DFG-Schwerpunktprogramm 1324

„Extraktion quantifizierbarer Information aus komplexen Systemen”

The Mixed Regularity of Electronic Wave Functions in Fractional Order and Weighted Sobolev Spaces

H.-C. Kreusler, H. Yserentant

Preprint 94

Edited by

AG Numerik/Optimierung
Fachbereich 12 - Mathematik und Informatik
Philipps-Universität Marburg
Hans-Meerwein-Str.
35032 Marburg

DFG-Schwerpunktprogramm 1324

„Extraktion quantifizierbarer Information aus komplexen Systemen"

The Mixed Regularity of Electronic Wave Functions in Fractional Order and Weighted Sobolev Spaces

H.-C. Kreusler, H. Yserentant

Preprint 94

The mixed regularity of electronic wave functions in fractional order and weighted Sobolev spaces

Hans-Christian Kreusler · **Harry Yserentant**

June 5, 2011

Abstract We continue the study of the regularity of electronic wave functions in Hilbert spaces of mixed derivatives. It is shown that the eigenfunctions of electronic Schrödinger operators and their exponentially weighted counterparts possess, roughly speaking, square integrable mixed weak derivatives of fractional order ϑ for $\vartheta < 3/4$. The bound $3/4$ is best possible and can neither be reached nor surpassed. Such results are important for the study of sparse grid-like expansions of the wave functions and show that their asymptotic convergence rate measured in terms of the number of ansatz functions involved does not deteriorate with the number of electrons.

Mathematics Subject Classification (2000) 35J10 · 35B65 · 41A25 · 41A63

1 Introduction

Quantum mechanics is the key to any deeper understanding of atomic and molecular systems. The basic problem is to find the solutions of the Schrödinger equation for a system of electrons and nuclei that interact by electrostatic attraction and repulsion forces. Due to the high-dimensionality of the problem, approximating these solutions is inordinately challenging and not possible with the standard methods of numerical mathematics. A further problem is the oscillatory character of the solutions and the many different time scales on which they vary and which can range over many orders of magnitude. Following Born and Oppenheimer the problem is therefore usually split into the electronic Schrödinger equation describing the motion of the electrons in the field of given clamped nuclei, and an equation for the motion of the nuclei in a potential field that is determined by solutions of the electronic equation. The present article is concerned with the mixed regularity of the solutions of the electronic

This research was supported by the DFG-Priority Program 1324 and the DFG-Research Center MATHEON

Institut für Mathematik, Technische Universität Berlin, 10623 Berlin, Germany
E-mail: kreusler, yserentant@math.tu-berlin.de

Schrödinger equation, the eigenfunctions of the electronic Hamilton operator

$$H \,=\, -\,\frac{1}{2}\sum_{i=1}^{N}\Delta_i - \sum_{i=1}^{N}\sum_{\nu=1}^{K}\frac{Z_\nu}{|x_i-a_\nu|} + \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\frac{1}{|x_i-x_j|}. \tag{1.1}$$

It extends the earlier work [14–16] of the second author. The mixed regularity of these solutions, the electronic wave functions, and of their correspondingly exponentially weighted counterparts can be used to expand them in sparse grid-like manner into tensor products for example of three-dimensional eigenfunctions of Schrödinger-like operators [16], orthogonal wavelets [18], or Gaussian frames [8]. Based on such regularity and decay properties and taking into account the partial antisymmetry of the wave functions enforced by the Pauli principle it has been shown that the convergence rates of such expansions measured in terms of the number of basis functions involved surprisingly do not fall below that for systems of only two electrons [16]. The present results can be used to improve the estimates for the convergence rates further.

The solution space of the electronic Schrödinger equation is the Hilbert space H^1 that consists of the one times weakly differentiable, square integrable functions

$$u:(\mathbb{R}^3)^N\to\mathbb{R}:(x_1,\ldots,x_N)\to u(x_1,\ldots,x_N) \tag{1.2}$$

with square integrable first-order weak derivatives; the dimension of their domain increases with the number N of electrons. The norm $\|\cdot\|_1$ on H^1 is composed of the L_2-norm $\|\cdot\|_0$ induced by the L_2-inner product $(\cdot,\cdot)$ and the L_2-norm of the gradient. The space H^1 is the space of the wave functions for which the total position probability remains finite and the expectation value of the kinetic energy can be given a meaning. To describe our results, we need to introduce a scale of norms that is defined in terms of Fourier transforms. We first introduce the polynomials

$$P_{\mathrm{iso}}(\omega) \,=\, 1+\sum_{i=1}^{N}|\omega_i|^2, \quad P_{\mathrm{mix}}(\omega) \,=\, \prod_{i=1}^{N}\big(1+|\omega_i|^2\big). \tag{1.3}$$

The $\omega_i\in\mathbb{R}^3$ forming together the variable $\omega\in(\mathbb{R}^3)^N$ can be associated with the momentums of the electrons. The expressions $|\omega_i|$ are their euclidean norms given by

$$|\omega_i|^2 \,=\, \sum_{\nu=1}^{3}\omega_{i,\nu}^2. \tag{1.4}$$

The norms describing the smoothness properties of the solutions are now given by

$$|||u|||_{\vartheta,m}^2 \,=\, \int P_{\mathrm{iso}}(\omega)^m P_{\mathrm{mix}}(\omega)^{\vartheta}\,|\widehat{u}(\omega)|^2\,\mathrm{d}\omega. \tag{1.5}$$

They are defined on the Hilbert spaces $H^{\vartheta,m}_{\mathrm{mix}}$ that consist of the square integrable functions (1.2) for which these expressions remain finite. For nonnegative integer values m and ϑ, the norms measure the L_2-norm of weak partial derivatives. The spaces L_2 and H^1 are special cases of such spaces. The rapidly decreasing functions and even the infinitely differentiable functions with compact support form dense subsets of all these spaces. This can be seen first approximating the functions in these spaces by band-limited functions and these then, multiplying them by appropriately chosen cut-off functions, by infinitely differentiable functions with compact support. Our main result is that the eigenfunctions u of the electronic Schrödinger operator (1.1) are contained in the intersection of such spaces, in

$$H^{1,0}_{\mathrm{mix}} \,\cap \bigcap_{\vartheta<3/4} H^{\vartheta,1}_{\mathrm{mix}}. \tag{1.6}$$

In the general case, the bound $3/4$ can neither be completely reached nor improved further. An exception are systems of electrons of the same spin, for which the wave functions are completely antisymmetric under the exchange of the positions of the electrons and vanish at the singular points of the interaction potential. It has been shown in [14–16] that these wave functions are at least contained in the space $H^{1,1}_{\mathrm{mix}}$. An alternative proof based on techniques as developed here is given in [11].

