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Wavelet Approximation in Weighted Sobolev Spaces of Mixed Order with Applications to the Electronic Schrödinger Equation

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Wavelet approximation in weighted Sobolev spaces of mixed order with applications to the electronic Schrödinger equation

Andreas Zeiser*

September 18, 2011

Abstract

We study the approximation of functions in weighted Sobolev spaces of mixed order by anisotropic tensor products of biorthogonal, compactly supported wavelets. As a main result we characterize these spaces in terms of wavelet coefficients which also enables us to explicitly construct approximations. In particular we derive approximation rates for functions in exponentially weighted Sobolev spaces discretized on optimized general sparse grids. Under certain regularity assumptions the rate of convergence is independent of the number of dimensions. We apply these results to the electronic Schrödinger equation and obtain a convergence rate which is independent of the number of electrons; numerical results for the helium atom are presented.

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1 Introduction

Approximating multi-variate functions defined on bounded domains in N dimensions using classical discretization schemes is infeasible for higher dimensions: the number of grid points grows exponentially in the number of dimensions, i.e. n^N, where n is the number of grid points in one dimension. One possible way to overcome these difficulties is to use sparse grids or hyperbolic cross spaces where the complexity reduces to $n(\log n)^{N-1}$ or even n. Such approximation spaces go back to [3, 40] and were studied for example in [29, 14, 48, 41, 15, 30, 22, 23, 38, 25], see also the survey [7] and references therein. Provided that the function possesses in a certain sense more regularity the approximation rate is independent of or up to logarithmic factors independent of the number of dimensions. In particular the functions have to be a member of so-called spaces of dominating mixed smoothness which were first introduced by Nikol′skiĭ and studied by several authors, see the monographs [29, 2, 35] and references therein, as well as the more recent work [43].

Approximating multi-variate functions defined on the *whole space* complicates the situation. In order to obtain an approximation in a finite number of terms one needs further information on the decay of the functions. One possible way to describe such a behavior is to introduce weighted spaces. Combining both requirements leads to weighted Sobolev spaces of mixed order.

In the present work we study the approximation of functions in such spaces by anisotropic tensor products of wavelets. In particular we are interested in the approximation rate which can be achieved. Similar results have been obtained in [24], where only the function itself is square integrable with respect to a polynomial weight function. Approximation results in unweighted Besov-Sobolev-Triebel-Lizorkin spaces of dominating mixed order defined on the whole space have been studied in [25].

In our approach we construct wavelet bases in higher dimensions by building anisotropic tensor-products of a biorthogonal and compactly supported multi-resolution analysis [28] in one or a few variables, see also [23] in the case of a bounded domain. As wavelets one may take Daubechies wavelets [12], the biorthogonal wavelet bases of B-splines [11], as well as orthogonal and piecewise polynomial multi-wavelets [17].

As a central result of this article we characterize weighted Sobolev spaces of mixed order in terms of wavelet coefficients. We restrict ourselves to weight functions which do not vary too much on any cube of fixed size, including weight functions of exponential [36] and polynomial [24] type. In fact these functions are a subset of A_1^{loc}-weights [34]. As a main tool we use localized norms, see for example [42]. A similar result for unweighted Sobolev spaces on a bounded domain has been obtained in [22, 23]. For the more general class of Besov-Sobolev-Triebel-Lizorkin spaces a characterization in terms of wavelets has been studied in the case of unweighted spaces with dominating mixed smoothness in [43] and for weighted spaces in [26], but only in the case of isotropic regularity.

With the help of the equivalent discrete norm we are able to identify potentially important contributions in the wavelet decomposition and are therefore able to construct efficient approximations, see also [23, 25]. In order to obtain quantitative results on the approximation rate we restrict ourselves to a class of weight functions of exponential type. Finally we arrive at a sparse grid in both the spatial coordinate as well as the level of the wavelet. Under certain regularity assumptions one obtains approximation rates which are independent of the number of dimensions. However the constant in the error estimate may depend exponentially on the number of dimensions, which renders the method applicable only for a moderate number of dimensions. In these cases, due to the stability and the compact support of the basis functions, these spaces are a good choice as ansatz spaces for a Galerkin discretization of corresponding operator equations.

Our motivation and main application is the electronic Schrödinger equation, see for example [44] and references therein for an introduction to the subject. Interpreting the regularity result in terms of exponentially weighted Sobolev spaces of mixed order, we can show that the wave functions of bounded states can indeed be approximated at a rate which is independent of the number of electrons. However, again, the constants show an exponential dependence on the number of electrons limiting the applicability of this discretization to the case of small atoms or molecules.

We will proceed along the following line. In Section 2 we will define weighted Sobolev spaces of mixed order and construct localized norms. In Section 3 the norm equivalence between the weighted Sobolev spaces of mixed order and a weighted sum of wavelet coefficients is derived. Based on this norm equivalence convergence rates in the case of an exponential weight functions are derived in Section 4. In the last Section 5 the bounded states of the electronic Schrödinger equation are approximated on an antisymmetrized sparse grid; finally numerical results for the helium ground state are presented.

2 Weighted Sobolev spaces of mixed order

In this section weighted Sobolev spaces of mixed order are defined. Classically weighted Sobolev spaces occur for example in the analysis of elliptic partial differential equations, see for example [27]. In our case, however, we concentrate on functions defined on the whole space, where the weight quantifies the decay property of the function and its derivatives. Such spaces are well known and can also be generalized to weighted Besov- or Triebel-Lizorkin spaces [34]. However isotropic regularity, as treated in the latter work, does not lead to efficient approximations of multi-variate functions. For that reason we combine the idea of weighted spaces with spaces of dominating mixed smoothness that occur naturally in the approximation of multi-variate functions on sparse grids, see for example [29, 2, 35, 43] for the treatment of spaces of dominating mixed smoothness, as well as the survey [7] and references therein. Such spaces were already considered in [24] for the approximation of bounded states of the electronic Schrödinger equation. In addition to the existence of mixed derivatives the function was supposed to be bounded with respect to an L^2-space with polynomial weights.

In our case we define weighted Sobolev spaces of mixed order over a more general class of weight functions, including weights of exponential type. More specifically we consider a subset of A_1^{loc} norms defined in [34]. Besides the function itself also its derivatives up to the given order should also be bounded with respect to the weighted L^2-norm. In our definition we are guided by the regularity results for the bounded states of the electronic Schrödinger equation proved recently in [44], which can be interpreted in terms of these spaces, see Section 5.

Following the definition we construct an equivalent norm on these spaces. Thereby we use the so called localization principle, see for example [42]. As a consequence the weighted norm can be written equivalently as a weighted sum of unweighted norms on overlapping cubes. Later in Section 3 this will be the key for the characterization of these spaces in terms of weighted wavelet coefficients.

2.1 Definition

In the following we define the weighted Sobolev space of mixed order and specify the class of weight functions we will investigate. Though we will later only consider functions defined on the whole space we allow for an arbitrary open subset $\Omega \subset \mathbb{R}^{dN}$. This is because in Subsection 2.2 we will need the corresponding unweighted spaces on cubes for the formulation of the equivalent localized norm. For the definition of spaces of fractional order we use the real interpolation theory first given in [32]. In Appendix A we assembled the main definition as well as references.

In view of the main application, the regularity of bounded states in the electronic Schrödinger equation (Section 5), we partition the coordinate $\vec{\boldsymbol{x}} \in \mathbb{R}^{dN}$ in d-tupels, i.e.

$$\vec{\boldsymbol{x}} = (\boldsymbol{x}_1, \dots, \boldsymbol{x}_N), \quad \boldsymbol{x}_i \in \mathbb{R}^d \quad \text{for } i = 1, \dots, N.$$

In the case mentioned this reflects the fact that $\boldsymbol{x}_i$ is the position of the i-th electron in a three dimensional space ($d = 3$). In our notation N-dimensional variables are marked with an arrow while d-dimensional variables are written in bold. Furthermore we denote by $|\cdot|_p$ the ℓ^p norm, where $1 \leq p \leq \infty$.

Definition 1. Let $d, N \geq 1$, $m, k \in \mathbb{N}$, $\Omega \subset \mathbb{R}^{dN}$ be an open subset and w a positive weight function on Ω. Define the set $A^{k,m} \subset (\mathbb{N}^d)^N$ of multi-indices as

$$A^{k,m} = \big\{ \vec{\boldsymbol{\alpha}}_{\mathrm{mix}} + \vec{\boldsymbol{\alpha}}_{\mathrm{iso}} \;\big|\; \max_{i=1,\dots,N} |\boldsymbol{\alpha}_{\mathrm{mix},i}|_1 \leq k, \, \sum_{i=1}^{N} |\boldsymbol{\alpha}_{\mathrm{iso},i}|_1 \leq m \big\}. \tag{1}$$

The *weighted Sobolev space of mixed order* $H^{k,m}_{\mathrm{mix}}(\Omega, w)$ is given by the set of all measurable functions u such that $\langle u, u \rangle_{\mathrm{mix},w,k,m,\Omega}$ is finite where

$$\langle u, v \rangle_{\mathrm{mix},w,k,m,\Omega} := \sum_{\vec{\boldsymbol{\alpha}} \in A^{k,m}} \int_{\Omega} \partial^{\vec{\boldsymbol{\alpha}}} u(\vec{\boldsymbol{x}}) \partial^{\vec{\boldsymbol{\alpha}}} v(\vec{\boldsymbol{x}}) \; w(\vec{\boldsymbol{x}}) \; \mathrm{d}\vec{\boldsymbol{x}}.$$

Thereby $\langle \cdot, \cdot \rangle_{\mathrm{mix},w,k,m,\Omega}$ defines an inner product on $H^{k,m}_{\mathrm{mix}}(\Omega, w)$, with associated norm $\|\cdot\|_{\mathrm{mix},w,k,m,\Omega}$. For fractional order of smoothness $s \geq 0$ define the space through interpolation theory

$$H^{s,m}_{\mathrm{mix}}(\Omega, w) = \Big[H^{0,m}_{\mathrm{mix}}(\Omega, w), H^{k,m}_{\mathrm{mix}}(\Omega, w) \Big]_{\theta,2} \quad k = \lceil s \rceil, \; \theta = s/k.$$

In this definition, classical unweighted Sobolev spaces $H^s(\Omega)$, $\Omega \subset \mathbb{R}^d$, are included also for fractional s (take $N = 1$ and $m = 0$). In addition one may interpolate once more to obtain mixed spaces with fractional order of isotropic smoothness.

Classically one introduces unweighted Sobolev spaces of mixed order as the intersection of tensor product spaces [22, 23], i.e.

$$H^{s,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N\big) = \bigcap_{i=1}^{N} H^{m \cdot \vec{e}_i + s \cdot \vec{1}}\big((\mathbb{R}^d)^N\big), \quad H^{\vec{t}}\big((\mathbb{R}^d)^N\big) = \bigotimes_{i=1}^{N} H^{t_i}(\mathbb{R}^d) \tag{2}$$

where $\vec{e}_i$ is the i-th unit vector, $\vec{1} = (1, \dots, 1) \in \mathbb{R}^N$. and the tensor product of Hilbert spaces is used [33]. In Appendix A, Corollary 19, it is shown that both definitions are equivalent.

As already mentioned we will need the weighted spaces only in the case of functions defined on the whole space $\mathbb{R}^{dN}$. Furthermore we restrict ourselves to the following class of weight functions.

Definition 2. Let $d, N \geq 1$ and w be a positive weight function on $\mathbb{R}^{dN}$. Then w is called *locally slowly varying* if there exists a constant C_w such that for all $\vec{\boldsymbol{x}}, \vec{\boldsymbol{y}} \in \mathbb{R}^{dN}$ with $|\vec{\boldsymbol{x}} - \vec{\boldsymbol{y}}|_\infty \leq 1$

$$w(\vec{\boldsymbol{y}}) \leq C_w \, w(\vec{\boldsymbol{x}}). \tag{3}$$

In particular the point evaluation of w should be well defined.

For weight function of this type the maximum value inside a cube is bounded by a multiple of the value at the center. Moreover a short calculation directly shows that this is also true for the minimum; more precisely

$$C_w^{-1} \, w(\vec{\boldsymbol{x}}) \leq w(\vec{\boldsymbol{y}}) \leq C_w w(\vec{\boldsymbol{x}})$$

for all $\vec{\boldsymbol{x}}, \vec{\boldsymbol{y}} \in \mathbb{R}^{dN}$ such that $|\vec{\boldsymbol{x}} - \vec{\boldsymbol{y}}|_\infty \leq 1$. Furthermore if one applies the inequality recursively one can proof the existence of a γ dependent on C_w such that

$$w(\vec{\boldsymbol{x}}) \lesssim e^{\gamma |\vec{\boldsymbol{x}}|_\infty}$$

for all $\vec{\boldsymbol{x}} \in \mathbb{R}^{dN}$. Therefore the slowly varying weight functions can only grow exponentially. These kind of functions are a special case of A_1^{loc} weights defined in [34].

