmetric multi-linear form in* $\omega_1,\dots,\omega_{k+\ell}$, *i.e.,*

$$D_{k+\ell}(\alpha\omega_1' + \beta\omega_1'',\dots,\omega_{k+\ell}) = \alpha D_{k+\ell}(\omega_1',\dots,\omega_{k+\ell}) + \beta D_{k+\ell}(\omega_1'',\dots,\omega_{k+\ell}) \quad \text{for } \alpha,\beta\in\mathbb{C},$$

$$D_{k+\ell}(\dots,\omega_\lambda,\dots,\omega_\kappa,\dots) = D_{k+\ell}(\dots,\omega_\kappa,\dots,\omega_\lambda,\dots).$$

Its normalisation reads $D_{k+\ell}(1,\dots,1) = N^{k+\ell}$.

Proof: The linearity of $D_{k+\ell}$ with respect to each argument follows from its definition in (3.16). Concerning $D_{k+\ell}(\dots,\omega_\lambda,\dots,\omega_\kappa,\dots) = D_{k+\ell}(\dots,\omega_\kappa,\dots,\omega_\lambda,\dots)$ exchange the λth and κth rows and columns in $\det(\langle \phi_{j[\lambda']}, \omega_{\kappa'} * \phi_{j[\kappa']}\rangle_1)_{\lambda',\kappa'=1,\dots,k+\ell}$, which does not change the sign. Since $j[\lambda]$ and $j[\kappa]$ may change their names without altering $\sum_{j[1],j[2],\dots,j[k+\ell]=1}^{N}\det(\cdots)$, symmetry is proved. □

Case of $\#(M(T_I)\cap M(T_{II}))=1$. The sets $M(T_I)$ and $M(T_{II})$ are assumed to overlap by exactly one index, which we denote by b^*. Let $T_I = (j'[1],\dots,j'[k])$, $T_{II} = (j''[1],\dots,j''[\ell])$ and $b^* := j'[\kappa^*] = j''[\lambda^*]$ for some $\kappa^*\in\{1,\dots,k\}$ and $\lambda^*\in\{1,\dots,\ell\}$. We order the $k+\ell-1$ elements of $M(T_I)\cup M(T_{II})$ by

$$\begin{aligned}&(j[1],\dots,j[k+\ell-1])\\ &:= (b^*, j'[1],\dots,j'[\kappa^*-1], j'[\kappa^*+1],\dots,j'[k], j''[1],\dots,j''[\lambda^*-1], j''[\lambda^*+1],\dots,j''[\ell])\end{aligned}$$

(note that by Remark 3.6 the ordering is not essential).

The summation $\sum_{T_I}\sum_{T_{II}}\sum_{\sigma\in P_N(T_I;k)}\sum_{\tau\in P_N(T_{II};\ell)}$ under the side condition $\#(M(T_I)\cap M(T_{II})) = 1$ can be written as

$$(N-k)!(N-\ell)!\sum_{\kappa^*=1}^{k}\sum_{\lambda^*=1}^{\ell}\sum_{(j[1],j[2],\dots,j[k+\ell-1])},$$

where the summations over $P_N(T_I;k)$ and $P_N(T_{II};k)$ are replaced by the factors $(N-k)!$ and $(N-\ell)!$. The summation over $(j[1],\dots,j[k+\ell-1])$ involves all *pairwise disjoint* tuples from $\{1,\dots,N\}^{k+\ell-1}$. The determinants $\det(\langle\phi_{j[a]},\omega_{b,\kappa^*,\lambda^*} * \phi_{j[b]}\rangle_1)_{a,b=1,\dots,k+\ell-1}$ to be summed have the factors

$$\omega_{b,\kappa^*,\lambda^*} = \begin{cases} \varphi_{\alpha_{\kappa^*}} * \varphi_{\beta_{\lambda^*}} & \text{for } b=1 \\ \varphi_{\alpha_{b-1}} & \text{for } 2\le b\le\kappa^* \\ \varphi_{\alpha_b} & \text{for } \kappa^*+1\le b\le k \\ \varphi_{\beta_{b-k}} & \text{for } k+1\le b\le k+\lambda^*-1 \\ \varphi_{\beta_{b-k+1}} & \text{for } k+\lambda^*\le b\le k+\ell-1. \end{cases} \tag{3.17}$$

The dependence of the factors ω on κ^*, λ^* is obvious in the case of $b = 1$. Furthermore, the meaning of $j[1], \ldots, j[k+\ell-1]$ depends on κ^*, λ^*, as seen from the distinction of the cases $b \le \kappa^*$ and $b > \kappa^*$ as well as $b \le k + \lambda^* - 1$ and $b > k + \lambda^* - 1$.