It is instructive to compare these regularity properties of multi-particle wave functions to those in the single-particle case, like to those of the solutions of the equation

$$-\frac{1}{2}\Delta u - \frac{1}{|x|}\,u = \lambda u \tag{1.7}$$

for the hydrogen atom. In the one-particle case, the spaces $H^{\vartheta,1}_{\mathrm{mix}}$ coincide with the isotropic Sobolev spaces H^s, $s = 1+\vartheta$. The regularity of the solutions of the equation (1.7) in this scale of spaces can be calculated directly [15] and increases with increasing angular momentum of the electron. The ground state eigenfunction

$$u(x) = \frac{1}{\sqrt{\pi}}\,\mathrm{e}^{-|x|}, \quad \widehat{u}(\omega) = \frac{\sqrt{2}}{\pi}\,\frac{2}{(1+|\omega|^2)^2} \tag{1.8}$$

is that of minimum regularity. It is contained in the spaces H^s, $s = 1+\vartheta$, for all values $\vartheta < 3/2$, but not for the value $\vartheta = 3/2$ itself. This transfers to Born-Oppenheimer atoms in which the electron-electron interaction is neglected. The eigenfunctions are then linear combinations of tensor products of such hydrogen-like eigenfunctions. They are contained in $H^{\vartheta,1}_{\mathrm{mix}}$ for $\vartheta < 3/2$ and even in $H^{s,0}_{\mathrm{mix}}$ for $s < 5/2$. The presence of the electron-electron interaction terms thus halves the order of regularity.

Our proofs are based on a representation of the eigenfunctions u of the electronic Schrödinger operator (1.1) that has been derived in [17] and for the two-electron case in [1]. It has been shown in [17] that the eigenfunctions can be written as products

$$u(x) = \exp\left(\sum_{i<j}\phi(x_i - x_j)\right)v(x) \tag{1.9}$$

of more regular functions $v \in H^{1,1}_{\mathrm{mix}}$ and a universal factor that covers their singularities. The same kind of splitting has already been used in [6] and [9] to study the Hölder regularity of the eigenfunctions. Quantum chemists denote regularizing factors as in (1.9) as Jastrow factors. There is a lot of freedom in the choice of the function ϕ; only its behavior near the origin is fixed. It needs to be of the form

$$\phi(x) = \widetilde{\phi}(|x|), \quad \widetilde{\phi}'(0) = \frac{1}{2}, \tag{1.10}$$

where $\widetilde{\phi} : [0,\infty) \to \mathbb{R}$ is an infinitely differentiable function behaving sufficiently well at infinity. For the present purpose we can assume that this function vanishes for all r greater some bound. In fact, we will generally consider functions of the form (1.9), with v a function in $H^{1,1}_{\mathrm{mix}}$, not only eigenfunctions of the operator (1.1). We will show that such functions are contained in the space (1.6) and will additionally prove optimal estimates for certain mixed weak derivatives of these functions in weighted L_2-spaces. The regularity of the functions (1.9) is therefore determined and limited by that of the explicitly known factor in front of their part v.

We are interested in eigenfunctions u of the Hamilton operator (1.1) for eigenvalues below the bottom of the essential spectrum, a value less than or equal to zero. Such eigenfunctions decay exponentially in the L_2-sense, as has first been shown in [12]. That means there is a constant $\gamma > 0$ such that the functions

$$x \;\to\; \exp\left(\gamma \sum_{i=1}^{N} |x_i|\right) u(x), \tag{1.11}$$

are square integrable. This constant γ depends on the distance of the eigenvalue under consideration to the bottom of the essential spectrum. More details and references to the literature can be found in [16]. It has been shown in [17] that these exponentially weighted eigenfunctions admit the same kind of representation (1.9) as the eigenfunctions themselves. Thus they share with them the described regularity properties. This observation is very important for the convergence analysis of sparse grid-like expansions [16, 18]. We will come back to this point at the end of the paper.

2 Characterizations of the norms and function spaces

We begin our study with a closer inspection of the norms (1.5) and of the corresponding function spaces. The functions (1.2) that we examine depend on variables $x_1, \ldots, x_N$ in $\mathbb{R}^3$ that are associated with the positions of the electrons under consideration. The components of these vectors are the real numbers $x_{i,1}$, $x_{i,2}$, and $x_{i,3}$. Accordingly, we label partial derivatives doubly, that is, by multi-indices

$$\alpha = (\alpha_1, \ldots, \alpha_N) \in (\mathbb{Z}^3_{\geq 0})^N, \quad \alpha_i = (\alpha_{i,1}, \alpha_{i,2}, \alpha_{i,3}) \in \mathbb{Z}^3_{\geq 0}. \tag{2.1}$$

The differential operator D^α of order $|\alpha| = \sum_{i,k} \alpha_{i,k}$ is in this notation

$$\mathrm{D}^\alpha = \prod_{i=1}^{N} \prod_{k=1}^{3} \left(\frac{\partial}{\partial x_{i,k}}\right)^{\alpha_{i,k}}. \tag{2.2}$$

Multivariate polynomials x^α are defined correspondingly. We are particularly concerned with differential operators D^α with multi-indices α in the set

$$\mathscr{A} \;=\; \big\{(\alpha_1, \ldots, \alpha_N) \,\big|\, \alpha_i \in \mathbb{Z}^3_{\geq 0},\, \alpha_{i,1} + \alpha_{i,2} + \alpha_{i,3} \leq 1\big\}, \tag{2.3}$$

that is, that are of most first-order in each of the variables $x_i \in \mathbb{R}^3$ and altogether at most of order N. Introducing the differential operator

$$\mathscr{L} \;=\; \sum_{\alpha \in \mathscr{A}} (-1)^{|\alpha|} \mathrm{D}^{2\alpha} \;=\; \prod_{i=1}^{N} (\mathrm{I} - \Delta_i), \quad \Delta_i \;=\; \frac{\partial^2}{\partial x_{i,1}^2} + \frac{\partial^2}{\partial x_{i,2}^2} + \frac{\partial^2}{\partial x_{i,3}^2}, \tag{2.4}$$

and remembering that $(\mathrm{i}\omega)^\alpha \widehat{u}(\omega)$ is the Fourier transform of $\mathrm{D}^\alpha u$, one obtains

$$|||u|||_{1,0}^2 = (u, \mathscr{L}u), \quad |||u|||_{1,1}^2 = (u, (\mathrm{I}-\Delta)\mathscr{L}u) \tag{2.5}$$

for rapidly decreasing functions u. Integration by parts, possible at least for infinitely differentiable functions with compact support, yields

$$|||u|||_{1,0}^2 = \sum_{\alpha\in\mathscr{A}} \|\mathrm{D}^\alpha u\|_0^2, \quad |||u|||_{1,1}^2 = \sum_{\alpha\in\mathscr{A}} \|\mathrm{D}^\alpha u\|_1^2. \tag{2.6}$$

The representation (2.6) transfers to all functions in the spaces

$$X_0 = H^{1,0}_{\mathrm{mix}}, \quad X^1 = H^{1,1}_{\mathrm{mix}}, \tag{2.7}$$

since the infinitely differentiable functions with compact support are dense in these spaces. This shows that these spaces consist of square integrable functions with corresponding square integrable weak derivatives.