2.2 Localized norm

In the following we will derive an equivalent norm on the weighted Sobolev spaces of mixed order. This norm is a weighted sum of unweighted Sobolev norms of mixed order on cubes, where the cubes cover the whole space. This kind of decomposition is called the localization principle, see for example [42]. In order to prove the equivalence we rely on the properties of the slowly varying weight function, see Definition 2.

First let us define the localized norm on the weighted Sobolev spaces of mixed order.

Definition 3. Let $d, N \geq 1$, $m \in \mathbb{N}$, $s \geq 0$ be given and let w be a locally slowly varying weight function on $\mathbb{R}^{dN}$. Define for $\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}$ the cubes

$$Q_{\vec{\boldsymbol{\ell}}} = \left\{ \vec{\boldsymbol{x}} \in \mathbb{R}^{dN} \;\middle|\; |\vec{\boldsymbol{x}} - \vec{\boldsymbol{\ell}}|_\infty < 1 \right\}$$

centered at $\vec{\boldsymbol{\ell}}$ and the norm

$$\|u\|^2_{\text{mix},w,s,m,\text{loc}} = \sum_{\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}} w_{\vec{\boldsymbol{\ell}}} \, \|u\|^2_{\text{mix},s,m,Q_{\vec{\boldsymbol{\ell}}}}, \quad w_{\vec{\boldsymbol{\ell}}} = w(\vec{\boldsymbol{\ell}})$$

for smooth enough functions $u : \mathbb{R}^{dN} \to \mathbb{R}$.

Now for integer order spaces it is easy to see that the so defined norm is equivalent to the original one.

Lemma 4. *Let $d, N \geq 1$, $m, k \in \mathbb{N}$ and w be a locally slowly varying function on $\mathbb{R}^{dN}$. Then the norm equivalence*

$$C_w^{-1}\ \|u\|^2_{\mathrm{mix},w,k,m} \lesssim \|u\|^2_{\mathrm{mix},w,k,m,\mathrm{loc}} \lesssim C_w\ \|u\|^2_{\mathrm{mix},w,k,m}.$$

holds in the space $H^{k,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w\big)$, where C_w is defined in Equation (3)*. The constants are thereby independent of C_w and u.*

Proof. In the first step we prove the left inequality. Since the cubes $\{Q_{\vec{\boldsymbol{\ell}}} \mid \vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}\}$ cover the space $\mathbb{R}^{dN}$

$$\|u\|^2_{\mathrm{mix},w,k,m} \leq \sum_{\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}} \sum_{\vec{\boldsymbol{\alpha}} \in A^{k,m}} \int_{Q_{\vec{\boldsymbol{\ell}}}} |D^{\vec{\boldsymbol{\alpha}}} u(\vec{\boldsymbol{x}})|^2 w(\vec{\boldsymbol{x}})\ \mathrm{d}\vec{\boldsymbol{x}}.$$

Using the Hölder inequality and the properties of the weight function shows the left inequality. In order to show the right inequality note that for all multi-indices $\vec{\boldsymbol{\alpha}} \in A^{k,m}$

$$\sum_{\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}} w_{\vec{\boldsymbol{\ell}}} \int_{Q_{\vec{\boldsymbol{\ell}}}} |D^{\vec{\boldsymbol{\alpha}}} u(\vec{\boldsymbol{x}})|^2\ \mathrm{d}\vec{\boldsymbol{x}} = \int_{\mathbb{R}^{dN}} |D^{\vec{\boldsymbol{\alpha}}} u(\vec{\boldsymbol{x}})|^2 \big[\sum_{\vec{\boldsymbol{\ell}} : \vec{\boldsymbol{x}} \in Q_{\vec{\boldsymbol{\ell}}}} w_{\vec{\boldsymbol{\ell}}} \big]\ \mathrm{d}\vec{\boldsymbol{x}}.$$

Each summand in the square bracket can be estimated by $w_{\vec{\boldsymbol{\ell}}} \leq C_w\ w(\vec{\boldsymbol{x}})$, since $\vec{\boldsymbol{x}}$ and $\vec{\boldsymbol{\ell}}$ differ in the $|\cdot|_\infty$-norm at most by one. Summing up the multi-indices proves the assertion. ◻

To show that also for fractional s both norms are equivalent one uses interpolation theory, see Appendix A.

Theorem 5. *Let $d, N \geq 1$, $m \in \mathbb{N}$, $s \geq 0$ and w be a locally slowly varying weight function on $\mathbb{R}^{dN}$. Then the norm equivalence*

$$C_w^{-1}\ \|u\|^2_{\mathrm{mix},w,s,m} \lesssim \|u\|^2_{\mathrm{mix},w,s,m,\mathrm{loc}} \lesssim C_w\ \|u\|^2_{\mathrm{mix},w,s,m}$$

holds for functions u in $H^{s,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w\big)$, where C_w is defined in Equation (3)*. The constants are thereby independent of C_w and u.*

Proof. In the case of $s \in \mathbb{N}$ Lemma 4 shows the assertion. Otherwise let $k = \lceil s \rceil$, i.e. the smallest integer bigger or equal s, and $\theta = s/k$. The K-functionals

$$\begin{aligned} K^2(t,u) &= \inf_{v \in H^{k,m}_{\mathrm{mix}}\left((\mathbb{R}^d)^N, w\right)} \|u - v\|^2_{\mathrm{mix},w,0,m} + t^2\ \|v\|^2_{\mathrm{mix},w,k,m} \\ K^2(t,u,Q_{\vec{\boldsymbol{\ell}}}) &= \inf_{v \in H^{k,m}_{\mathrm{mix}}(Q_{\vec{\boldsymbol{\ell}}})} \|u - v\|^2_{\mathrm{mix},0,m,Q_{\vec{\boldsymbol{\ell}}}} + t^2\ \|v\|^2_{\mathrm{mix},k,m,Q_{\vec{\boldsymbol{\ell}}}}. \end{aligned}$$

are central in the proof. The first K-functional is used for constructing the norms on $H^{s,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w\big)$ defined on the whole space $\mathbb{R}^{dN}$. The second K-functional leads to unweighted norms on the spaces $H^{s,m}_{\mathrm{mix}}(Q_{\vec{\boldsymbol{\ell}}})$ defined on the cubes $Q_{\vec{\boldsymbol{\ell}}}$, which will be used for the localized norm.

In the first part of the proof we show the right inequality. For all $t \geq 0$ let $v^*(t) \in H^{k,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w\big)$ be a function such that

$$\|u - v^*(t)\|^2_{\mathrm{mix},w,0,m} + t^2 \, \|v^*(t)\|^2_{\mathrm{mix},w,k,m} \leq 2K^2(t,u). \tag{4}$$

It follows that

$$\begin{aligned}
\|u\|^2_{\mathrm{mix},w,s,m,\mathrm{loc}} &= \sum_{\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}} w_{\vec{\boldsymbol{\ell}}} \int_0^\infty t^{-1-2\theta} \, K^2(t,u,Q_{\vec{\boldsymbol{\ell}}}) \, \mathrm{d}t \\
&\leq \sum_{\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}} w_{\vec{\boldsymbol{\ell}}} \int_0^\infty t^{-1-2\theta} \left[\|u - v^*(t)\|^2_{\mathrm{mix},0,m,Q_{\vec{\boldsymbol{\ell}}}} + t^2 \, \|v^*(t)\|^2_{\mathrm{mix},k,m,Q_{\vec{\boldsymbol{\ell}}}} \right] \mathrm{d}t.
\end{aligned}$$

Now due to the Theorem of Monotone Convergence

$$\begin{aligned}
\|u\|^2_{\mathrm{mix},w,s,m,\mathrm{loc}} &\leq \int_0^\infty t^{-1-2\theta} \left[\|u - v^*(t)\|^2_{\mathrm{mix},w,0,m,\mathrm{loc}} + t^2 \, \|v^*(t)\|^2_{\mathrm{mix},w,k,m,\mathrm{loc}} \right] \mathrm{d}t \\
&\lesssim C_w \int_0^\infty t^{-1-2\theta} \left[\|u - v^*(t)\|^2_{\mathrm{mix},w,0,m} + t^2 \, \|v^*(t)\|^2_{\mathrm{mix},w,k,m} \right] \mathrm{d}t,
\end{aligned}$$

where in the second step the norm equivalence of Lemma 4 was used. Using Equation (4) shows the first assertion.

In the second part we show the left inequality. For that purpose let $v^*_{\vec{\boldsymbol{\ell}}}(t) \in H^{k,m}_{\mathrm{mix}}(Q_{\vec{\boldsymbol{\ell}}})$ be given for all $\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}$ and all $t > 0$ such that

$$\|u - v^*_{\vec{\boldsymbol{\ell}}}(t)\|^2_{\mathrm{mix},0,m,Q_{\vec{\boldsymbol{\ell}}}} + t^2 \|v^*_{\vec{\boldsymbol{\ell}}}(t)\|^2_{\mathrm{mix},k,m,Q_{\vec{\boldsymbol{\ell}}}} \leq 2K^2(t,u,Q_{\vec{\boldsymbol{\ell}}}). \tag{5}$$

Furthermore let φ be an infinitely differentiable function such that

$$\varphi_{\vec{\boldsymbol{\ell}}} := \varphi(\cdot - \vec{\boldsymbol{\ell}}), \quad \operatorname{supp}(\varphi_{\vec{\boldsymbol{\ell}}}) \subset Q_{\vec{\boldsymbol{\ell}}}, \quad \vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}$$

forms a partition of unity. The function

$$v^*(t) := \sum_{\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}} \varphi_{\vec{\boldsymbol{\ell}}} v^*_{\vec{\boldsymbol{\ell}}}(t)$$

is an element of $H^{k,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w\big)$, which we will show in the following. Using the properties of the partition of unity and the locally slowly varying weight function gives

$$\|v^*(t)\|^2_{\mathrm{mix},w,k,m} \lesssim \sum_{\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}} \|\varphi_{\vec{\boldsymbol{\ell}}} v^*_{\vec{\boldsymbol{\ell}}}(t)\|^2_{\mathrm{mix},w,k,m} \lesssim \sum_{\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}} w_{\vec{\boldsymbol{\ell}}} \|v^*_{\vec{\boldsymbol{\ell}}}(t)\|^2_{\mathrm{mix},k,m,Q_{\vec{\boldsymbol{\ell}}}}. \tag{6}$$