Using again the argument of Remark 3.3, we can also allow tuples $(j[1], j[2], \ldots, j[k+\ell-1])$ which are not pairwise disjoint. This leads to the following result.

Lemma 3.8. *a) Let $\omega_{b,\kappa^*,\lambda^*}$ be defined as in (3.17). The part of $I_{\alpha_1\ldots\alpha_k;\beta_1\ldots\beta_\ell}$ corresponding to tuples T_I, T_{II} with $\#(M(T_I) \cap M(T_{II})) = 1$ is given by the sum*

$$N!(N-k)!(N-\ell)! \sum_{\kappa^*=1}^{k} \sum_{\lambda^*=1}^{\ell} \sum_{j[1],\ldots,j[k+\ell-1]=1}^{N} \det\left(\left\langle \phi_{j[a]}, \omega_{b,\kappa^*,\lambda^*} * \phi_{j[b]} \right\rangle_1\right)_{a,b=1,\ldots,k+\ell-1}. \tag{3.18}$$

b) If $\varphi_\alpha, \varphi_\beta$ are finite element functions, most of the products $\varphi_{\alpha_{\kappa^*}} * \varphi_{\beta_{\lambda^*}}$ vanish because of the disjoint supports $\operatorname{supp} \varphi_\alpha$ *and* $\operatorname{supp} \varphi_\beta$.

In terms of the function $D_{k+\ell-1}$ introduced in Lemma 3.7, the sum $\sum_{j[1],j[2],\ldots,j[k+\ell-1]=1}^{N} \det(\cdots)$ in (3.18) equals $D_{k+\ell-1}(\varphi_{\alpha_{\kappa^*}} * \varphi_{\beta_{\lambda^*}}, \varphi_{\alpha_1}, \ldots, \varphi_{\beta_\ell})$, where $\varphi_{\alpha_{\kappa^*}}$ and $\varphi_{\beta_{\lambda^*}}$ are omitted from the list $\varphi_{\alpha_1}, \ldots, \varphi_{\beta_\ell}$. Because of the symmetry (cf. Lemma 3.7b), the ordering of $(\varphi_{\alpha_{\kappa^*}} * \varphi_{\beta_{\lambda^*}}, \varphi_{\alpha_1}, \ldots, \varphi_{\beta_\ell})$ is arbitrary.

Case of $\#(M(T_I) \cap M(T_{II})) > 1$. If $\#M(T_I) \cap M(T_{II}) > 1$, one obtains similar expression as in (3.16) or (3.18). The determinant is of the format $(k+\ell-m) \times (k+\ell-m)$, where $m := \#(M(T_I) \cap M(T_{II}))$.

4. Reformulated Problem

The expressions (3.16) and (3.18) as well as those arising from (2.9) are of the form $D_K(\psi_1 \ldots, \psi_K)$. In the case of (3.16), we have $K := k + \ell$ and $\psi_\kappa = \omega_\kappa$ defined in (3.14), while in the case of (3.18), $K := k + \ell - 1$ and $(\psi_1 \ldots, \psi_K) = (\varphi_{\alpha_{\kappa^*}} * \varphi_{\beta_{\lambda^*}}, \varphi_{\alpha_1}, \ldots, \varphi_{\beta_\ell})$ (see sentence following Lemma 3.8).

In the next subsections we fix the K-tuple $(\psi_1 \ldots, \psi_K)$. The required entries of the determinants are $a_{ij}^{(\ell)} := \langle \phi_i, \psi_\ell * \phi_j \rangle_1$ $(1 \le \ell \le K,\ 1 \le i, j \le N)$.