For values $0 < \vartheta < 1$, the spaces $H^{\vartheta,1}_{\mathrm{mix}}$ can be characterized as interpolation spaces between H^1 and X^1. To show this, we need to recall the notion of the K-functional. The K-functional of a function $u \in H^1$ is in our case given by

$$K(t,u) = \inf_{v\in X^1} \{ \|u-v\|_1^2 + t^2 \, |||v|||_{1,1}^2 \}^{1/2}. \tag{2.8}$$

The faster $K(t,u)$ tends to zero for $t \to 0+$ the smoother u is. The K-functional is needed to define the interpolation spaces

$$[H^1, X^1]_\vartheta, \quad 0 < \vartheta < 1, \tag{2.9}$$

the spaces for which the interpolation norm defined by

$$\|u\|^2 = \int_0^\infty [\, t^{-\vartheta} K(t,u)]^2 \, \frac{\mathrm{d}t}{t} \tag{2.10}$$

remains finite. This is a very general, far-reaching construction. More information on interpolation spaces can be found in [2] and [3]. In the present case, the interpolation norm given by (2.10) coincides, up to a known factor, with the norm (1.5). The interpolation spaces (2.9) are therefore the spaces $H^{\vartheta,1}_{\mathrm{mix}}$.

Lemma 2.1 *The interpolation norm given by (2.10) of a function $u \in H^1$ remains finite if and only if u is contained in the space $H^{\vartheta,1}_{\mathrm{mix}}$. In this case,*

$$\int_0^\infty [\, t^{-\vartheta} K(t,u)]^2 \, \frac{\mathrm{d}t}{t} = \int_0^\infty \frac{t^{1-2\vartheta}}{1+t^2} \, \mathrm{d}t \, |||u|||_{\vartheta,1}^2. \tag{2.11}$$

Proof For functions $u \in H^1$ and $v \in X^1$,

$$\|u-v\|_1^2 + t^2 \, |||v|||_{1,1}^2 = \int P_{\mathrm{iso}}(\omega) \big\{ |\widehat{u}(\omega) - \widehat{v}(\omega)|^2 + t^2 P_{\mathrm{mix}}(\omega) \, |\widehat{v}(\omega)|^2 \big\} \, \mathrm{d}\omega.$$

The integrand is, for $\widehat{u}(\omega)$ a given value, minimized by the value

$$\widehat{v}(\omega) = \frac{\widehat{u}(\omega)}{1 + t^2 P_{\mathrm{mix}}(\omega)}.$$

This expression defines, for $u \in H^1$ given, a function $v \in X^1$ at which the infimum in the definition of the K-functional is attained. Inserting this function above, we have found a closed representation of $K(t,u)$ in terms of the Fourier transform of u:

$$K(t,u)^2 = \int P_{\mathrm{iso}}(\omega)\,\frac{t^2 P_{\mathrm{mix}}(\omega)}{1+t^2 P_{\mathrm{mix}}(\omega)}\,|\widehat{u}(\omega)|^2\,\mathrm{d}\omega.$$

The proposition follows from this representation with Fubini's theorem. □

The factor relating the two norms differs at most by the factor two from

$$\frac{1}{2\vartheta(1-\vartheta)}, \tag{2.12}$$

as can be seen replacing the denominator $1+t^2$ of the integrand on the right hand side of (2.11) by 1 for $t \le 1$ and t^2 for $t > 1$. It tends to infinity when ϑ approaches the values 0 or 1 but remains uniformly bounded and uniformly bounded away from zero on every closed subinterval of the open interval $0 < \vartheta < 1$.

The mapping $u \to K(t,u)$ has, for $t > 0$ given, all properties of a norm. It defines a norm on H^1 that is equivalent to the original H^1-norm and satisfies the estimate

$$\frac{t}{\sqrt{1+t^2}}\,\|u\|_1 \le K(t,u) \le \|u\|_1. \tag{2.13}$$

This follows from the representation of the K-functional from the proof of the lemma and from $P_{\mathrm{mix}}(\omega) \ge 1$. The mapping is thus in particular continuous with respect to the H^1-norm. The mixed regularity of a function $u \in H^1$ is conversely almost characterized by the behavior of its K-functional $K(t,u)$ in the limit $t \to 0+$:

Lemma 2.2 *If u is contained in the space $H^{\vartheta,1}_{\mathrm{mix}}$ for a ϑ between 0 and 1,*

$$K(t,u) \le t^{\vartheta}\,|||u|||_{\vartheta,1}. \tag{2.14}$$

If conversely $K(t,u) = \mathscr{O}(t^{\delta})$ in the limit $t \to 0+$ for a given positive $\delta \le 1$, the function $u \in H^1$ is contained in the spaces $H^{\vartheta,1}_{\mathrm{mix}}$ for $\vartheta < \delta$.

Proof The first part follows from the representation of the K-functional from the proof of Lemma 2.1 and the observation that for $0 \le \vartheta \le 1$

$$\left(\frac{t^2 P_{\mathrm{mix}}(\omega)}{1+t^2 P_{\mathrm{mix}}(\omega)}\right)^{1-\vartheta}\left(\frac{t^2 P_{\mathrm{mix}}(\omega)}{1+t^2 P_{\mathrm{mix}}(\omega)}\right)^{\vartheta} \le t^{2\vartheta} P_{\mathrm{mix}}(\omega)^{\vartheta}.$$

The other direction follows from $K(t,u) \le \|u\|_1$, the finiteness of the integrals

$$\int_0^1 \frac{t^{2\delta}}{t^{2\vartheta+1}}\,\mathrm{d}t, \qquad \int_1^\infty \frac{1}{t^{2\vartheta+1}}\,\mathrm{d}t$$

for the values $0 < \vartheta < \delta$, and the representation (2.11) of the norm on $H^{\vartheta,1}_{\mathrm{mix}}$. □