Here the boundedness of φ and its derivatives was used. Each summand can be estimated by

$$\begin{aligned}
t^2 \, \|v^*_{\vec{\boldsymbol{\ell}}}(t)\|^2_{\mathrm{mix},k,m,Q_{\vec{\boldsymbol{\ell}}}} &\leq 2\, K^2(t,u,Q_{\vec{\boldsymbol{\ell}}}) = 4\theta t^{2\theta} \int_t^\infty \tau^{-1-2\theta} K^2(t,u,Q_{\vec{\boldsymbol{\ell}}}) \, \mathrm{d}\tau \\
&\leq 4\theta t^{2\theta} \int_0^\infty \tau^{-1-2\theta} K^2(\tau,u,Q_{\vec{\boldsymbol{\ell}}}) \, \mathrm{d}\tau = 4\theta t^{2\theta} \|u\|^2_{\mathrm{mix},s,m,Q_{\vec{\boldsymbol{\ell}}}}
\end{aligned}$$

due to the monotonicity of the K-functional. Inserting this inequality in Equation (6) gives the estimate $\|v^*(t)\|^2_{\mathrm{mix},w,k,m} \lesssim \|u\|^2_{\mathrm{mix},w,s,m,\mathrm{loc}}$, where the constant depends on t. Using the estimate $\|u\|^2_{\mathrm{mix},w,s,m,\mathrm{loc}} \lesssim C_w \|u\|^2_{\mathrm{mix},w,s,m}$ of the first part of the proof shows that $v^*(t)$ is an element of $H^{k,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w\big)$ for all $t > 0$. Therefore one can use $v^*(t)$ to estimate the K-functional:

$$\begin{aligned} K^2(t,u) &\leq \|u - v^*(t)\|^2_{\mathrm{mix},w,0,m} + t^2 \|v^*(t)\|^2_{\mathrm{mix},w,k,m} \\ &\lesssim \sum_{\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}} \Big[\big\|\varphi_{\vec{\boldsymbol{\ell}}}\big(u - v^*_{\vec{\boldsymbol{\ell}}}(t)\big)\big\|^2_{\mathrm{mix},w,0,m} + t^2 \|\varphi_{\vec{\boldsymbol{\ell}}} v^*_{\vec{\boldsymbol{\ell}}}(t)\|^2_{\mathrm{mix},w,k,m} \Big], \end{aligned}$$

where we again used the properties of the partition of unity. Now since $\mathrm{supp}(\varphi_{\vec{\boldsymbol{\ell}}}) \subset Q_{\vec{\boldsymbol{\ell}}}$,

$$\begin{aligned} K^2(t,u) &\lesssim C_w \sum_{\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}} w_{\vec{\boldsymbol{\ell}}} \left[\|u - v^*_{\vec{\boldsymbol{\ell}}}(t))\|^2_{\mathrm{mix},0,m,Q_{\vec{\boldsymbol{\ell}}}} + t^2 \|v^*_{\vec{\boldsymbol{\ell}}}(t)\|^2_{\mathrm{mix},k,m,Q_{\vec{\boldsymbol{\ell}}}} \right] \\ &\lesssim C_w \sum_{\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}} w_{\vec{\boldsymbol{\ell}}}\, K^2(t,u,Q_{\vec{\boldsymbol{\ell}}}), \end{aligned}$$

where in the last inequality Equation (5) was used. Hence

$$\|u\|^2_{\mathrm{mix},w,s,m} \lesssim C_w \int_0^\infty t^{-1-2\theta} \big[\sum_{\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}} w_{\vec{\boldsymbol{\ell}}}\, K^2(t,u,Q_{\vec{\boldsymbol{\ell}}}) \big] \,\mathrm{d}t.$$

Finally using the Theorem of Monotone Convergence gives the assertion. □

3 Wavelet characterization of weighted Sobolev spaces of mixed order

In this section we characterize weighted Sobolev spaces of mixed order by a weighted sum of wavelet coefficients. These norm equivalences are later the key for constructing efficient approximations, see Section 4. Due to their localization in space and frequency wavelets are a suitable tool for the study of function spaces, see for example [9, 13] for an introduction to wavelets. Wavelets constitute a stable basis for a wide variety of function spaces, comprising isotropic Sobolev and Besov spaces (see for example [9]), weighted Besov- and Triebel-Lizorkin spaces [26], as well as Sobolev [30, 22, 23] and Besov-Triebel-Lizorkin spaces [43] of mixed order. In this work we study the case of Hilbert spaces with anisotropic smoothness as in [23] combined with weighted norms [26]. However we restrict ourselves to the simpler case of Sobolev spaces and weights given in Definition 2. It remains for future work to extend the obtained results to Besov and Triebel-Lizorkin spaces of mixed order and more general weights.

3.1 Wavelet bases

In this part we construct an anisotropic basis for the dN-dimensional spaces by tensorizing compactly supported biorthogonal wavelets in d dimensions. For $d \geq 1$ assume that two sets of functions in $L^2(\mathbb{R}^d)$

$$\Psi = \big\{ \psi_\lambda \mid \lambda \in \nabla \big\}, \quad \tilde{\Psi} = \big\{ \tilde{\psi}_\lambda \mid \lambda \in \nabla \big\}.$$

are given, where ∇ is a suitable set of indices. The elements $\psi_\lambda \in \Psi$ and $\tilde{\psi}_\lambda \in \tilde{\Psi}$ are called *primal* and *dual wavelets*, respectively. The sets are assumed to be biorthogonal in $L^2(\mathbb{R}^d)$, i.e.

$$\langle \psi_\lambda, \tilde{\psi}_{\lambda'} \rangle_{L^2(\mathbb{R}^d)} = \delta_{\lambda,\lambda'} \quad \lambda, \lambda' \in \nabla.$$

We assume that the multi-indices $\lambda = (\varepsilon, j, \boldsymbol{k}) \in \nabla$ consists of three parts: $\varepsilon \in \{0, 1, \dots, n_\varepsilon\}$ specifies the *type* of function, $j \in \mathbb{N}$ the *level* and $\boldsymbol{k} \in \mathbb{Z}^d$ the *translation*. Each function ψ_λ is then given by

$$\psi_\lambda(\boldsymbol{x}) = 2^{jd/2} \psi^{(\varepsilon)}(2^j \boldsymbol{x} - \boldsymbol{k}), \quad \lambda = (\varepsilon, j, \boldsymbol{k})$$

and analogously also for $\tilde{\psi}_\lambda$. In this way classical constructions like Daubechies wavelets [12], biorthogonal wavelets [11], as well as multi-wavelets like [17] are included.

Furthermore the wavelets are assumed to be uniformly compactly supported, i.e. there exists a constant ξ such that for all $\varepsilon \in \{0, 1, \dots, n_\varepsilon\}$

$$\operatorname{supp} \psi^{(\varepsilon)}, \operatorname{supp} \tilde{\psi}^{(\varepsilon)} \subset B_\xi(0), \tag{7}$$

where $B_r(\boldsymbol{x})$ denotes a ball centered in $\boldsymbol{x}$ with radius r. Consequently the support of the wavelet ψ_λ, $\lambda = (\varepsilon, j, \boldsymbol{k})$, is contained in a ball centered at $\boldsymbol{x}_\lambda = 2^{-j}\boldsymbol{k}$ with radius $2^{-j}\xi$. The term $\boldsymbol{x}_\lambda = 2^{-j}\boldsymbol{k}$ is called the *center* of the wavelet.

In addition we assume that Ψ is a stable basis for a whole range of Sobolev spaces. More precisely we assume that there exits a constant $\tau > 0$ such that for all $0 \le s < \tau$ the norm equivalence

$$\|u\|_s^2 \sim \sum_{\lambda \in \nabla} 2^{2sj(\lambda)} \, |u_\lambda|^2, \quad u_\lambda = \langle \tilde{\psi}_\lambda, u \rangle_{L^2(\mathbb{R}^d)} \tag{8}$$

holds for all $u \in H^s(\mathbb{R}^d)$. Here $j(\lambda)$ gives the level j of a multi index $\lambda = (\varepsilon, j, \boldsymbol{k})$.

The existence of such bases is well known, see for example [9]. Especially the bases mentioned above, i.e. Daubechies wavelets [12], biorthogonal wavelets [11] and the orthogonal multi-wavelets based on B-splines [17], fulfill the prerequisites.

Now given such a set of biorthogonal bases in d variables we construct a biorthogonal set of bases for dN variables. For that purpose define a multi-index $\vec{\lambda} = (\lambda_1, \dots, \lambda_N) \in \nabla^N$ and the corresponding functions

$$\psi_{\vec{\lambda}} = \bigotimes_{i=1}^N \psi_{\lambda_i}, \quad \tilde{\psi}_{\vec{\lambda}} = \bigotimes_{i=1}^N \tilde{\psi}_{\lambda_i}$$

through the tensor product. Then the sets

$$\Psi = \{\psi_{\vec{\lambda}} \mid \vec{\lambda} \in \nabla^N\}, \quad \tilde{\Psi} = \{\tilde{\psi}_{\vec{\lambda}} \mid \vec{\lambda} \in \nabla^N\}$$

are biorthogonal bases in $L^2\big((\mathbb{R}^d)^N\big)$ as can be readily shown. Now the level of a wavelet $\psi_{\vec{\lambda}}$ is given by a vector $\vec{j}(\vec{\lambda}) = \big(j(\lambda_1), \dots, j(\lambda_N)\big)$. Furthermore define the *center* of the wavelet by $\vec{\boldsymbol{x}}_{\vec{\lambda}} = \big(\boldsymbol{x}_{\lambda_1}, \dots, \boldsymbol{x}_{\lambda_N}\big)$.

3.2 Norm equivalence

Having fixed the prerequisites for the wavelet basis in dN variables we will show that these bases are stable for a wide range of weighted Sobolev spaces of mixed order. As a first step we will show that the wavelet coefficients characterize the unweighted Sobolev spaces of mixed order. For that purpose we proceed along the lines of [23] where the case of a bounded domain was studied. The key to the proof is the fact that the unweighted Sobolev spaces of mixed order, Definition 1, can be written as an intersection of tensor product spaces, see Corollary 19. With this result one can proceed as in [23] which leads to the following result.

Theorem 6. *Let $m \in \mathbb{N}$ and $s \geq 0$ be given such that $m + s < \tau$, where τ is the upper bound of the norm equivalence* (8)*. For ease of notation define*

$$\kappa_{\mathrm{mix}}(\vec{\lambda}) = 2^{|\vec{j}(\vec{\lambda})|_1}, \quad \kappa_{\mathrm{iso}}(\vec{\lambda}) = 2^{|\vec{j}(\vec{\lambda})|_\infty}, \quad \kappa_{s,m}(\vec{\lambda}) = \kappa^s_{\mathrm{mix}}(\vec{\lambda}) \cdot \kappa^m_{\mathrm{iso}}(\vec{\lambda})$$

and the discrete norm

$$|||u|||^2_{\mathrm{mix},s,m} = \sum_{\vec{\lambda} \in \nabla^N} \kappa^2_{s,m}(\vec{\lambda})\, |u_{\vec{\lambda}}|^2, \quad u_{\vec{\lambda}} = \langle \tilde{\psi}_{\vec{\lambda}}, u \rangle_{L^2(\mathbb{R}^{dN})}.$$

Then the norm equivalence $\|u\|_{\mathrm{mix},s,m} \sim |||u|||_{\mathrm{mix},s,m}$ holds in the case of unweighted Sobolev space $H^{s,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N\big)$ of mixed order.

Note that in general the constants in the norm equivalence $\|\cdot\|_{\mathrm{mix},s,m} \sim |||\cdot|||_{\mathrm{mix},s,m}$ depend exponentially on the number of dimensions. The factors $\kappa_{\mathrm{mix/iso}}$ correspond to the mixed/isotropic regularity, see also the index set $A^{k,m}$ in Equation (1). In a second step we prove the case of weighted spaces by reducing it to the case of unweighted spaces. This is achieved by using the localized norm of Subsection 2.2 and the compact support of both the primal and dual wavelet.

Theorem 7. *Let $d, N \geq 1$, $m \in \mathbb{N}$ and $s \geq 0$ such that $m + s < \tau$, where τ is the upper bound of the norm equivalence* (8)*. Furthermore let w be a locally slowly varying weight function on $\mathbb{R}^{dN}$. Define the discrete norm*

$$|||u|||^2_{\mathrm{mix},w,s,m} = \sum_{\vec{\lambda} \in \nabla^N} w(\vec{\boldsymbol{x}}_{\vec{\lambda}})\, \kappa^2_{s,m}(\vec{\lambda})\, |u_{\vec{\lambda}}|^2, \quad u_{\vec{\lambda}} = \langle \tilde{\psi}_{\vec{\lambda}}, u \rangle_{L^2(\mathbb{R}^{dN})}.$$

Then the norm equivalence in $H^{s,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w\big)$

$$C_w^{-n_\xi}\, \|u\|^2_{\mathrm{mix},w,s,m} \lesssim |||u|||^2_{\mathrm{mix},w,s,m} \lesssim C_w^{n_\xi}\, \|u\|^2_{\mathrm{mix},w,s,m} \tag{9}$$

holds. Here $n_\xi = \lceil \xi \rceil + 4$, where ξ determines the size of the support of the wavelets, see Equation (7)*.*