4.1. Basic Problem

The function $D_K(\psi_1 \ldots, \psi_K)$ (with fixed $(\psi_1 \ldots, \psi_K)$) is redefined in

Problem 4.1. *Let $N \times N$-matrices $A^{(\ell)} = (a_{ij}^{(\ell)})_{1 \le i,j \le N}$ be given for $\ell = 1, \ldots, K$, where $K \le N$ is a natural number. We abbreviate the K-tuple of matrices by $\mathscr{A} := (A^{(1)}, \ldots, A^{(K)})$. The number to be computed is*

$$\det_K(\mathscr{A}) := \sum_{1\le i_1,i_2,\ldots,i_K\le N} \det\left(a^{(\beta)}_{i_\alpha,i_\beta}\right)_{\alpha,\beta=1,\ldots,K}. \tag{4.1}$$

Note that the $K \times K$-determinants involve columns from different matrices $A^{(\beta)}$. It may happen that some of the matrices $A^{(1)},\ldots,A^{(K)}$ coincide, but we will not exploit this fact.

Remark 4.2. (*a*) *If for some term in* (4.1) *at least two indices* i_γ *coincide* (*i.e.*, $i_\gamma = i_{\gamma'}$ *for* $\gamma \ne \gamma' \in \{1,\ldots,K\}$), *the determinant has two identical rows* ($\alpha = \gamma,\gamma'$) *and vanishes so that* (4.1) *is identical to*

$$\det_K(\mathscr{A}) = \sum_{(i_1,i_2,\ldots,i_K)} \det\left(a^{(\beta)}_{i_\alpha,i_\beta}\right)_{\alpha,\beta=1,\ldots,K}, \tag{4.2}$$

where the sum is taken over all pairwise different *K-tuples* $(i_1,i_2,\ldots,i_K) \in \{1,\ldots,N\}^K$.

(*b*) *For* $a^{(\beta)}_{i_\alpha,i_\beta} := \langle\phi_{j[\alpha]},\omega_\beta * \phi_{j[\beta]}\rangle_1$ $(i_\alpha = j[\alpha], i_\beta = j[\beta])$, *the function in* (4.2) *coincides with the expression* (3.16).

(*c*) *For* $a^{(\beta)}_{i_\alpha,i_\beta} := \langle\phi_{j[\alpha]},\omega_{\beta,\kappa^*,\lambda^*} * \phi_{j[\beta]}\rangle_1$ $(i_\alpha = j[\alpha], i_\beta = j[\beta])$ *with fixed* κ^*,λ^*, *we obtain the sum from* (3.18):

$$\sum_{(j[1],j[2],\ldots,j[k+\ell-1])} \det\left(\left\langle\phi_{j[a]},\omega_{b,\kappa^*,\lambda^*} * \phi_{j[b]}\right\rangle_1\right)_{a,b=1,\ldots,k+\ell-1}.$$

We always assume that K is small compared with N. The idea is that K remains fixed, while $N \to \infty$. The expression $O(\cdot)$ is understood in this sense.

Since the number of the input data is KN^2 (≥ 1 = number of output data), we conclude part a) of

Remark 4.3. *a*) *The lower bound for the complexity of any algorithm computing* $\det_K$ is $O(N^2)$.

b) *The direct evaluation of the right-hand side in* (4.1) *leads to the complexity* $O(N^K)$.

Proof: b) By assumption on K, the cost for the evaluation of $\det(a^{(\beta)}_{i_\alpha,j_\beta})_{\alpha,\beta=1,\ldots,K}$ is $O(1)$, while the number of indices $1 \le i_1,i_2,\ldots,i_K \le N$ amounts to N^K.