3 Hardy inequalities in three space dimensions

Hardy inequalities play a very important role in our argumentation. An detailed analysis of Hardy inequalities is given in [13]. We prove in this section the Hardy inequality on which everything is based and derive some corollaries from it. Starting point is:

Lemma 3.1 *For all exponents s in the semi-infinite interval $s < 3/2$ and all infinitely differentiable functions $v : \mathbb{R}^3 \to \mathbb{R}$ that have a compact support,*

$$\int \frac{1}{|x|^{2s}} v^2 \,\mathrm{d}x \;\leq\; \Big(\frac{2}{3-2s}\Big)^2 \int \frac{1}{|x|^{2s-2}} |\nabla v|^2 \,\mathrm{d}x. \tag{3.1}$$

Proof Let $d(x) = |x|$ for abbreviation. To avoid any difficulty, we assume at first that the function v vanishes on a neighborhood of the origin. If $s \neq 1/2$,

$$\frac{1}{d^{2s}} \;=\; -\frac{1}{2s-1} \nabla\Big(\frac{1}{d^{2s-1}}\Big) \cdot \nabla d.$$

Integration by parts then yields

$$\int \frac{1}{d^{2s}} v^2 \,\mathrm{d}x \;=\; \frac{1}{2s-1} \int \frac{1}{d^{2s-1}} \nabla \cdot (v^2 \nabla d) \,\mathrm{d}x$$

or, using $\Delta d = 2/d$ and resolving for the left-hand side, the representation

$$\int \frac{1}{d^{2s}} v^2 \,\mathrm{d}x \;=\; -\frac{2}{3-2s} \int \frac{1}{d^{2s-1}} \, v \nabla d \cdot \nabla v \,\mathrm{d}x$$

of the integral to be estimated. This relation holds for all exponents $s \neq 3/2$, also for the first excluded exponent $s = 1/2$ as can be shown letting s tend to $1/2$ on both sides of the equation. The Cauchy-Schwarz inequality yields

$$\int \frac{1}{d^{2s}} v^2 \,\mathrm{d}x \;\leq\; \frac{2}{|3-2s|} \Big(\int \frac{1}{d^{2s}} v^2 \,\mathrm{d}x\Big)^{1/2} \Big(\int \frac{1}{d^{2s-2}} |\nabla d \cdot \nabla v|^2 \,\mathrm{d}x\Big)^{1/2}$$

or, using $|\nabla d| = 1$, the estimate (3.1) for functions v vanishing near the origin and even all $s \neq 3/2$. To complete the proof, let $\chi : \mathbb{R}^3 \to [0,1]$ be an infinitely differentiable function with $\chi(x) = 0$ for $|x| \leq 1/2$ and with $\chi(x) = 1$ for $|x| \geq 1$. Let v now be an arbitrary infinitely differentiable function with compact support and set

$$v_k(x) = \chi(kx)v(x).$$

The estimate (3.1) then holds for the functions v_k as just proved. Using

$$|\chi(kx)| \leq 1, \quad |k(\nabla\chi)(kx)| \leq \frac{c}{|x|}$$

with a constant c independent of k and the local integrability of

$$x \;\to\; \frac{1}{|x|^{2s}}, \quad s < 3/2,$$

(3.1) follows from the dominated convergence theorem letting k go to infinity. □

An estimate of this kind cannot hold for exponents $s \geq 3/2$ as the singular part of the integrand on the left hand side of the inequality is not locally integrable for these values of s. The constant thus needs to tend to infinity as s goes to $3/2$. It cannot be improved as the following example shows. Let $v : \mathbb{R}^3 \to \mathbb{R}$ be an infinitely differentiable functions that takes the values $v(x) = r^{3/2-s}$ for $r \geq 1$, where $r = |x|$ has been set. Let $\chi : [0,\infty) \to \mathbb{R}$ be an infinitely differentiable function with values $\chi(r) = 1$ for $r \leq 1$ and $\chi(r) = 0$ for $r \geq 2$. The functions

$$v_R(x) = \chi\Big(\frac{r}{R}\Big)v(x), \quad R > 1, \tag{3.2}$$

are then infinitely differentiable and vanish outside the balls of radius $2R$ around the origin. The quotient of the integrals on the left and the right side of (3.1) tends in this case to the constant in (3.1) as R goes to infinity, which is therefore optimal.

The estimate from Lemma 3.1 will later be applied for exponents in the half-open interval $1 \leq s < 3/2$. A special case of the estimate is the classical Hardy inequality

$$\int \frac{1}{|x|^2}\, v^2\,\mathrm{d}x \;\leq\; 4\int |\nabla v|^2\,\mathrm{d}x \tag{3.3}$$

for the infinitely differentiable functions $v : \mathbb{R}^3 \to \mathbb{R}$ with compact support or more generally the functions $v \in H^1$. This inequality plays a central role in the derivation of the results from [17] on which this paper is based.

To get rid of singular terms as on the right hand side of (3.1), we need the estimate

$$\int \frac{1}{|x|^{2s-2}}\, v^2\,\mathrm{d}x \;\leq\; \int v^2\,\mathrm{d}x \,+\, 4\int |\nabla v|^2\,\mathrm{d}x. \tag{3.4}$$

that holds for the functions $v \in H^1$ and all exponents $1 \leq s \leq 2$. It follows from the trivial inequality $1/r^{2s-2} \leq 1 + 1/r^2$ and the Hardy inequality (3.3). The inequality (3.4) is adapted to our needs but obviously no longer invariant under a rescaling of the variables. To remove this deficiency, one can estimate the integral by a fractional order norm of the function v expressed in terms of its Fourier transform [11].

4 Estimates of mixed derivatives

We are now in the position to prove that a good deal of the smoothness of the regular part v of the wave functions (1.9) transfers to the wave functions themselves. The arguments are rather general and do not utilize that the functions under consideration solve the Schrödinger equation. We only assume that they are of the form

$$u(x) = \Big\{\prod_{i<j} F(x_i - x_j)\Big\}\, v(x), \tag{4.1}$$

where $v : (\mathbb{R}^3)^N \to \mathbb{R}$ is a function in one of the spaces (2.7), i.e., possessing square integrable weak derivatives $\mathrm{D}^\alpha v$, $\alpha \in \mathscr{A}$, in L_2 respectively H^1. The product in front of v takes the role of the singular part of the wave function (1.9). We assume that

$$F : \mathbb{R}^3 \to \mathbb{R} : x \to f(r), \quad r = |x|, \tag{4.2}$$

is rotationally symmetric and takes the value $F(x) = 1$ for all x outside some ball around the origin and $f : [0,\infty) \to \mathbb{R}$ is infinitely differentiable.