Proof. In the first part of the proof we show the left inequality. For that purpose define

$$\nabla_{\vec{\boldsymbol{\ell}}} = \big\{ \vec{\lambda} \in \nabla^N \;\big|\; \mathrm{supp}(\psi_{\vec{\lambda}}) \cap Q_{\vec{\boldsymbol{\ell}}} \neq \emptyset \big\}, \quad \vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN},$$

i.e. the set of all indices, such that the support of the corresponding wavelet intersects the cube $Q_{\vec{\boldsymbol{\ell}}}$. Then

$$\|u\|_{\mathrm{mix},s,m,Q_{\vec{\boldsymbol{\ell}}}} = \Big\| \sum_{\vec{\lambda} \in \nabla_{\vec{\boldsymbol{\ell}}}} u_{\vec{\lambda}} \psi_{\vec{\lambda}} \Big\|_{\mathrm{mix},s,m,Q_{\vec{\boldsymbol{\ell}}}} \leq \Big\| \sum_{\vec{\lambda} \in \nabla_{\vec{\boldsymbol{\ell}}}} u_{\vec{\lambda}} \psi_{\vec{\lambda}} \Big\|_{\mathrm{mix},s,m},$$

where in the last step we used the fact that also the mixed norm of fractional order grows if the domain is increased. Using the norm equivalence from Theorem 6 gives

$$\|u\|^2_{\mathrm{mix},s,m,Q_{\vec{\boldsymbol{\ell}}}} \lesssim \sum_{\vec{\lambda}\in\nabla_{\vec{\boldsymbol{\ell}}}} \kappa^2_{s,m}(\vec{\lambda})\,|u_{\vec{\lambda}}|^2.$$

Summing up all translations $\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}$ with the appropriate weights $w_{\vec{\boldsymbol{\ell}}}$ leads to

$$\|u\|^2_{\mathrm{mix},w,s,m,\mathrm{loc}} \lesssim \sum_{\vec{\lambda}\in\nabla^N} \Big[\sum_{\vec{\boldsymbol{\ell}}:\vec{\lambda}\in\nabla_{\vec{\boldsymbol{\ell}}}} w_{\vec{\boldsymbol{\ell}}}\Big]\,\kappa^2_{s,m}(\vec{\lambda})\,|u_{\vec{\lambda}}|^2.$$

A fixed wavelet index $\vec{\lambda} \in \nabla^N$ is contained only in those index sets $\nabla_{\vec{\boldsymbol{\ell}}}$, where $|\vec{\boldsymbol{x}}_{\vec{\lambda}} - \vec{\boldsymbol{\ell}}|_\infty \le \xi + 1$. Now due to the locally slowly varying weight function it follows that

$$\|u\|^2_{\mathrm{mix},w,s,m,\mathrm{loc}} \lesssim C_w^{\lceil\xi\rceil+1} \sum_{\vec{\lambda}\in\nabla^N} w(\vec{\boldsymbol{x}}_{\vec{\lambda}})\,\kappa^2_{s,m}(\vec{\lambda})\,|u_{\vec{\lambda}}|^2.$$

Using the norm equivalence of Theorem 5 and taking $C_w^{\lceil\xi\rceil+4}$ instead of $C_w^{\lceil\xi\rceil+2}$ for reasons of symmetry ($C_w \ge 1$) one obtains the left inequality.

In the second part we prove the right inequality. Central to the proof is the fact that the projectors $\langle\tilde{\psi}_{\vec{\lambda}}, u\rangle_{L^2(\mathbb{R}^{dN})}$ act only locally due to the compact support of the dual wavelets. Define by

$$\tilde{\nabla}_{\vec{\boldsymbol{\ell}}} = \big\{\vec{\lambda}\in\nabla^N \;\big|\; \vec{\boldsymbol{x}}_{\vec{\lambda}} \in Q_{\vec{\boldsymbol{\ell}}}\big\}, \quad \vec{\boldsymbol{\ell}}\in\mathbb{Z}^{dN}$$

the set of all indices, such that the center $\vec{\boldsymbol{x}}_{\vec{\lambda}}$ of the corresponding wavelet is contained in the cube $Q_{\vec{\boldsymbol{\ell}}}$. Based on these sets define the union of all supports of the corresponding dual wavelets, i.e.

$$\tilde{Q}_{\vec{\boldsymbol{\ell}}} = \bigcup\big\{\operatorname{supp}\tilde{\psi}_{\vec{\lambda}} \;\big|\; \vec{\lambda}\in\tilde{\nabla}_{\vec{\boldsymbol{\ell}}}\big\}.$$

Using the properties of the weight function gives

$$\sum_{\vec{\lambda}\in\tilde{\nabla}_{\vec{\boldsymbol{\ell}}}} w(\vec{\boldsymbol{x}}_{\vec{\lambda}})\,\kappa^2_{s,m}(\vec{\lambda})\,|u_{\vec{\lambda}}|^2 \lesssim C_w \sum_{\vec{\lambda}\in\tilde{\nabla}_{\vec{\boldsymbol{\ell}}}} w_{\vec{\boldsymbol{\ell}}}\,\kappa^2_{s,m}(\vec{\lambda})\,|u_{\vec{\lambda}}|^2, \tag{10}$$

where the coefficients are defined by $u_{\vec{\lambda}} = \langle\tilde{\psi}_{\vec{\lambda}}, u\rangle_{L^2(\mathbb{R}^{dN})}$. Since the dual wavelets $\tilde{\psi}_{\vec{\lambda}}$ have compact support, the coefficients $u_{\vec{\lambda}}$ for $\vec{\lambda}\in\tilde{\nabla}_{\vec{\boldsymbol{\ell}}}$ only depend on the function values of u on $\tilde{Q}_{\vec{\boldsymbol{\ell}}}$. Now construct an infinitely continuous differentiable function φ such that

$$\varphi(\vec{\boldsymbol{x}}) = \begin{cases} 1 & \vec{\boldsymbol{x}}\in\tilde{Q}_{\vec{\boldsymbol{0}}} \\ 0 & \inf_{\vec{\boldsymbol{y}}\in\tilde{Q}_{\vec{\boldsymbol{0}}}} |\vec{\boldsymbol{x}}-\vec{\boldsymbol{y}}|_\infty \ge 1 \end{cases}$$

and define the corresponding translations $\varphi_{\vec{\boldsymbol{\ell}}} = \varphi(\cdot - \vec{\boldsymbol{\ell}})$ for $\vec{\boldsymbol{\ell}}\in\mathbb{Z}^{dN}$. Since $\varphi_{\vec{\boldsymbol{\ell}}}$ is equal to one on $\tilde{Q}_{\vec{\boldsymbol{\ell}}}$

$$u_{\vec{\lambda}} = \langle\tilde{\psi}_{\vec{\lambda}}, \varphi_{\vec{\boldsymbol{\ell}}}\,u\rangle_{L^2(\mathbb{R}^{dN})}, \quad \vec{\lambda}\in\tilde{\nabla}_{\vec{\boldsymbol{\ell}}}$$

for all $\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}$. Inserting this into Equation (10) gives

$$\sum_{\vec{\lambda} \in \tilde{\nabla}_{\vec{\boldsymbol{\ell}}}} w(\vec{\boldsymbol{x}}_{\vec{\lambda}})\, \kappa_{s,m}^2(\vec{\lambda})\, |u_{\vec{\lambda}}|^2 \leq C_w\, w_{\vec{\boldsymbol{\ell}}} \sum_{\vec{\lambda} \in \nabla^N} \kappa_{s,m}^2(\vec{\lambda})\, |\langle \tilde{\psi}_{\vec{\lambda}}, \varphi_{\vec{\boldsymbol{\ell}}}\, u \rangle_{L^2(\mathbb{R}^{dN})}|^2,$$

where the sum has already been extended to all indices $\vec{\lambda} \in \nabla^N$. Now using the norm equivalence for the unweighted case, see Theorem 6, it follows

$$\sum_{\vec{\lambda} \in \tilde{\nabla}_{\vec{\boldsymbol{\ell}}}} w(\vec{\boldsymbol{x}}_{\vec{\lambda}})\, \kappa_{s,m}^2(\vec{\lambda})\, |u_{\vec{\lambda}}|^2 \lesssim C_w\, w_{\vec{\boldsymbol{\ell}}}\, \|\varphi_{\vec{\boldsymbol{\ell}}}\, u\|_{\mathrm{mix},s,m}^2 \lesssim C_w\, w_{\vec{\boldsymbol{\ell}}}\, \|u\|_{\mathrm{mix},s,m,\mathrm{supp}\,\varphi_{\vec{\boldsymbol{\ell}}}}^2,$$

where the Hölder inequality was used. Summing up all $\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}$ gives

$$\sum_{\vec{\lambda} \in \nabla^N} w(\vec{\boldsymbol{x}}_{\vec{\lambda}})\, \kappa_{s,m}^2(\vec{\lambda}) |u_{\vec{\lambda}}|^2 \lesssim C_w \sum_{\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}} w_{\vec{\boldsymbol{\ell}}}\, \|u\|_{\mathrm{mix},s,m,\mathrm{supp}\,\varphi_{\vec{\boldsymbol{\ell}}}}^2.$$

Here we used the fact that each index $\vec{\lambda}$ is contained in only finite many index sets $\tilde{\nabla}_{\vec{\boldsymbol{\ell}}}$. Now we cover $\mathrm{supp}\varphi_{\vec{\boldsymbol{\ell}}}$ with the cubes $Q_{\vec{\boldsymbol{\ell}}}$ and obtain

$$\sum_{\vec{\lambda} \in \nabla^N} w(\vec{\boldsymbol{x}}_{\vec{\lambda}})\, \kappa_{s,m}^2(\vec{\lambda}) |u_{\vec{\lambda}}|^2 \lesssim C_w \sum_{\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}} \Big[\sum_{\vec{\boldsymbol{\ell}}' :\ Q_{\vec{\boldsymbol{\ell}}} \cap \mathrm{supp}\,\varphi_{\vec{\boldsymbol{\ell}}'} \neq \emptyset} w_{\vec{\boldsymbol{\ell}}'} \Big]\, \|u\|_{\mathrm{mix},s,m,Q_{\vec{\boldsymbol{\ell}}}}^2.$$

Due to definition of $\varphi_{\vec{\boldsymbol{\ell}}}$, for fixed $\vec{\boldsymbol{\ell}}$ all indices $\vec{\boldsymbol{\ell}}'$ contained in the sum fulfill $|\vec{\boldsymbol{\ell}} - \vec{\boldsymbol{\ell}}'|_\infty \leq \xi + 2$. Hence

$$\sum_{\vec{\lambda} \in \nabla^N} w(\vec{\boldsymbol{x}}_{\vec{\lambda}})\, \kappa_{s,m}^2(\vec{\lambda}) |u_{\vec{\lambda}}|^2 \lesssim C_w^{\lceil \xi \rceil + 3} \sum_{\vec{\boldsymbol{\ell}} \in \mathbb{Z}^{dN}} w_{\vec{\boldsymbol{\ell}}}\, \|u\|_{\mathrm{mix},s,m,Q_{\vec{\boldsymbol{\ell}}}}^2.$$

Using the norm equivalence of Theorem 5 finishes the proof. □

Again, in general the constants in the norm equivalence depend exponentially on the number of dimensions. This fact will limit the applicability of the discretization scheme to a moderate number of dimensions.

4 Approximation results

In this section we construct approximation spaces for functions in weighted Sobolev spaces of mixed order. In the most general setting let a pair of weighted Sobolev spaces of mixed order $Y \subset X$ be given, where

$$X = H_{\mathrm{mix}}^{s',m'}\big((\mathbb{R}^d)^N, w'\big), \quad Y = H_{\mathrm{mix}}^{s,m}\big((\mathbb{R}^d)^N, w\big)$$

for appropriate orders and weight functions. Given a function $u \in Y$ and a tolerance $\varepsilon > 0$ we want to find an approximation u_ε given by a finite linear combination of wavelets such that the error $\|u - u_\varepsilon\|_X$ measured with respect to the norm on X is below ε. In particular we are interested in the rate of convergence with respect to the terms needed in the linear combination of wavelets. More precisely we want to determine the asymptotic behavior of the quantities

$$E_n = \inf_{\substack{V_n \subset X \\ \dim V_n = n}} \sup_{\|u\|_Y = 1} \inf_{u_n \in V_n} \|u - u_n\|_X$$

describing the approximation error for the best linear space generated by n wavelets for the unit ball in Y. Similar results, also in the case of best n-term approximations, were obtained for example in [41, 15, 30, 22, 23, 25].

For the construction of corresponding approximation spaces we proceed as in [22, 23] leading to optimized sparse grid spaces [6]. In particular we use the norm equivalence derived in the last section to identify the important contributions.

Since the functions are defined on the whole space $\mathbb{R}^{dN}$ one has to assume certain decay properties of the function in order to achieve finite dimensional approximation spaces. In terms of weight functions, w has to increase in a certain sense more rapidly than w'. As a consequence we end up with sparse grid spaces where both the level and the center of the wavelets are restricted simultaneously. Similar approximation results with respect to a redundant set of functions have been obtained in [24], where however only the function itself and not its derivatives decayed in a polynomial sense; see the end of this section for a discussion of this case.