4.2. Auxiliary Problems A, B

The following auxiliary problem arises. Let $\mathscr{I}$ be the set of k-tuples

$$I = (\kappa_1,\ldots,\kappa_k) \subset \{1,\ldots,K\}^k \text{ with } \kappa_2 < \cdots < \kappa_k \text{ for arbitrary } k \in \{1,\ldots,K\}.$$

Except the first component, the k-tuples $I \in \mathscr{I}$ are ordered with respect to the size of their components. Finally, let $\mathscr{I}_0$ be the subset of the completely ordered k-tuples, i.e.,

$$\mathscr{I}_0 := \{I \in \mathscr{I} : \kappa_1 < \kappa_2, \text{ if } k = \operatorname{card}(I) \geq 2\}.$$

The Basic Problem 4.1 will occur for the k-tuples $\mathscr{A}(I) := \left(A^{(\kappa_1)}, \ldots, A^{(\kappa_k)}\right)$, i.e., $\det_k(\mathscr{A}(I))$ is to be computed. This defines the first auxiliary problem.

Problem 4.4 (Problem A). *Let* $I = (\kappa_1, \ldots, \kappa_k) \in \mathscr{I}_0$ *and* $k = \operatorname{card}(I)$. *Compute*

$$\det_k(I) := \sum_{1 \leq i_1, i_2, \ldots, i_k \leq N} \det\left(a^{(\kappa_\beta)}_{i_\alpha, i_\beta}\right)_{\alpha,\beta=1,\ldots,k}. \tag{4.3}$$

Besides *Problem A* we have the following auxiliary task.

Problem 4.5 (Problem B). (*a*) *Let* $I = (\kappa_1, \ldots, \kappa_k) \in \mathscr{I}$ *and* $2 \leq k = \operatorname{card}(I) \leq K - 1$. *Further, two indices* $i_1, j_1 \in \{1, \ldots, N\}$ *are given. Compute*

$$\det_k(I; i_1, j_1) := \sum_{1 \leq i_2, \ldots, i_k \leq N} \det\left(a^{(\kappa_\beta)}_{i_\alpha, j_\beta}\right)_{\alpha,\beta=1,\ldots,k}, \quad \text{where } j_\beta := i_\beta \text{ for } \beta = 2, \ldots, k. \tag{4.4}$$

(*b*) *Compute* $\det_k(I; i_1, j_1)$ *for all* $i_1, j_1 \in \{1, \ldots, N\}$ *and all* $I \in \mathscr{I}$ *with* $\operatorname{card}(I) = k$.

Note that the summation in (4.4) involves the $k-1$ indices $i_2, \ldots, i_k$ but not i_1. The connection of both problems is explained in

Remark 4.6. (*a*) *The Basic Problem* 4.1 *is the special case* $\det_K((1, \ldots, K))$ *of Problem A for* $I = (1, \ldots, K)$ *and* $k = K$.

(*b*) $\det_k(I) = \sum_{1 \leq i_1 \leq N} \det_k(I; i_1, i_1)$.

(*c*) *The ordering of the indices* $i_2, \ldots, i_k$ *in* (4.4) *is irrelevant*.

4.3. Simultaneous Solution of Problems A and B

We start the induction at $k = 2$, i.e., with pairs I. The sum in $\det_2(I; i_1, j_1)$ is taken only over $i_2 \in \{1, \ldots, N\}$ and therefore needs $O(N)$ operations per $i_1, j_1 \in \{1, \ldots, N\}$. Note that in Problem A the indices $i_1, j_1 \in \{1, \ldots, N\}$ may be different so that N^2 pairs exist. Thus the computation of $\det_2(I; i_1, j_1)$ for all i_1, j_1 requires $O(N^3)$ operations. Due to the relation mentioned in Remark 4.6b, $\det_2(I)$ can be obtained by N further additions. This proves the following *induction hypothesis* for $k = 2$:

$$\text{Problems A and Bb (for induction variable } k\text{) require } O(N^3) \text{ operations.} \tag{4.5}$$

The computed quantities $\det_2(I; i_1, j_1)$ should be stored for all $i_1, j_1 \in \{1, \ldots, N\}$ together with $\det_2(I)$. Obviously, this leads to the second hypothesis:

$$\text{Problems A and Bb require } O(N^2) \text{ storage size.} \tag{4.6}$$

Since K is a constant, the assertions (4.5) and (4.6) hold also if the *Problems A,B* are posed for *all* k-tuples from $\mathscr{I}$. Since the number of quantities to be computed is $O(N^2)$, the storage size (4.6) follows.