Denoting by x_1, x_2, and x_3 for a moment the components of $x \in \mathbb{R}^3$, the first and second order partial derivatives of the function F are, for $x \neq 0$,

$$\frac{\partial}{\partial x_k} F(x) = \frac{x_k}{r} f'(r), \quad \frac{\partial^2}{\partial x_k \partial x_\ell} F(x) = \frac{x_k}{r}\frac{x_\ell}{r} f''(r) + \Big(\delta_{k\ell} - \frac{x_k}{r}\frac{x_\ell}{r}\Big)\frac{1}{r} f'(r) \tag{4.3}$$

and its third order partial derivatives can outside the origin be written as

$$\frac{\partial^3}{\partial x_k \partial x_\ell \partial x_m} F(x) = \frac{x_k}{r}\frac{x_\ell}{r}\frac{x_m}{r} f'''(r) + a_{k\ell m}(x)\Big(\frac{1}{r} f''(r) - \frac{1}{r^2} f'(r)\Big), \tag{4.4}$$

where we have utilized the abbreviation

$$a_{k\ell m}(x) = \delta_{\ell m}\frac{x_k}{r} + \delta_{km}\frac{x_\ell}{r} + \delta_{k\ell}\frac{x_m}{r} - 3\,\frac{x_k}{r}\frac{x_\ell}{r}\frac{x_m}{r}. \tag{4.5}$$

Since the derivatives of $r \to f(r)$ are bounded for $r \geq 0$ and vanish for all r greater than some $r_0 > 0$, we can deduce from that that their derivatives can be bounded via

$$\Big|\frac{\partial}{\partial x_k} F(x)\Big| \lesssim 1, \quad \Big|\frac{\partial^2}{\partial x_k \partial x_\ell} F(x)\Big| \lesssim \frac{1}{r}, \quad \Big|\frac{\partial^3}{\partial x_k \partial x_\ell \partial x_m} F(x)\Big| \lesssim \frac{1}{r^2} \tag{4.6}$$

and vanish outside the given ball. Here we have used the notation "$a \lesssim b$", which means that a can be estimated by b up to a positive constant that is independent of the parameters under consideration.

We will also need a regularized, smooth counterpart of the product function in front of v in (4.1). For this purpose, let $x \to B(r)$, $B(r) > 0$, be an infinitely differentiable, radially symmetric function. Assume that $B(r) = r$ for $r > 1$ and set, for $\varepsilon > 0$,

$$F_\varepsilon(x) = f(B_\varepsilon(r)), \quad B_\varepsilon(r) = \varepsilon B\big(\frac{r}{\varepsilon}\big). \tag{4.7}$$

The infinitely differentiable function F_ε coincides outside the ball of radius ε around the origin with the function F. Inside this ball, its derivatives can be estimated as

$$\Big|\frac{\partial}{\partial x_k} F_\varepsilon(x)\Big| \lesssim 1, \quad \Big|\frac{\partial^2}{\partial x_k \partial x_\ell} F_\varepsilon(x)\Big| \lesssim \frac{1}{\varepsilon}, \quad \Big|\frac{\partial^3}{\partial x_k \partial x_\ell \partial x_m} F_\varepsilon(x)\Big| \lesssim \frac{1}{\varepsilon^2}, \tag{4.8}$$

with constants that are independent of the smoothing parameter $\varepsilon > 0$. These estimates follow from (4.3) and (4.4) replacing the function f by its smoothed counterparts $r \to f(B_\varepsilon(r))$ and using that $B'(0) = 0$. As follows from (4.6) and (4.8),

$$\Big|\frac{\partial^3}{\partial x_k \partial x_\ell \partial x_m} F_\varepsilon(x)\Big| \lesssim \varepsilon^{s-2}\,\frac{1}{r^s} \tag{4.9}$$

for all values $0 < s < 2$ and all $x \neq 0$, with a constant independent of ε. This estimate will later play a decisive role. Finally for all $x \in \mathbb{R}^3$,

$$|F(x) - F_\varepsilon(x)| \lesssim \varepsilon \tag{4.10}$$

so that the functions F_ε tend uniformly to F as ε goes to zero.

Theorem 4.1 *Let $v : (\mathbb{R}^3)^N \to \mathbb{R}$ be a function that possesses weak derivatives $\mathrm{D}^\alpha v$ in L_2 for all multi-indices α in the set $\mathscr{A}$ from (2.3). The function (4.1) then possesses weak derivatives $\mathrm{D}^\alpha u$, $u \in \mathscr{A}$, in L_2 as well, which can be estimated as*

$$|||u|||_{1,0} \lesssim |||v|||_{1,0} \tag{4.11}$$

by the corresponding derivatives of the function v.

Proof We first assume that v is an infinitely differentiable function with compact support and consider the regularized, themselves infinitely differentiable functions

$$u_\varepsilon(x) = \left\{ \prod_{i<j} F_\varepsilon(x_i - x_j) \right\} v(x). \tag{4.12}$$

Their partial derivatives $\mathrm{D}^\alpha u_\varepsilon$, $\alpha \in \mathscr{A}$, consist of sums of products of partial derivatives of the factors $F_\varepsilon(x_i - x_j)$ with respect to the components of x_i and x_j of orders up to two and of partial derivatives of v. According to (4.6) and (4.8), the partial derivatives of these factors of orders up to one are uniformly bounded in $\varepsilon > 0$ and thus do not require special attention. Their second order derivatives can be bounded via

$$\left| \frac{\partial^2}{\partial x_{i,k} \partial x_{j,\ell}} F_\varepsilon(x_i - x_j) \right| \lesssim \frac{1}{|x_i - x_j|} \tag{4.13}$$

uniformly in ε. If such a second order derivative appears neither x_i nor x_j can appear in another such factor. Letting ε tend to zero, one therefore recognizes, with help of the dominated convergence theorem and the definition of weak derivatives, that the weak derivatives $\mathrm{D}^\alpha u$, $u \in \mathscr{A}$, exist and can formally be obtained by the product rule. The derivatives of the factors $F(x_i - x_j)$ have here to be interpreted pointwise outside the singular set and the derivatives of v still classically.

The estimate (4.11) follows from Fubini's theorem and the Hardy inequality (3.3), where one has to take into account that with the appearance of a second order derivative as in (4.13) the function v is not differentiated with respect to the components of x_i and x_j, and again that neither x_i nor x_j can appear in another such singular factor. With that we have proven the proposition for infinitely differentiable functions v with compact support. The rest follows from the density of these functions in X_0. Let $v_1, v_2, v_3, \ldots$ be such functions tending to v in X_0. The assigned u_n form then a Cauchy sequence in X_0 and tend with that to a limit functions u both in X_0 and L_2. This limit function then necessarily coincides with the corresponding function (4.1) which is therefore itself contained in X_0 and satisfies the estimate (4.11). □

The theorem particularly implies that, for every function v with the given properties, the assigned function $u = \mathsf{F}v$ from (4.1) is contained in H^1. We keep in mind that its weak gradient and with that its first order weak derivatives are given by

$$\nabla u = \mathsf{F}\, \nabla v + v \nabla \mathsf{F}, \tag{4.14}$$

where the gradient of v is understood in the weak sense and that of F pointwise.