In a first step we will construct approximation spaces for the general problem. Afterwards we determine the rate of convergence only for a certain family of weight functions. In view of our main example, the electronic Schrödinger equation (Section 5), we restrict ourselves to a family of weight functions of exponential type.

We begin with the definition of a general index set of wavelet coefficients for constructing an approximation.

Definition 8. Let $T < 1$ and a function $\rho : \mathbb{R}^{dN} \to \mathbb{R}$ be given. For all $J \geq 0$ define the index set

$$\Lambda_\rho^T(J) = \big\{ \vec{\lambda} \in \nabla^N \;\big|\; -\rho(\vec{\boldsymbol{x}}_{\vec{\lambda}}) - |\vec{j}(\vec{\lambda})|_1 + T|\vec{j}(\vec{\lambda})|_\infty \geq -J + TJ \big\} \tag{11}$$

of wavelet coefficients. The corresponding spaces $\{\psi_{\vec{\lambda}} \,|\, \vec{\lambda} \in \Lambda_\rho^T(J)\}$ are called *optimized general sparse grid spaces.*

One sees that simultaneous restrictions on both the level $\vec{j}(\vec{\lambda})$ and the position $\vec{\boldsymbol{x}}_{\vec{\lambda}}$ of the wavelet are imposed. Based on this index set we construct an approximation and use the norm equivalence of the last section to estimate the accuracy.

Theorem 9. *Let $d, N \geq 1$, $m, m' \in \mathbb{N}$ and $s, s' \geq 0$ such that $s + m, s' + m' < \tau$, where τ is the upper bound of the norm equivalence* (8). *Furthermore assume that $s - s' > m' - m$. Let w' and w be locally slowly varying weight functions. Given a function $u \in H^{s,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w\big)$ define for $J \geq 0$ an approximation*

$$u_J := \sum_{\vec{\lambda} \in \Lambda_\rho^T(J)} u_{\vec{\lambda}}\, \psi_{\vec{\lambda}}, \quad u_{\vec{\lambda}} = \langle \tilde{\psi}_{\vec{\lambda}}, u \rangle_{L^2(\mathbb{R}^{dN})},$$

where the parameters of the index set $\Lambda_\rho^T(J)$, Equation (11)*, are given by*

$$T = \frac{m' - m}{s - s'}, \quad \rho = \frac{\log_2(w/w')}{2\,(s - s')}.$$

Setting $\sigma = (s - s') - (m' - m)$ the error can be bounded by

$$\|u - u_J\|_{\mathrm{mix},w',s',m'} \lesssim C_{w'}^{n_\xi/2}\, C_w^{n_\xi/2}\, 2^{-\sigma J} \|u\|_{\mathrm{mix},w,s,m}$$

asymptotically for $J \to \infty$, where the constants are independent of J, w' and w. Here C_w and $C_{w'}$ are the constants of the locally varying weight functions w and w', see Definition 2, and n_ξ is defined in Theorem 7.

Proof. Using the norm equivalence from Equation (9) it follows from the definition of u_J that

$$\begin{aligned}\|u - u_J\|^2_{\mathrm{mix},w',s',m'} &= \Big\| \sum_{\vec{\lambda} \notin \Lambda_\rho^T(J)} u_{\vec{\lambda}} \psi_{\vec{\lambda}} \Big\|^2_{\mathrm{mix},w',s',m'} \\ &\lesssim C_{w'}^{n_\xi} \sum_{\vec{\lambda} \notin \Lambda_\rho^T(J)} w'(\vec{\boldsymbol{x}}_{\vec{\lambda}})\, \kappa^2_{s',m'}(\vec{\lambda}) |u_{\vec{\lambda}}|^2.\end{aligned}$$

Now the definition of $\Lambda_\rho^T(J)$ implies that

$$\frac{w(\vec{\boldsymbol{x}}_{\vec{\lambda}})\, \kappa^2_{s,m}(\vec{\lambda})}{w'(\vec{\boldsymbol{x}}_{\vec{\lambda}})\, \kappa^2_{s',m'}(\vec{\lambda})} \geq 2^{2\sigma J}, \quad \vec{\lambda} \notin \Lambda_\rho^T(J).$$

Hence

$$\|u - u_J\|^2_{\mathrm{mix},w',s',m'} \lesssim C_{w'}^{n_\xi}\, 2^{-2\sigma J} \sum_{\vec{\lambda} \in \nabla^N} w(\vec{\boldsymbol{x}}_{\vec{\lambda}})\ \kappa^2_{s,m}(\vec{\lambda})\ |u_{\vec{\lambda}}|^2$$

Using the norm equivalence once more proves the assertion. □

The theorem shows that arbitrary accuracy can be achieved provided that J is chosen big enough. Note however that the index set is not universal: for a function $u \in H^{s,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w\big)$ the orders of differentiability s and m as well as the weight function w enter into the definition of the index set $\Lambda_\rho^T(J)$. In the determination of convergence rates this fact is of no importance, whereas in applications one has to estimate the corresponding parameters. However the function to be approximated is often given implicitly as the solution of a corresponding equation. In this case one may use adaptive methods to determine the index set for example by using adaptive wavelet methods [10], even in high space dimensions [37]. In this way one benefits from a possibly higher non-linear approximation rate.

Now in order to determine the approximation rate we have to relate the approximation error to the cardinality of the index set $\Lambda_\rho^T(J)$ as defined in the theorem. For that purpose we have to specify the weight functions w and w'. In view of our main example, the electronic Schrödinger equation (Section 5), we restrict ourselves to a family of weight functions of exponential type. However also for other weight functions, i.e. of polynomial type, one can deduce approximation rates in a similar way.

Definition 10. Let $d, N \geq 1$ and $\gamma > 0$. Define the weight function

$$w_\gamma(\vec{\boldsymbol{x}}) = \prod_{i=1}^N e^{\gamma |\boldsymbol{x}_i|_2}$$

on $\mathbb{R}^{dN}$. For $m \in \mathbb{N}$ and $s \geq 0$ the space $H^{s,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w_\gamma\big)$ is called *exponentially weighted Sobolev space of mixed order*.

It can be directly verified that w_γ is indeed a slowly varying weight function since

$$w_\gamma(\vec{\boldsymbol{y}}) \leq C_\gamma w_\gamma(\vec{\boldsymbol{x}}), \quad C_\gamma = e^{\gamma\sqrt{d}N}. \tag{12}$$

for all $\vec{\boldsymbol{x}}, \vec{\boldsymbol{y}} \in \mathbb{R}^{dN}$ such that $|\vec{\boldsymbol{x}} - \vec{\boldsymbol{y}}|_\infty \leq 1$. Note that the constant C_γ depends exponentially on the number of dimensions.

In the rest of the work we restrict ourselves to the case that both weight functions w and w' are of this type. As only the quotient of both enters into the discussion we can assume without loss of generality that the pair of subspaces is now given by

$$X = H^{s',m'}_{\text{mix}}\big((\mathbb{R}^d)^N\big), \quad Y = H^{s,m}_{\text{mix}}\big((\mathbb{R}^d)^N, w_\gamma\big).$$

for some $\gamma > 0$. Now for this choice the function ρ in the index set $\Lambda^T_\rho(J)$ from Theorem 9 is given by

$$\rho(\vec{\boldsymbol{x}}) = \frac{\gamma \log_2 e}{2(s-s')}\,\rho_1(\vec{\boldsymbol{x}}), \quad \rho_1(\vec{\boldsymbol{x}}) := \sum_{i=1}^N |\boldsymbol{x}_i|_2. \tag{13}$$

In Figure 1 for $N = 2$ and $d = 1$ the sets $\Lambda^T_{\rho_1}(J)$ are sketched for the parameters $T = 0.5, 0, -1$ and $J = 3, 6$. There each dot corresponds to the center of a wavelet. As J increases the region of discretization grows and as well as wavelets of finer levels are included in the sparse grid spaces.

In order to derive approximation rates it remains to estimate the number of elements in $\Lambda^T_\rho(J)$ with respect to the level J. We begin by proving a few preparatory results about combinatorics.

Lemma 11. *Let $j \in \mathbb{N}$. Then*

$$\sharp\big\{\vec{j} \in \mathbb{N}^N \,\big|\, |\vec{j}|_1 = j\big\} \lesssim (j+1)^{N-1} \tag{14}$$

where the constant is independent of j. Furthermore for $0 \leq k \leq j$

$$\sharp\big\{\vec{j} \in \mathbb{N}^N \,\big|\, |\vec{j}|_1 = j,\ |\vec{j}|_\infty = k\big\} \lesssim (j-k+1)^{N-2} \tag{15}$$

and for $k \geq 0$

$$\sharp\big\{\vec{j} \in \mathbb{N}^N \,\big|\, |\vec{j}|_1 = j,\ |\vec{j}|_\infty \leq j/N + k\big\} \lesssim (k+1)^{N-1}, \tag{16}$$

where the constants are independent of j and k.

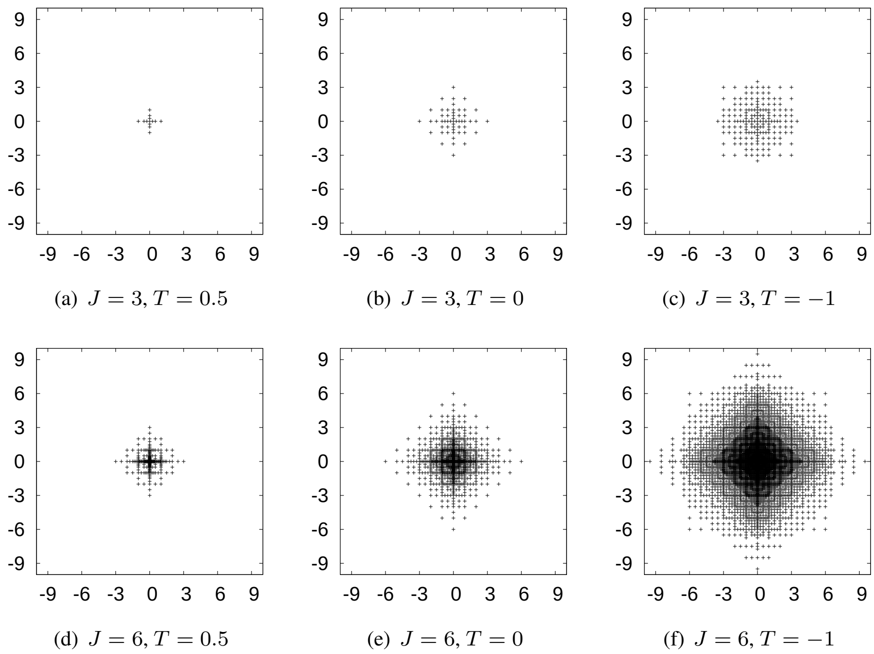
Proof. The first statement directly follows from the number of possibilities for distributing j balls into N places, see also [7].

For the second estimate setting one entry of $\vec{j}$ to k the rest of the entries sum up to $j-k$. Using the last result it follows that there are at most $\lesssim (j-k+1)^{N-2}$ possibilities.

For the last assertion it suffices to take j as a multiple of N. For $k = 0$ all entries of $\vec{j}$ are equal to j/N. Now in order to fulfill $|\vec{j}|_\infty \leq j/N + k$ one may increase ℓ entries, $1 \leq \ell \leq N-1$, at most by k. The total sum of added values, at most ℓk, has to be balanced by the remaining $N-\ell$ entries. Using combinatorics one may estimate the number of elements in the set by

$$\sum_{\ell=1}^{N-1} \binom{N}{\ell} k^\ell \binom{k\ell + (N-\ell) - 1}{(N-\ell)-1} \lesssim \sum_{\ell=1}^{N-1} \binom{N}{\ell} k^\ell\,(k\ell+1)^{N-\ell-1} \lesssim (k+1)^{N-1},$$

which finishes the proof. $\square$



(a) $J = 3, T = 0.5$ (b) $J = 3, T = 0$ (c) $J = 3, T = -1$

(d) $J = 6, T = 0.5$ (e) $J = 6, T = 0$ (f) $J = 6, T = -1$

Figure 1: Sketch of the index sets $\Lambda^T_{\rho_1}(J)$ for $N = 2$, $d = 1$ and the weight ρ_1, Equation (13), for different parameters $T = 0.5, 0, -1$ and $J = 3, 6$. Each dot corresponds to the center of support of a wavelet.

The constant in the last estimate, Equation (16), however depends exponentially on the number of dimensions N. For a discussion see the end of this section. In addition we need the following result.