By induction we want to show: If (4.5) holds for $k-1 < K$, then the assertion hold also for k. By Remark 4.6b, the solution of *Problem A* is an $O(N)$-problem as soon as *Problem Bb* is solved. Therefore, only *Problem B* is to be discussed. Consider the determinant $\det(a^{(\kappa_\beta)}_{i_\alpha, j_\beta})_{\alpha,\beta=1,\ldots,k}$, which is one of the terms in (4.4). Expansion by the first column yields

$$\det\left(a^{(\kappa_\beta)}_{i_\alpha, j_\beta}\right)_{\alpha,\beta=1,\ldots,k} = \sum_{\alpha=1,\ldots,k} (-1)^{\alpha+1} a^{(\kappa_1)}_{i_\alpha, j_1} * \det\left(a^{(\kappa_\beta)}_{i_a, j_\beta}\right)_{a=1,\ldots,\alpha-1,\alpha+1,\ldots,k;\ \beta=2,\ldots,k}. \tag{4.7}$$

Case $\alpha = 1$: The summand on the right-hand side has the form $(-1)^{\alpha+1} a^{(\kappa_1)}_{i_1, j_1} * \det(a^{(\kappa_\beta)}_{i_a, j_\beta})_{a,\beta=2,\ldots,k} = a^{(\kappa_1)}_{i_1, j_1} * \det(a^{(\kappa_\beta)}_{i_a, i_\beta})_{a,\beta=2,\ldots,k}$, since $i_\alpha = j_\alpha$ for $\alpha = 2, \ldots, k$. The summation $\sum_{1 \le i_2, \ldots, i_k \le N}$ from (4.4) leads to

$$\begin{aligned} a^{(\kappa_1)}_{i_1, j_1} * \sum_{1 \le i_2, \ldots, i_k \le N} \det\left(a^{(\kappa_\beta)}_{i_a, i_\beta}\right)_{a,\beta=2,\ldots,k} \\ = a^{(\kappa_1)}_{i_1, j_1} * \det_{k-1}(I_1) \quad \text{with } I_1 = (\kappa_\beta)_{\beta=2,\ldots,k}, \end{aligned} \tag{4.8}$$

where by induction $\det_{k-1}(I_1)$ is already computed and stored.

Case $\alpha > 1$: In the following we exploit $i_\alpha = j_\alpha$. The β-indices in det $(a^{(\kappa_\beta)}_{i_a, i_\beta})_{a=1,\ldots,\alpha-1,\alpha+1,\ldots,k;\ \beta=2,\ldots,k}$ must be reordered: In the sequence $\{2, \ldots, k\}$ of the β-values the index α is placed at the top position: $\{\alpha, 2, \ldots, \alpha-1, \alpha+1, \ldots, k\}$. This rearrangement of the columns corresponds to a permutation with sign $(-1)^\alpha$. Hence,

$$\begin{aligned} (-1)^{\alpha+1} \det\left(a^{(\kappa_\beta)}_{i_a, i_\beta}\right)_{a=1,\ldots,\alpha-1,\alpha+1,\ldots,k;\ \beta=2,\ldots,k} \\ = -\det\left(a^{(\kappa_b)}_{i_a, i_b}\right)_{a=1,\ldots,\alpha-1,\alpha+1,\ldots,k;\ b=\alpha,2,\ldots,\alpha-1,\alpha+1,\ldots,k}. \end{aligned} \tag{4.9}$$

After the rearrangement the index tuples $(i_a)_{a=1,\ldots,\alpha-1,\alpha+1,\ldots,k}$ and $(i_b)_{b=\alpha,2,\ldots,\alpha-1,\alpha+1,\ldots,k}$ coincide up to the first component. The $(k-1)$-tuple $I_\alpha := (\kappa_b)_{b=\alpha,2,\ldots,\alpha-1,\alpha+1,\ldots,k}$ belongs to $\mathscr{I}$. If we omit the summation over i_α in $\Sigma_{1 \le i_2, \ldots, i_k \le N}$, we obtain the value $\det_{k-1}(I_\alpha; i_1, i_\alpha)$ which by induction is already determined as a part of *Problem Bb*.