If the weak derivatives $\mathrm{D}^\alpha v$, $\alpha \in \mathscr{A}$, of the regular part of the function (4.1) are in H^1, the corresponding derivatives of the function (4.1) itself, however, do not need to be located in H^1 as the singularities arising in front of the derivatives of v are too strong. To cover the behavior of these derivatives of the wave functions near the singular set where two or more electrons meet, we introduce the weight function

$$\Omega(x) = \min\Big\{ \min_{i<j} |x_i - x_j|, 1 \Big\}. \tag{4.15}$$

Theorem 4.2 *Let $v : (\mathbb{R}^3)^N \to \mathbb{R}$ be a square integrable function that possesses weak derivatives $\mathrm{D}^\alpha v$ in H^1 for all multi-indices α in the set $\mathscr{A}$ from (2.3). The weak derivatives $\mathrm{D}^\alpha u$, $\alpha \in \mathscr{A}$, of the function (4.1) are then themselves one times weakly differentiable outside the singular set Γ where two or more components x_i coincide. Their first order weak derivatives defined outside this singular set satisfy an estimate*

$$\|\Omega^\mu \nabla \mathrm{D}^\alpha u\|_0 \lesssim \frac{1}{2\mu - 1} \, |||v|||_{1,1} \tag{4.16}$$

for all exponents $1/2 < \mu \leq 1$, with a constant that is independent of μ.

Proof The arguments are similar to that in the proof of the previous theorem and are based on the estimates (4.6) for the first, second, and third-order derivatives of the function F. The corresponding weak derivatives of u on the complement of the singular set Γ can be formally calculated with help of the product rule and consist of sums of products of partial derivatives of the factors $F(x_i - x_j)$ up to order three and the corresponding weak derivatives of v.

The first order derivatives of the factors $F(x_i - x_j)$ are bounded and do not require special attention. The situation is different with the second and third-order derivatives of these factors that behave, according to (4.6), on the neighborhood of Γ like

$$\lesssim \frac{1}{|x_i - x_j|}, \quad \lesssim \frac{1}{|x_i - x_j|^2}.$$

In any of the products of which the components of $\nabla \mathrm{D}^\alpha u$, $\alpha \in \mathscr{A}$, are composed, a variable x_i can only appear in one of these singular terms. In this case, v is not differentiated with respect to a component of x_i. The pairs x_i, x_j for which the derivatives of the factors behaves like $\sim 1/|x_i - x_j|$ can therefore be treated with the classical Hardy inequality (3.3). A factor involving a third-order derivative of the function F can appear at most once in each of these products and is therefore to a sufficient extent compensated by the weight function. Since, with $1 \leq s = 2 - \mu < 3/2$,

$$\Omega(x)^{2\mu} \frac{1}{|x_i - x_j|^4} \leq \frac{1}{|x_i - x_j|^{2s}},$$

(4.16) follows with help of Fubini's theorem from the Hardy inequality (3.1) in combination with the estimate (3.4) and the classical Hardy inequality (3.3). $\square$

An estimate like (4.16) cannot hold for exponents $\mu \leq 1/2$. This follows from the fact that the function $x \to 1/r^{4-2\mu}$ is locally integrable in three space dimensions if and only if $\mu > 1/2$. The lower bound $\mu > 1/2$ can therefore not be improved further.

The results of this section can be summarized in the estimate

$$\sum_{\alpha\in\mathscr{A}} \Big\{ \|\mathrm{D}^\alpha u\|_0^2 + \|\Omega^\mu \nabla \mathrm{D}^\alpha u\|_0^2 \Big\} \lesssim \Big(\frac{1}{2\mu-1} \Big)^2 \sum_{\alpha\in\mathscr{A}} \|\mathrm{D}^\alpha v\|_1^2 \tag{4.17}$$

that holds for $1/2 < \mu < 1$ with a constant independent of μ and reflects the behavior of the mixed derivatives of the function (4.1) in the neighborhood of the singular set. The eigenfunctions u of the electronic Schrödinger operator (1.1) for eigenvalues below the bottom of the essential spectrum possess therefore square integrable weak derivatives $\mathrm{D}^\alpha u$ for all multi-indices $\alpha \in \mathscr{A}$, that is, are contained in $H^{1,0}_{\mathrm{mix}}$. Their weighted weak derivatives $\Omega^\mu \nabla \mathrm{D}^\alpha u$, $\alpha \in \mathscr{A}$, exist outside the singular set where two ore more electrons meet and are square integrable for all exponents $\mu > 1/2$.

5 The K-functional and estimates in fractional order spaces

The next theorem shows, in combination with the results from [17], that the solutions of the electronic Schrödinger equation are contained in the spaces $H^{\vartheta,1}_{\mathrm{mix}}$ for all ϑ below $3/4$. It is based on an estimate of the K-functional (2.8) of the function under consideration, from the perspective of approximation theory the decisive quantity.

Theorem 5.1 *Let $v : (\mathbb{R}^3)^N \to \mathbb{R}$ be a square integrable function that possesses weak derivatives $\mathrm{D}^\alpha v$ in H^1 for all multi-indices α in the set $\mathscr{A}$ from (2.3). The function (4.1) is then contained in the spaces $H^{\vartheta,1}_{\mathrm{mix}}$ for all values $\vartheta < 3/4$. Moreover,*

$$K(t,u) \lesssim -\ln(t)\, t^{3/4}\, |||v|||_{1,1}, \quad t \to 0+, \tag{5.1}$$

which means that $K(t,u)$ tends faster to zero in t than any power t^ϑ, $\vartheta < 3/4$.

Proof We assume first that the given function v is an infinitely differentiable function with compact support. The idea is to estimate the K-functional by the expression

$$K(t,u) \le \{ \|u - u_\varepsilon\|_1^2 + t^2\, |||u_\varepsilon|||_{1,1}^2 \}^{1/2},$$

where $\varepsilon > 0$ will later be coupled to t and $u_\varepsilon = \mathsf{F}_\varepsilon v$ is the smoothed variant (4.12) in the space X^1 of the function $u = \mathsf{F}v$ from (4.1) in the space H^1. We recall that the weak gradient of u can be formally calculated with help of the product rule (4.14).