Lemma 12. *Let $n, m \in \mathbb{N}$, $J \geq 0$ and $\alpha > 0$. Then*

$$\sum_{j=0}^{\lfloor J \rfloor} (j+1)^n \, (J-j+1)^m \, e^{\alpha j} \lesssim J^n e^{\alpha J} \tag{17}$$

for $J \to \infty$, where the constant is independent of J.

Proof. For all $m, n \in \mathbb{N}$

$$\sum_{j=0}^{\lfloor J \rfloor} j^n \, (J-j)^m \, e^{\alpha j} \lesssim \int_0^J x^n \, (J-x)^m \, e^{\alpha x} \, \mathrm{d}x = {}_1F_1(1+n, 2+m+n, \alpha J),$$

where ${}_1F_1$ is the the Kummer confluent hypergeometric function. For $J \to \infty$ the right hand side converges to $m! \, J^n e^{\alpha J}$ [1, Equation 13.1.4]. Now expanding $(j+1)$ and $(J-j+1)$ in Equation (17) into powers of j and $(J-j)$, respectively, the assertion follows. $\square$

Finally we can estimate the cardinality of the index set $\Lambda^T_\rho(J)$ defined in Theorem 9.

Lemma 13. *Let $d, N \geq 1$, $T < 1$ and $\gamma > 0$. Then the number of elements in the index set $\Lambda_\rho^T(J)$ for ρ defined as in Equation* (13) *is given by*

$$\sharp\Lambda_\rho^T(J) \lesssim \gamma^{-dN} \begin{cases} 2^{dJ} & 0 < T < 1 \\ J^{N-1}\, 2^{dJ} & T = 0 \\ 2^{(1-T)/(1-T/N)\, dJ} & T < 0 \end{cases}$$

asymptotically for $J \to \infty$, where the constant is independent of J and γ.

Proof. For a given $\vec{j} \in \mathbb{N}^N$ set $j = |\vec{j}|_1$ and $k = |\vec{j}|_\infty$. A wavelet index $\vec{\lambda}$ with $\vec{j}(\vec{\lambda}) = \vec{j}$ is in the set $\Lambda_\rho^T(J)$ if the center of support $\vec{\boldsymbol{x}}_{\vec{\lambda}}$ satisfies

$$\rho_1(\vec{\boldsymbol{x}}_{\vec{\lambda}}) \leq R_{j,k}^T(J), \quad R_{j,k}^T(J) := \frac{2(s-s')}{\gamma \log_2 e}\, \big[(J-j) - T(J-k)\big].$$

The cardinality of the index set

$$\big\{\vec{\lambda} \in \nabla^N \,\big|\, \vec{j}(\vec{\lambda}) = \vec{j},\ \rho_1(\vec{\boldsymbol{x}}) \leq R_{j,k}^T(J))\big\}$$

can be bounded by

$$\prod_{i=1}^N \sharp\big\{\lambda \in \nabla \,\big|\, j(\lambda_i) = j_i,\ |\boldsymbol{x}_{\lambda_i}|_2 \leq R_{j,k}^T(J)\big\} \lesssim \prod_{i=1}^N \big(R_{j,k}^T(J)+1\big)^d\, 2^{dj_i}.$$

Therefore the number of elements in $\Lambda_\rho^T(J)$ can be estimated by

$$\sharp\Lambda_\rho^T(J) \lesssim \sum_{j,k} \sharp\big\{\vec{j} \,|\, |\vec{j}|_1 = j,\ |\vec{j}|_\infty = k\big\}\, \big(R_{j,k}^T(J)+1\big)^{dN}\, 2^{dj} \tag{18}$$

where the summation runs over appropriate indices j and k. The case $N = 1$ can be readily shown using Lemma 12, hence from now on let $N \geq 2$.

The case $T = 0$: Using Equation (14) gives

$$\sharp\Lambda_\rho^0(J) \lesssim \sum_{j=0}^{\lfloor J \rfloor} (j+1)^{N-1}\, \gamma^{-dN}\, (J-j+1)^{dN}\, 2^{dj} \lesssim \gamma^{-dN}\, J^{N-1} 2^{dJ},$$

where in the second step Lemma 12 was applied.

The case $0 < T < 1$: Since $\rho \geq 0$ it follows from Equation (11) that the summation indices j, k in Equation (18) are restricted by

$$0 \leq j \leq J \ \text{ and } \ \max\big(J - \frac{J-j}{T},\ j/N\big) \leq k \leq j.$$

Now in the lower bound of k the first term in the maximum is active if

$$j \geq \frac{1-T}{1-T/N}\, J = \tilde{J}.$$

We split the summation in Equation (18) according to

$$\sum_{j=0}^{\lceil \tilde{J} \rceil - 1} \sum_{k=\lceil j/N \rceil}^{j} + \sum_{j=\lceil \tilde{J} \rceil}^{\lfloor J \rfloor} \sum_{k=\lceil J-(J-j)/T \rceil}^{j}.$$

Based on Equation (15) and Lemma 12 we crudely estimate the first sum by

$$\lesssim \sum_{j=0}^{\lceil \tilde{J} \rceil -1} \sum_{k=\lceil j/N \rceil}^{j} (j-k+1)^{N-2} \gamma^{-dN} (J-j+1)^{dN} 2^{dj} \lesssim \gamma^{-dN} J^{(d+1)N} 2^{d\tilde{J}}$$

and finally by $\lesssim \gamma^{-dN} 2^{dJ}$ since $J > \tilde{J}$. Here we bounded $R^T_{j,k}(J) \lesssim \gamma^{-1}(J-j)$. For the second sum

$$\sum_{j=\lceil \tilde{J} \rceil}^{\lfloor J \rfloor} \sum_{k=\lceil J-(J-j)/T \rceil}^{j} (j-k+1)^{N-2} \gamma^{-dN} (J-j+1)^{dN} 2^{dj}$$

we use a finer estimate for the sum over k:

$$\sum_{k=\lceil J-(J-j)/T \rceil}^{j} (j-k+1)^{N-2} \lesssim \Big[j - \big(J - \frac{J-j}{T}\big) + 1 \Big]^{N-1} \lesssim (J-j+1)^{N-1}.$$

Applying Lemma 12 proves the second case.

The case $T < 0$: In this case the summation indices in Equation (18) are restricted by

$$0 \le j \le \frac{1-T}{1-T/N} J =: \bar{J}, \quad j/N \le k \le \min\big(j, J - \frac{J-j}{T}\big).$$

In the upper bound of k the second term in the minimum is active if $j \ge J$. Now the summation over the indices j and k in Equation (18) is split according to

$$\sum_{j=0}^{\lceil J \rceil -1} \sum_{k=\lceil j/N \rceil}^{j} + \sum_{j=\lceil J \rceil}^{\lfloor \bar{J} \rfloor} \sum_{k=\lceil j/N \rceil}^{\lfloor J-(J-j)/T \rfloor}.$$

Proceeding as in the case $0 < T < 1$ the first sum can be bounded by $2^{d\bar{J}}$ since $\bar{J} > J$. In the second sum the index k is restricted by

$$\frac{j}{N} \le k \le J - \frac{J-j}{T} = \frac{j}{N} + (\bar{J} - j)\Big(\frac{1}{N} - \frac{1}{T}\Big).$$

Using Equation (16) the second sum can therefore be bounded by

$$\lesssim \sum_{j=\lceil J \rceil}^{\lfloor \bar{J} \rfloor} \sum_{k=\lceil j/N \rceil}^{\lfloor J-(J-j)/T \rfloor} (\bar{J}-j+1)^{N-1} \gamma^{-dN} \big[(J-j) - T(J-k) + 1\big]^{dN} 2^{dj}.$$

The summation over k gives

$$\sum_{k=\lceil j/N \rceil}^{\lfloor J-(J-j)/T \rfloor} \big[(J-j) - T(J-k) + 1\big]^{dN} \lesssim \big[(J-j) - T(J-j/N) + 1\big]^{dN+1}$$
$$\lesssim (\bar{J}-j+1)^{dN+1}.$$

Applying Lemma 12 once more finishes the proof. □

Combining the error estimate and the bound on the number of degrees of freedom we finally can evaluate the approximation rate.

Theorem 14. *Let $d, N \geq 1$, $\gamma > 0$, $m, m' \in \mathbb{N}$ and $s', s \geq 0$ such that $s'+m', s+m < \tau$, where τ is the upper bound of the norm equivalence* (8)*. Furthermore assume that $s - s' > m' - m$. Given a function $u \in H^{s,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N, w_\gamma\big)$ for each $\varepsilon > 0$ there exists a finite linear combination u_ε of functions $\{\psi_{\vec{\lambda}} \mid \vec{\lambda} \in \nabla^N\}$ of the form given in Theorem 9 such that*

$$\|u - u_\varepsilon\|_{\mathrm{mix},s',m'} \leq \varepsilon \, \|u\|_{\mathrm{mix},w_\gamma,s,m}. \tag{19}$$

Set

$$\sigma = (s - s') - (m' - m), \quad \beta = \frac{1-T}{1-T/N}, \quad T = \frac{m'-m}{s-s'}.$$

Then asymptotically the number of summands in u_ε can be bounded by

$$\sharp u_\varepsilon \lesssim \gamma^{-dN} \begin{cases} C_\gamma^{dn_\xi/(2\sigma)} \; \varepsilon^{-d/\sigma} & m' > m \\ C_\gamma^{dn_\xi/(2\sigma)} \; |\log \varepsilon|^{N-1} \; \varepsilon^{-d/\sigma} & m' = m \\ C_\gamma^{\beta dn_\xi/(2\sigma)} \; \varepsilon^{-\beta d/\sigma} & m' < m \end{cases}$$

for $\varepsilon \to 0$, where the constants are independent of ε and γ. Here n_ξ is defined in Theorem 7 and C_γ in Equation (12)*.*

Proof. Theorem 9 applied to the present situation gives an error bound

$$\|u - u_J\|_{\mathrm{mix},s',m'} \lesssim C_\gamma^{n_\xi/2} \, 2^{-\sigma J} \|u\|_{\mathrm{mix},w_\gamma,s,m}.$$

Denote by c the constant in the inequality which is a multiple of $C_\gamma^{n_\xi/2}$. Now let $u_\varepsilon = u_J$ with $J = (-\log_2 \varepsilon + \log_2 c)/\sigma$. Then Equation (19) is fulfilled and the number of elements can then be estimated using Lemma 13 which shows the assertion. ☐

Solving for the degrees of freedom n gives the estimate

$$\|u - u_n\|_{\mathrm{mix},s,m} \lesssim \begin{cases} n^{-\sigma/d} & m' > m \\ (\log n)^{\sigma(N-1)} \cdot n^{-\sigma/d} & m' = m \\ n^{-\sigma/(\beta d)} & m' < m \end{cases} \tag{20}$$

where u_n denotes an approximation with n terms. As a consequence the approximation rate for the case $m' > m$ is independent of the number of dimensions N and deteriorates only by a logarithmic factor for the case $m' = m$. In the case $T \to -\infty$, i.e. no additional mixed smoothness, the approximation rate $dN/(m - m')$ of classical approximation schemes is recovered.

Note however that the constants in Theorem 14 might depend exponentially on the number of dimensions. This unfavorable scaling is rooted on the one hand in the constants in norm equivalence, Theorem 7, and on the other hand in the estimate of the cardinality of the index. Moreover even the mixed norm might grow exponentially in the number of dimensions, like in the case of normalized Gaussian functions. This limits the applicability of the discretization scheme to a moderate number of dimensions.

Despite the unbounded domain the approximation rates equal those for the bounded domain obtained in [23]. In our case $1/\gamma$ plays the role of a characteristic length scale in real space. In contrast to [23], however, we did not study negative differential orders and only integer orders of isotropic smoothness. The latter restriction can be removed by using interpolation theory once more.

Similar approximation results for the unbounded domain have been obtained in [24]. There a function in a Sobolev space of mixed order was approximated, where only the function itself decays in a polynomial sense. More precisely u satisfies

$$\|u\|^2_{H^{s,m}_{\mathrm{mix}}((\mathbb{R}^d)^N)} + \|u\|^2_{L^2((\mathbb{R}^d)^N,w)} < \infty, \quad w(\vec{\boldsymbol{x}}) = \prod_{i=1}^{N}(1 + |\boldsymbol{x}_i|_2)^t \tag{21}$$

for orders $m'+s' < m+s$ and $s-s' > 0$ and polynomial degrees $t \in \mathbb{N}, t > 0$. The approximation was constructed using a smooth dyadic partition of the Fourier space and a subsequent multi-level approximation on each patch. As a consequence the approximation results apply to all considered orders m, m', s, s' and are not restricted by the regularity of the multi-scale approximation at the price that the ansatz functions are not compactly supported in real space. The obtained approximation rates deteriorate with the polynomial degree t and converges to the rates of Theorem 14 up to logarithmic factors for the case $t \to \infty$.