Combining (4.7), (4.8) and (4.9), we are led to

$$\begin{aligned}\det_k(I;i_1,j_1) &= \sum_{1\le i_2,\ldots,i_k\le N} \det\left(a^{(\kappa_\beta)}_{i_\alpha,j_\beta}\right)_{\alpha,\beta=1,\ldots,k}\\ &= a^{(\kappa_1)}_{i_1,j_1} * \det_{k-1}(I_1) - \sum_{\alpha=2,\ldots,k}\sum_{1\le i_\alpha\le N} a^{(\kappa_1)}_{i_\alpha,j_1} * \det_{k-1}(I_\alpha;i_1,i_\alpha). \qquad (4.10)\end{aligned}$$

Obviously, the latter row of this equality can be determined by $O(N)$ operations. Computing these expressions for all $i_1, j_1 \in \{1,\ldots,N\}$, the total cost amounts to $O(N^3)$. Hence, assertion (4.5) is proved by induction.

4.4. Solution Process

In Subsections §4.1–4.3, the computation of $D_K(\psi_1\ldots,\psi_K)$ and of the auxiliary function $D_K(\psi_1\ldots,\psi_K;i,j)$ for a fixed K-tuple is discussed. Here we sketch the overall procedure. However, in order to avoid too complicated notations, we consider only a part of the problem. First, we consider the problem (3.5) characterised by $k=\ell=2$ implying $K=4$. The related products $\varphi_\alpha(x_1)*\varphi_\beta(x_2)$ of sparse grid functions belong to the pair of spaces $(V_\lambda, V_{L-\lambda})$ for $\lambda=1,\ldots,\lfloor L/2\rfloor$. Similarly, $\varphi_\gamma(x_1)*\varphi_\delta(x_2)$ corresponds to $(V_\kappa, V_{L-\kappa})$ for another $\kappa\in\{1,\ldots,\lfloor L/2\rfloor\}$. Second, we fix two values $\lambda,\kappa\in\{1,\ldots,\lfloor L/2\rfloor\}$ and assume $\lambda\le\kappa$. Note that $\lambda>\kappa$ does not appear because of symmetry (cf. Lemma 3.7b). If $\lambda=\kappa$, simplifications are possible (see Remark 4.8a below).

We replace the notation of the basis function φ_α by its index α. The index sets are J_ℓ (cf. (3.2)). Note that $\#J_\ell = \dim V_\ell = b^\ell$. Correspondingly, the function $\det_4(I)$ from Problem A with $I=(1,2,3,4)$ is written as

$$\det_4(\alpha,\beta,\gamma,\delta) = D_4(\varphi_\alpha,\varphi_\beta,\varphi_\gamma,\varphi_\delta) \quad \text{for } \alpha\in J_{L-\lambda}, \beta\in J_{L-\kappa}, \gamma\in J_\lambda, \delta\in J_\kappa. \quad (4.11)$$

The number of cases is $\#J_{L-\lambda} * \#J_{L-\kappa} * \#J_\lambda * \#J_\kappa = b^{2L}$.

Due to Remark 4.6b, all $\det_4(\alpha,\beta,\gamma,\delta)$ can be computed from

$$\det_4(\alpha,\beta,\gamma,\delta;i,i) \quad \text{for } \alpha\in J_{L-\lambda}, \beta\in J_{L-\kappa}, \gamma\in J_\lambda, \delta\in J_\kappa, 1\le i\le N. \qquad (4.12)$$

Here, $\det_4(\alpha,\beta,\gamma,\delta;i,i)$ corresponds to the function $\det_4(I;i,i)$ from Problem B. The number of cases in (4.12) is $N*b^{2L}$.

The computation of $\det_4(\alpha,\beta,\gamma,\delta;i,i)$ by means of (4.10) requires the data $\det_3(\beta,\gamma,\delta)$ and

$$\det_3(\beta,\gamma,\delta;i,j), \det_3(\gamma,\beta,\delta;i,j), \det_3(\delta,\beta,\gamma;i,j) \quad \text{for } \beta\in J_{L-\kappa}, \gamma\in J_\lambda, \delta\in J_\kappa, 1\le i,j\le N. \qquad (4.13)$$

Since $\det_3(\beta,\gamma,\delta)$ can be obtained immediately from $\det_3(\beta,\gamma,\delta;i,i)$, it is not explicitly listed in (4.13).