The function $u - u_\varepsilon$ vanishes outside the union of the sets Γ_{ij} that consist of those x for which $|x_i - x_j| \le \varepsilon$. The H^1-distance of u and u_ε over Γ_{ij} can be estimated as

$$\|u - u_\varepsilon\|_{1,\Gamma_{ij}} \le \|(\mathsf{F} - \mathsf{F}_\varepsilon)\nabla v\|_{0,\Gamma_{ij}} + \|(\nabla\mathsf{F} - \nabla\mathsf{F}_\varepsilon)v\|_{0,\Gamma_{ij}} + \|(\mathsf{F} - \mathsf{F}_\varepsilon)v\|_{0,\Gamma_{ij}}.$$

As $|(\mathsf{F} - \mathsf{F}_\varepsilon)(x)| \lesssim \varepsilon$ and $|(\nabla\mathsf{F} - \nabla\mathsf{F}_\varepsilon)(x)| \lesssim 1$, the squares of the first two terms on the right hand side can, for arbitrary s in the interval $1 \le s < 3/2$, be estimated by

$$\varepsilon^{2s} \int_{\Gamma_{ij}} \frac{1}{|x_i - x_j|^{2s-2}}\, |\nabla v|^2 \,\mathrm{d}x, \quad \varepsilon^{2s} \int_{\Gamma_{ij}} \frac{1}{|x_i - x_j|^{2s}}\, v^2 \,\mathrm{d}x,$$

and the square of the last term correspondingly by the expression

$$\varepsilon^{2s} \int_{\Gamma_{ij}} \frac{1}{|x_i - x_j|^{2s-2}} \, v^2 \, \mathrm{d}x.$$

These expressions can be further estimated with help of (3.1) and (3.4). This yields

$$\|u - u_\varepsilon\|_1 \lesssim \frac{1}{3-2s} \, \varepsilon^s \, |||v|||_{1,1},$$

with a constant that depends neither on ε nor on the choice of s.

Estimating the norm $|||u_\varepsilon|||_{1,1}$ means estimating partial derivatives of u_ε. These partial derivatives split again into sums of products of partial derivatives of the factors $F_\varepsilon(x_i - x_j)$ with respect to the components of x_i and x_j of orders up to three and of partial derivatives of v. One proceeds as in the proof of Theorem 4.2, where the estimate (4.9) for the third order derivatives of F_ε enters into the estimates of the terms involving a third order derivative of one of the factors $F_\varepsilon(x_i - x_j)$. One obtains, with help of Fubini's theorem and the estimates from Sect. 3, the estimate

$$|||u_\varepsilon|||_{1,1} \lesssim \frac{1}{3-2s} \, \varepsilon^{s-2} \, |||v|||_{1,1},$$

where the constant depends as before neither on $1 \leq s < 3/2$ nor on ε.

The estimates for the two single parts can now be combined to an estimate for the K-functional. Choosing for both the same s and setting $\varepsilon = \sqrt{t}$, one obtains

$$K(t,u) \lesssim \frac{1}{3-2s} \, t^{s/2} \, |||v|||_{1,1},$$

with a constant independent of $1 \leq s < 3/2$. The estimate (5.1) now follows choosing

$$s = \frac{3}{2} + \frac{2}{\ln t};$$

for $t \leq \mathrm{e}^{-4}$ this s is located in the admissible interval and minimizes the right hand side of the inequality above. That the estimate (5.1) holds for all functions $v \in X^1$, not only for the infinitely differentiable functions v with compact support as just proved, follows from the density of these functions in X^1, the continuity of the mapping $v \rightarrow u$ as a mapping from X^1 to H^1, and the continuity of the mapping $u \rightarrow K(t,u)$ from H^1 to the real numbers. The rest of the proposition follows from Lemma 2.2. □

The estimate (5.1) for the K-functional implies the norm estimate

$$|||u|||_{\vartheta,1} \lesssim \left(\frac{1}{3-4\vartheta}\right)^{3/2} |||v|||_{1,1} \tag{5.2}$$

for the function (4.1) that holds for $0 \leq \vartheta < 3/4$, with a constant independent of ϑ. It suffices to prove the estimate for $\vartheta \geq 1/2$ as the norm on the left hand side of the equation increases with ϑ. This can be done using the representation (2.11) of this norm in terms of the K-functional and an argument as in the proof of Lemma 2.2.

6 A counterexample

The upper bound $\vartheta < 3/4$ from Theorem 5.1 is optimal and can never be reached nor surpassed. This can be seen by the example of the function

$$u(x) \;=\; \Big(1 + \frac{1}{2}\,|x_1 - x_2|\Big)\,\exp\Big(-\frac{1}{4}\,|x_1|^2 - \frac{1}{4}\,|x_2|^2\Big) \tag{6.1}$$

that falls into the considered category but is not contained in $H^{\vartheta,1}_{\mathrm{mix}}$ for $\vartheta \geq 3/4$. This function often serves as a model for electronic wave functions. Its singular behavior at the diagonal $x_1 = x_2$ is the same as that of the solutions of the electronic Schrödinger equation at the positions where two electrons of distinct spin meet [7]. The function represents at the same time the ground state of the so-called hookium or harmonium atom [10], an artificial two-electron system with the Hamiltonian

$$-\frac{1}{2}\,\Delta + \frac{1}{8}\,|x|^2 + \frac{1}{|x_1 - x_2|} \tag{6.2}$$

in which the potential of the nucleus is replaced by that of a harmonic oscillator.

To show that the function (6.1) cannot be contained in $H^{\vartheta,1}_{\mathrm{mix}}$ for $\vartheta \geq 3/4$, we first rotate the coordinate system by the matrix

$$Q = \frac{1}{\sqrt{2}}\begin{pmatrix} I & -I \\ I & I \end{pmatrix} \tag{6.3}$$

built up from the (3×3)-identity matrix and write u in the form $u(x) = w(Qx)$, where

$$w(x) \;=\; \Big(1 + \frac{1}{\sqrt{2}}\,|x_1|\Big)\exp\Big(-\frac{1}{4}\,|x_1|^2 - \frac{1}{4}\,|x_2|^2\Big). \tag{6.4}$$