Using the techniques presented in this section analog results for wavelet discretization can be obtained for functions satisfying (21). For that purpose in a first step Equation (21) is expressed equivalently in terms of wavelet coefficients:

$$\sum_{\vec{\lambda}\in\nabla^N} \left[\kappa^2_{s,m}(\vec{\lambda}) + w(\vec{\boldsymbol{x}}_{\vec{\lambda}})\right] |u_{\vec{\lambda}}|^2, \quad u_{\vec{\lambda}} = \langle \tilde{\psi}_{\vec{\lambda}}, u\rangle_{L^2(\mathbb{R}^{dN})}.$$

Based on the discrete weights, again, one may construct an efficient approximation by choosing important contributions. If one uses the exponential weight w_γ instead one recovers up to logarithmic terms the result of Theorem 14.

Furthermore the approximation results of Theorem 14 may be improved with respect to the restrictions on the orders, i.e. the requirement $m'+s', m+s < \tau$ can be weakened. For deriving approximation results it suffices to use a Jackson type estimate. Since in the wavelet setting the number of vanishing moments may be higher than the regularity of the wavelets, the approximation results may be valid for a bigger range of orders [16].

5 Application to the electronic Schrödinger equation

In this section we apply our result to the electronic Schrödinger equation and present a numerical example. We want to approximate bounded states of atoms or molecules and rely thereby on the regularity results obtained in [44]. We refer to this work for an introduction to this subject and pointers to literature.

For the quantum mechanical description of a molecule or atom one has to discretize the so called wave function, which is a function in $H^1(\mathbb{R}^{3N})$ if the system is composed of N electrons. Recently Yserentant [44] showed, that the wave function has mixed regularity. Using Theorem 6.9 and Theorem 6.12 of [44] basically one can show via interpolation theory that the wave function is an element of $H^{1/2,1}_{\mathrm{mix}}\big((\mathbb{R}^3)^N, w_\gamma\big)$, provided that γ is chosen appropriately.

The quality of the approximation is measured with respect to the energy norm in H^1. Therefore one can apply the approximation results for the case $T = 0$ of the previous section to derive the approximation rate. Denote by u the wave function and by u_n the approximation with n terms according to Theorem 14. It follows that

$$\|u - u_n\|_1 \lesssim (\log n)^{(N-1)/2}\, n^{-1/6},$$

that is up to logarithmic terms the approximation rate equals $1/6$.

However this result can still be improved by using symmetry properties of the wave function u. The Pauli principle requires that the function is antisymmetric with respect to interchange of certain variables. More specifically

$$u(P\vec{\boldsymbol{x}}) = \operatorname{sign}(P)\, u(\vec{\boldsymbol{x}}), \tag{22}$$

where P is any permutation in the symmetric group S_N satisfying

$$P(\vec{\sigma}) = \vec{\sigma}, \quad \vec{\sigma} = (\underbrace{+{}^1\!/\!_2, \dots, +{}^1\!/\!_2}_{N_+ \text{ times}}, \underbrace{-{}^1\!/\!_2, \dots, -{}^1\!/\!_2}_{N - N_+ \text{ times}}). \tag{23}$$

for a fixed spin configuration $\vec{\sigma}$. One can directly verify that the operator

$$(\mathsf{A}_{\vec{\sigma}} u)(\vec{\boldsymbol{x}}) = \frac{1}{N_+!\,(N - N_+)!} \sum_{P : P\vec{\sigma} = \vec{\sigma}} \operatorname{sign}(P) u(P\vec{\boldsymbol{x}}),$$

is an H^1-orthogonal projector on the space of all functions with the corresponding symmetry. Therefore it follows directly that for an approximation $u_\varepsilon \in H^1(\mathbb{R}^{3N})$

$$\|u - u_\varepsilon\|_1^2 = \|u - \mathsf{A}_{\vec{\sigma}} u_\varepsilon\|_1^2 + \|(\mathrm{Id} - \mathsf{A}_{\vec{\sigma}}) u_\varepsilon\|_1^2. \tag{24}$$

As a consequence the best approximation of an antisymmetric function is itself again antisymmetric.

Now instead of approximating u on sparse grids introduced in the last section, we take the antisymmetrized sparse grid spaces

$$G_{\vec{\sigma}}(J) = \operatorname{span}\bigl\{\mathsf{A}_{\vec{\sigma}} \psi_{\vec{\lambda}} \mid \vec{\lambda} \in \Lambda_\rho^0(J)\bigr\},$$

where ρ is given in Equation (13) and Λ_ρ^0 in Equation (11). Since different $\vec{\lambda}$ and $\vec{\lambda}'$ may span the same subspace, i.e. $\mathsf{A}_{\vec{\sigma}} \psi_{\vec{\lambda}} = \pm \mathsf{A}_{\vec{\sigma}} \psi_{\vec{\lambda}'}$, or may even vanish, i.e. $\mathsf{A}_{\vec{\sigma}} \psi_{\vec{\lambda}} = 0$, the given set of indices is redundant. Therefore one needs fewer indices to span the antisymmetrized sparse grid. In the following we estimate the number of degrees of freedom.

Lemma 15. *Let $N \geq 1$, $\gamma > 0$ and $\vec{\sigma}$ be a spin configuration, see Equation* (23)*. Define the set of all indices $\Lambda_{\vec{\sigma}}(J)$ as the set of all indices $\vec{\lambda} \in \Lambda_\rho^0(J)$ such that the levels in each spin group, i.e.*

$$\bigl(j(\lambda_i)\bigr)_{i=1,\dots,N_+} \text{ and } \bigl(j(\lambda_i)\bigr)_{i=N_+ + 1,\dots,N}$$

are monotonically decreasing. Then $G_{\vec{\sigma}}(J) = \operatorname{span}\bigl\{\mathsf{A}_{\vec{\sigma}} \psi_{\vec{\lambda}} \mid \vec{\lambda} \in \Lambda_{\vec{\sigma}}(J)\bigr\}$ and the degrees of freedom can be estimated by

$$\sharp \Lambda_{\vec{\sigma}}(J) \lesssim \gamma^{-3N} \cdot e^{4\sqrt{2J}}\, 2^{3J}$$

asymptotically in J. Here the constant is independent of γ and J.

Proof. Due to the properties of the operator $\mathsf{A}_{\vec{\sigma}}$ it is clear that we can restrict ourselves to indices where the levels in each spin group decrease. For estimating the number of elements in $\Lambda_{\vec{\sigma}}(J)$ one basically proceeds as in the proof of Lemma 13 in the case $T = 0$. Instead of estimating $\sharp\{\vec{j} \in \mathbb{N}^N \mid |\vec{j}|_1 = j\}$ in Equation (18) we only consider those indices $\vec{j}$ which are in addition monotonically decreasing in each group $1, \ldots, N_+$ and $N_+ + 1, \ldots, N$. This can be done by using the partition number. For $\ell \in \mathbb{N}$ this number $p(\ell)$ is defined as the number of monotonically decreasing sequences $\ell_1 \geq \ell_2 \geq \ldots$ of non-negative integers such that the sum $\ell_1 + \ell_2 + \ldots$ equals ℓ. One may estimate this number by

$$p(\ell) \lesssim \frac{e^{2\sqrt{2\ell}}}{\ell}$$

where the constant is independent of ℓ, see for example [44]. Now since $|\vec{j}|_1 = j$ the indices in both groups too sum up to at most j. Therefore the number of sequences can be estimated by $\left(e^{2\sqrt{2j}}\right)^2 = e^{4\sqrt{2j}}$. Summing up like in the proof of Lemma 13 shows the assertion. $\square$

Given the estimate on the accuracy and the number of elements needed we can easily estimate the convergence rate.

Theorem 16. *Let $s, \gamma > 0$ and $u \in H^{s,1}_{\mathrm{mix}}\big((\mathbb{R}^3)^N, w_\gamma\big)$ which is antisymmetric in the sense of Equation* (22) *for a fixed spin configuration $\vec{\sigma}$. In addition let $1 + s < \tau$ where τ is the upper bound of the norm equivalence* (8)*. Then for every $\varepsilon > 0$ the antisymmetrized approximation $\tilde{u}_\varepsilon = \mathsf{A}_{\vec{\sigma}} u_\varepsilon$ from Theorem 9 (set $m' = 1$, $s' = 0$) satisfies $\|u - \tilde{u}_\varepsilon\|_1 \leq \varepsilon \, \|u\|_{\mathrm{mix}, w_\gamma, s, 1}$. Asymptotically the number of summands in $\tilde{u}_\varepsilon$ can be bounded by*

$$\sharp\tilde{u}_\varepsilon \lesssim C_\gamma^{3n_\xi/(2s)} \cdot \gamma^{-3N} \cdot e^{4\sqrt{2|\log_2 \varepsilon|}} \cdot \varepsilon^{-3/s}$$

for $\varepsilon \to 0$, where the constant is independent of ε and γ.

Proof. The approximation $\tilde{u}_\varepsilon$ approximates u at least as well as u_ε, see Equation (24). Therefore the estimate of accuracy from Theorem 9 carries over to the antisymmetric case. The number of elements can then be calculated using Lemma 15. $\square$

Now since the bounded states u of an atom or molecule are in $H^{1/2,1}_{\mathrm{mix}}\big((\mathbb{R}^3)^N, w_\gamma\big)$ the wave function u can be approximated with a rate

$$\|u - u_n\|_1 \lesssim e^{2\sqrt{2/3\ \log_2 n}} \cdot n^{-1/6},$$

where u_n is a linear combination of n terms. In the case of the transcorrelated equation one can show that the solution u is an element of $H^{1,1}_{\mathrm{mix}}\big((\mathbb{R}^3)^N, w_\gamma\big)$ [45]. Proceeding as above one can show that

$$\|u - u_n\|_1 \lesssim e^{4/3\sqrt{2/3\ \log_2 n}} \cdot n^{-1/3}$$

for an approximation u_n consisting of n terms. For a discussion of a wavelet discretization of this equation see also [4].

If one compares this result to the one without antisymmetry (for $T = 0$) one sees that the exponent N of the logarithmic term has vanished. Therefore the rate is indeed

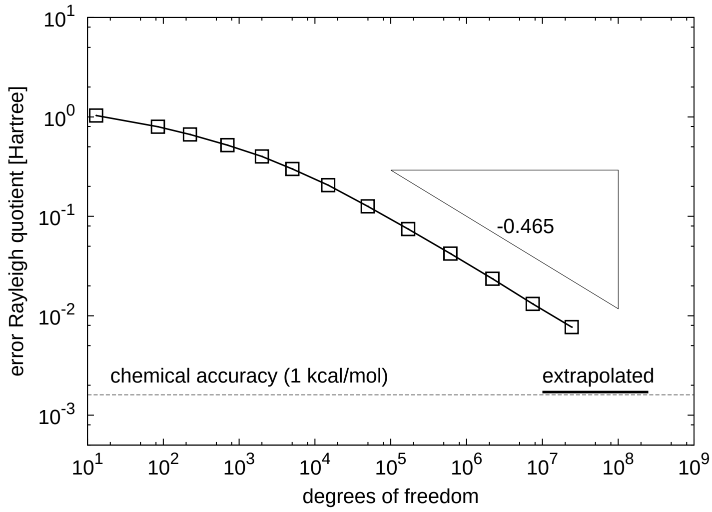


Figure 2: Error of the eigenvalue approximation in atomic units of the lowest eigenvalue of helium with respect to the degrees of freedom, where the reference value is taken from [39]. The approximation is calculated by a Galerkin discretization using adaptively refined anisotropic sparse grids based on linear prewavelets [8]. The chemical accuracy is given by $1\mathrm{kcal}/\mathrm{mol}$. The extrapolated value is calculated using the last three steps.

independent of the number of electrons N. However, the constant behind $\lesssim$ might depend exponentially on N limiting the applicability of the discretization scheme to small atoms or molecules.