Remark 4.7. *The function* $\det_K(\alpha_1, \ldots, \alpha_K; i, j)$ *is symmetric with respect to the arguments* $\alpha_2, \ldots, \alpha_K$ (α_1 *must be excluded*). *The corresponding function* $D_K(\varphi_{\alpha_1}, \ldots, \varphi_{\alpha_K}; i, j)$ *is multi-linear.*

The number of data in (4.13) is $3N^2 b^{L+\lambda}$.

Again due to Remark 4.6b, the data in (42) can be computed from $\det_2(\gamma, \delta)$, $\det_2(\beta, \delta)$, $\det_2(\beta, \gamma)$ and

$$\begin{aligned}&\det_2(\gamma, \delta; i, j), \det_2(\delta, \gamma; i, j), \det_2(\beta, \delta; i, j), \det_2(\delta, \beta; i, j),\\ &\quad \det_2(\beta, \gamma; i, j), \det_2(\gamma, \beta; i, j) \quad \text{for all } \beta \in J_{L-\kappa}, \gamma \in J_\lambda, \delta \in J_\kappa, 1 \le i, j \le N. \end{aligned} \tag{4.14}$$

The number of terms is $2N^2 * (b^{\lambda+\kappa} + b^L + b^{L-\kappa+\lambda}) \le 6N^2 b^L$. Each value $\det_2$ can be computed by $O(N)$ operations.

The solution process would run from the bottom to the top. The quantities are to be computed in the order (4.14), (4.13), (4.12) and (4.11).

Remark 4.8. *a*) *If* $\kappa = \lambda$, *the functions* $\det_4(\alpha, \beta, \gamma, \delta; i, i)$ *in* (4.12) *and* $\det_3(\beta, \gamma, \delta; i, j)$ *in* (4.13) *are symmetric with respect to* $\gamma, \delta \in J_\lambda$. *This fact halves the number of cases.*

b) *Another reduction of operations is due to the inclusion* $V_\ell \subset V_{\ell+1}$. *Assume that one of the previous* (*multi-linear*) *functions is already evaluated on* $\cdots \times V_{\ell+1} \times \cdots$, *i.e.*, $\det_K(\ldots, \alpha, \ldots)$ *is computed for all* $\alpha \in J_{\ell+1}$ (*and certain arguments at the place of* "$\ldots$"). *Take any* $\beta \in J_\ell$ *and note that* $\varphi_\beta \in V_\ell$ *can be written as linear combination* $\varphi_\beta = \sum_{\alpha \in J_{\ell+1}} \omega_\alpha \varphi_\alpha$ (*usually the number of non-zero terms is* $O(1)$). *Then*

$$\det_K(\ldots, \beta, \ldots) = \sum_{\alpha \in J_{\ell+1}} \omega_\alpha \det_K(\ldots, \alpha, \ldots)$$

provides a cheap method to evaluate $\det_K$ *in* $\cdots \times V_\ell \times \cdots$.

4.5. Parallelisation

The major part of the computation time and storage is due to the quantities $\det_k(I; i, j)$ or $\det_k(\ldots; i, j)$, respectively, because of the N^2 different pairs (i, j). However, the recursion of $\det_k(\ldots; i, j)$ is easy to parallelise. Formula (4.10) states that $\det_k(\ldots; i, \cdot)$ depends only on $\det_{k-1}(\ldots; i, \cdot)$ for the same $i \in \{1, \ldots, N\}$. Hence, N processors can be used without communication except finally when the data from (4.12) (only $\det_{K-1}(\ldots; i, i)$ for $j = i$) are summed up to the final results in (4.11). Then the overall computing time is $O(Nb^{2L} + N^2 b^{L+\lambda})$ in the example from above. Also the storage is well-distributed among the N processors and amounts to $O(b^{2L} + Nb^{L+\lambda})$ per processor.

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