In the following we present numerical results of the computation of the ground state of helium. For the solution of the six-dimensional Schrödinger equation we used a sparse grid based on linear prewavelets [8] in a Galerkin discretization, where we set $d = 1$ and $N = 6$. This was done to speed up the application of a vector to the discretization matrix, see also [47]. One can show that up to logarithmic factors the same approximation rates can be reached. In addition the regularity assumptions can be weakened such that the upper bound τ of the norm equivalence (8) fulfills $1 + s/3 < \tau$ at the cost of additional logarithmic terms [46].

In Figure 2 the error of the approximation of the lowest eigenvalue with respect to the degrees of freedom is shown. The reference value is obtained from [39]. The asymptotic convergence behaviour starts around 10^5 and is determined numerically to be approximately 0.465. Since the Hamilton operator is self-adjoint the convergence rate of the eigenvalue is doubled compared to the convergence of the function with respect to the energy norm, i.e. H^1. This value is above the expected rate of convergence of $1/3$ which follows from the fact that the wave function is in $H^{1/2,1}_{\mathrm{mix}}$. Indeed the rate is closer to $1/2$ which would correspond to a regularity of the wave function of $H^{3/4,1}_{\mathrm{mix}}$.

Despite the nice convergence rate the error does not reach the chemical accuracy of $1\ \mathrm{kcal}/\mathrm{mol}$ (approximately 1.6 mHartree in atomic units) needed in quantum chemistry. Using around 25 million degrees of freedom results in an error of around 7.7 mHartree.

Chemical accuracy is expected to be reached as late as using one billion degrees of freedom. One may, however, use the convergence behaviour to extrapolate the eigenvalue to obtain an approximation with an error of 1.7 mHartree just above the chemical accuracy. This computation improves the result calculated by the sparse grid combination technique [20], where an error of approximately 19 mHartree in the lowest eigenvalue of helium was obtained using about 25 million degrees of freedom in a corresponding sparse grid.

These results show that even in the most simple case of a helium atom classical sparse grid constructions reach the desired accuracy only with great effort. Moreover it is expected that the larger the number of electrons the later the asymptotic regime sets in.

A possible way out may be to use sparse grid techniques in combination with well established discretization schemes in quantum chemistry. A good starting point is the Hartree-Fock wave function which is the best rank one approximation of the eigenfunction corresponding to the lowest eigenvalue. In the so called Jastrow ansatz the wave function is approximated by a product of the Hartree-Fock solution and a function to be determined. Using anisotropic wavelets with around 300 basis function chemical accuracy can be reached [18, 19]. A draw back of this approach is that the Hartree-Fock solution fixes the zeros of the approximate wave function. This will likely prevent convergence to the exact wave function. To overcome this effect one may use the Hartree-Fock wave function as an enrichment to sparse grid spaces [24, 21]. In this way the efficiency of the Hartree-Fock solution is combined with guaranteed convergence rates of the sparse grid setting. With this approach small atoms and molecules may be computed with sufficient accuracy; in the case of helium chemical accuracy is reached using less than two thousand basis functions. However the discretization scheme is like all linear methods not size consistent and thus prevents this method from being applied to larger systems.

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A Appendix Interpolation theory

In this appendix we biefly fix the notation needed for applying real interpolation theory as introduced by Peetre [32, 31]. For an overview see also for example [5]. Moreover we prove that the definition of the unweighted Sobolev spaces of fractional mixed order, Definition 1, coincides with the usual definition via intersection of tensor product spaces, see Equation (2) and for example [23].

We begin with the definition of interpolation spaces and restrict ourselves to the case of Hilbert spaces $(X, \|\cdot\|_X)$ and $(Y, \|\cdot\|_Y)$ where $Y \subset X$ is continuously embedded in X:

$$\|f\|_X \leq c\,\|f\|_Y \quad \text{for all } f \in Y.$$

Here the constant c does not depend on f. With the help of the interpolation theory we can construct a family of Hilbert spaces $[X, Y]_{\theta,2}$ where $0 < \theta < 1$ that lie between Y and X, i.e. $Y \subset [X, Y]_{\theta,2} \subset X$. In the following we state this more precisely.

Theorem 17. *Let the Hilbert spaces X and Y be given as above. Define the K-*functional *as*

$$K^2 : X \times \mathbb{R}^+ \to \mathbb{R}, \quad (f,t) \mapsto K^2(f,t) = \inf_{g\in Y} \left[\|f-g\|_X^2 + t^2\,\|g\|_Y^2\right].$$

Based on this functional define for $0<\theta<1$ the norm

$$\|f\|^2_{[X,Y]_{\theta,2}} = \int_0^\infty t^{-2\theta-1}\,K^2(f,t)\,\mathrm{d}t.$$

and the corresponding interpolation space $[X,Y]_{\theta,2}$ *as*

$$[X,Y]_{\theta,2} = \bigl\{f\in X \mid \|f\|_{[X,Y]_{\theta,2}} < \infty\bigr\}.$$

Then $[X,Y]_{\theta,2}$ is a Hilbert space.

Note that we have restricted ourselves to the case of nested Hilbert spaces and the interpolation with $q=2$. An important example is given by the fact that the fractional order Sobolev spaces can be characterized as interpolation spaces:

$$\bigl[L^2(\mathbb{R}^d), H^m(\mathbb{R}^d)\bigr]_{\theta,2} = H^{\theta m}(\mathbb{R}^d)$$

for $m\in\mathbb{N}$ and $0<\theta<1$. Proofs for these facts can be found in [5] for example.

In Definition 1 we introduced the fractional order weighted Sobolev spaces of mixed order via interpolation theory. In the following we show that in the unweighted case these spaces coincide with the classical definition of Sobolev spaces of mixed order through the intersection of tensor product spaces.

In a first step we derive an equivalent norm in terms of the Fourier transform of the function.

Theorem 18. *Let $d,N\ge 1$, $m\in\mathbb{N}$ and $s\ge 0$. Then the norm equivalence*

$$\|u\|^2_{\mathrm{mix},s,m} \sim \int_{\mathbb{R}^{dN}} \bigl(1+|\vec{\boldsymbol{\omega}}|_2^2\bigr)^m \cdot \prod_{i=1}^N \bigl(1+|\boldsymbol{\omega}_i|_2^2\bigr)^s \cdot |\hat{u}(\vec{\boldsymbol{\omega}})|^2\,\mathrm{d}\vec{\boldsymbol{\omega}},$$

holds in the space $H^{s,m}_{\mathrm{mix}}\bigl((\mathbb{R}^d)^N\bigr)$. Here $\hat{u}$ denotes the Fourier transform of u.

Proof. First we prove the norm equivalence for the spaces of integer order $H^{k,m}_{\mathrm{mix}}\bigl((\mathbb{R}^d)^N\bigr)$, where $k\in\mathbb{N}$. It follows from Definition 1 and the properties of the Fourier transform that

$$\|u\|^2_{\mathrm{mix},k,m} = \int_{\mathbb{R}^{dN}} \Bigl[\sum_{\vec{\boldsymbol{\alpha}}\in A^{k,m}} \vec{\boldsymbol{\omega}}^{2\vec{\boldsymbol{\alpha}}}\Bigr] |\hat{u}(\vec{\boldsymbol{\omega}})|^2\,\mathrm{d}\vec{\boldsymbol{\omega}}.$$

Now due to the structure of $A^{k,m}$

$$\sum_{\vec{\boldsymbol{\alpha}}\in A^{k,m}} \vec{\boldsymbol{\omega}}^{2\vec{\boldsymbol{\alpha}}} = \Bigl[\sum_{\sum_i |\boldsymbol{\alpha}_i|_1\le m} \vec{\boldsymbol{\omega}}^{2\vec{\boldsymbol{\alpha}}}\Bigr] \cdot \Bigl[\sum_{|\boldsymbol{\alpha}_1|_1\le k} {\boldsymbol{\omega}_1}^{2\boldsymbol{\alpha}_1}\Bigr] \cdot\ldots\cdot \Bigl[\sum_{|\boldsymbol{\alpha}_N|_1\le k} {\boldsymbol{\omega}_N}^{2\boldsymbol{\alpha}_N}\Bigr].$$

The first factor is equivalent to $\bigl(1+|\vec{\boldsymbol{\omega}}|_2^2\bigr)^m$ while the others are equivalent to $(1+|\boldsymbol{\omega}_i|_2^2)^k$, respectively. This finishes the proof in the case of integer order.

Now we turn to the case $H^{s,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N\big)$ where $s \notin \mathbb{N}$. According to Definition 1 the norm of these spaces is given by

$$\|u\|^2_{\mathrm{mix},s,m} = \int_0^\infty t^{-1-2\theta} \inf_{v\in H^{k,m}_{\mathrm{mix}}} \left[\|u-v\|^2_{\mathrm{mix},0,m} + t^2\|v\|^2_{\mathrm{mix},k,m}\right] \mathrm{d}t,$$

where $k = \lceil s \rceil$ and $\theta = s/k$. Using the result in the case of integer order from above

$$\inf_{v\in H^{k,m}_{\mathrm{mix}}} \int_{\mathbb{R}^{dN}} \left(1+|\vec{\boldsymbol{\omega}}|_2^2\right)^m \left[|\hat{u}(\vec{\boldsymbol{\omega}}) - \hat{v}(\vec{\boldsymbol{\omega}})|^2 + t^2 \prod_{i=1}^N \left(1+|\boldsymbol{\omega}_i|_2^2\right)^k |\hat{v}(\vec{\boldsymbol{\omega}})|^2\right] \mathrm{d}\vec{\boldsymbol{\omega}}.$$

is equivalent to the infimum in the integrand. Now evaluating the infimum pointwise one gets

$$\hat{v}(\vec{\boldsymbol{\omega}}) = \frac{1}{1+t^2\prod_{i=1}^N \left(1+|\boldsymbol{\omega}_i|_2^2\right)^k}\ \hat{u}(\vec{\boldsymbol{\omega}}).$$

One can show that for all $t > 0$ the function v is indeed an element of $H^{k,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N\big)$. Finally with the help of this function one may calculate the interpolation norm explicitly leading to the desired assertion. □

With the help of this theorem one may now show that the unweighted Sobolev spaces of mixed order are intersections of certain tensor product spaces, see also [23] in the case of bounded domains. For the definition of tensor products of Hilbert spaces see for example [33, Section II.4] or [38, Thm. 2.1] for the more general case.

Corollary 19. *Let* $d, N \geq 1$, $m \in \mathbb{N}$ *and* $s \geq 0$. *Then*

$$H^{s,m}_{\mathrm{mix}}\big((\mathbb{R}^d)^N\big) = \bigcap_{i=1}^N H^{m\cdot\vec{e}_i + s\cdot\vec{1}}\big((\mathbb{R}^d)^N\big), \quad H^{\vec{t}}\big((\mathbb{R}^d)^N\big) = \bigotimes_{i=1}^N H^{t_i}(\mathbb{R}^d),$$

where $\vec{e}_i$ *is the* i*-th unit vector and* $\vec{1} = (1,\dots,1) \in \mathbb{R}^N$.

Proof. First the norm on $H^{\vec{t}}$ may be expressed equivalently as

$$\|u\|^2_{H^{\vec{t}}\left((\mathbb{R}^d)^N\right)} \sim \int_{\mathbb{R}^{dN}} \prod_{i=1}^N \left(1+|\boldsymbol{\omega}_i|_2^2\right)^{t_i} |\hat{u}(\vec{\boldsymbol{\omega}})|_2^2 \,\mathrm{d}\vec{\boldsymbol{\omega}},$$

see [38, Def. A.2, A.5]. Denote by $\|\cdot\|_{\bigcap H^{\vec{t}}}$ the norm on the intersection of the space $H^{\vec{t}}\big((\mathbb{R}^d)^N\big)$ as defined above. Then

$$\|u\|^2_{\bigcap H^{\vec{t}}} \sim \int_{\mathbb{R}^{dN}} \left[\sum_{j=1}^N \prod_{i=1}^N \left(1+|\boldsymbol{\omega}_i|_2^2\right)^{s+\delta_{ij}\cdot m}\right] \cdot |\hat{u}(\vec{\boldsymbol{\omega}})|_2^2 \,\mathrm{d}\vec{\boldsymbol{\omega}}.$$

Now the first factor in the integrand may be written as

$$\left[\sum_{j=1}^N \left(1+|\boldsymbol{\omega}_j|_2^2\right)^m\right] \cdot \prod_{i=1}^N \left(1+|\boldsymbol{\omega}_i|_2^2\right)^s.$$

Since the term in the square bracket is equivalent to $\left(1+|\vec{\boldsymbol{\omega}}|_2^2\right)^m$ the assertion directly follows from Theorem 18. □

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