As Q is orthogonal the Fourier transform of u is then $\widehat{u}(\omega) = \widehat{w}(Q\omega)$. Therefore

$$\int P(\omega)|\widehat{u}(\omega)|^2\,\mathrm{d}\omega \;=\; \int P(Q^T\omega)|\widehat{w}(\omega)|^2\,\mathrm{d}\omega \tag{6.5}$$

for every symbol $P(\omega)$. Since $|Q^T\omega| = |\omega|$ thus we have to show that the function

$$\omega \;\to\; (1+|\omega|^2)\,P_{\mathrm{mix}}(Q^T\omega)^{\vartheta}\,|\widehat{w}(\omega)|^2 \tag{6.6}$$

cannot be integrable for exponents $\vartheta \geq 3/4$, where

$$P_{\mathrm{mix}}(Q^T\omega) \;=\; \Big(1 + \frac{1}{2}\,|\omega_1 - \omega_2|^2\Big)\Big(1 + \frac{1}{2}\,|\omega_1 + \omega_2|^2\Big). \tag{6.7}$$

To proceed, we need to know the asymptotic behavior of the Fourier transform of the function w. We rewrite w first in the form

$$w(x) \;=\; \phi(x_1)\,\mathrm{e}^{-|x_2|^2/4} \;=\; \widetilde{\phi}(|x_1|)\,\mathrm{e}^{-|x_2|^2/4} \tag{6.8}$$

with the univariate function

$$\widetilde{\phi}(r) \;=\; \Big(1 + \frac{1}{\sqrt{2}}\,r\Big)\,\mathrm{e}^{-r^2/4}. \tag{6.9}$$

The Fourier transform of w is in this notation

$$\widehat{w}(\omega) = \widehat{\phi}(\omega_1)\,(\sqrt{2})^3\,\mathrm{e}^{-|\omega_2|^2}. \tag{6.10}$$

The asymptotic behavior of the Fourier transform of ϕ is given by the following lemma that is of general nature and into which only the decay properties of $\widetilde{\phi}$ enter.

Lemma 6.1 *The Fourier transform of ϕ behaves for $|\omega|$ tending to infinity like*

$$\widehat{\phi}(\omega) = -2\sqrt{\frac{2}{\pi}}\,\frac{\widetilde{\phi}'(0)}{|\omega|^4} + \mathscr{O}\Big(\frac{1}{|\omega|^6}\Big). \tag{6.11}$$

Proof As ϕ is a rotationally symmetric function, $\widehat{\phi}(\omega) = \widehat{\phi}(Q\omega)$ for all orthogonal (3×3)-matrices Q. Particularly $\widehat{\phi}(\omega) = \widehat{\phi}(|\omega|e_3)$. Therefore

$$\widehat{\phi}(\omega) = \Big(\frac{1}{\sqrt{2\pi}}\Big)^3 \int \widetilde{\phi}(|x|)\,\mathrm{e}^{-\mathrm{i}\,|\omega|x_3}\,\mathrm{d}x.$$

Transforming the integral to polar coordinates, the representation

$$\widehat{\phi}(\omega) = \sqrt{\frac{2}{\pi}}\,\frac{1}{|\omega|}\int_0^\infty r\,\widetilde{\phi}(r)\sin(|\omega|r)\,\mathrm{d}r$$

of the Fourier transform of a rotationally symmetric function $\phi(x) = \widetilde{\phi}(|x|)$ in three space dimensions follows. If $r \to a(r)$ is an infinitely differentiable function with integrable derivatives tending to zero as r goes to infinity, integration by parts yields

$$\int_0^\infty a(r)\sin(|\omega|r)\,\mathrm{d}r = \frac{1}{|\omega|}\,a(0) - \frac{1}{|\omega|^2}\int_0^\infty a''(r)\sin(|\omega|r)\,\mathrm{d}r.$$

Applying this relation a second and third time, one obtains

$$\int_0^\infty a(r)\sin(|\omega|r)\,\mathrm{d}r = \frac{1}{|\omega|}\,a(0) - \frac{1}{|\omega|^3}\,a''(0) + \mathscr{O}\Big(\frac{1}{|\omega|^5}\Big)$$

as $|\omega|$ goes to infinity and therefore, inserting $a(r) = r\,\widetilde{\phi}(r)$, the proposition. □

We can now complete the proof and are ready to to show that the function (6.6) cannot be integrable for $\vartheta \geq 3/4$. For that it suffices to show that it cannot be integrable over the cylinder $|\omega_2| \leq 1$ for these values of ϑ. For $|\omega_2| \leq 1$,

$$\Big(1 + \frac{1}{2}\,|\omega_1 - \omega_2|^2\Big)\Big(1 + \frac{1}{2}\,|\omega_1 + \omega_2|^2\Big) \geq 1 + \frac{1}{4}\,|\omega_1|^4. \tag{6.12}$$

In our case $\widetilde{\phi}'(0) \neq 0$. With help of Lemma 6.1 one gets therefore, for ω in the given cylinder and sufficiently large $|\omega_1|$, the desired lower bound

$$\gtrsim \Big(\frac{1}{|\omega_1|}\Big)^{6-4\vartheta} \tag{6.13}$$

for the function (6.6). If $\vartheta \geq 3/4$, the function (6.6) thus cannot be integrable over the cylinder $|\omega_2| \leq 1$ and even less over the full space. This proves that the function (6.1) is indeed contained in none of the spaces $H^{\vartheta,1}_{\mathrm{mix}}$ for $\vartheta \geq 3/4$. Moreover, for this u,

$$K(t,u) \gtrsim t^{3/4}, \tag{6.14}$$

as can be shown in the same way, with help of the representation of the K-functional from the proof of Lemma 2.1 and the asymptotic behavior of the Fourier transform of the function w on the cylinder $|\omega_2| \leq 1$. This demonstrates that the estimate (5.1) from Theorem 5.1 is almost optimal and that at most the logarithm got lost there.

7 Exponential decay, approximability, and approximation order

We mentioned in the introduction that the eigenfunctions u of the operator (1.1) decay exponentially in the L_2-sense, which means that the functions (1.11) here denoted as

$$x \to \mathrm{e}^{\psi(x)}u(x), \quad \psi(x) = \gamma \sum_{i=1}^{N} |x_i|, \tag{7.1}$$

are square integrable for values $\gamma > 0$ below some bound that depends on the distance of the eigenvalue under consideration to the bottom of the essential spectrum. It has been shown in [17] that these exponentially weighted eigenfunctions admit the same kind of representation (1.9) as the eigenfunctions themselves. They are therefore like these contained in the spaces $H^{\vartheta,1}_{\mathrm{mix}}$ for $\vartheta < 3/4$. We outline in this section how this can be used to study the convergence behavior of approximation processes.

Lemma 7.1 *For all functions v for which $\mathrm{e}^{\psi}v$ is located in $H^{1,1}_{\mathrm{mix}}$, that is, in X^1,*

$$|||\mathrm{e}^{\psi}v|||^2_{1,1} \lesssim \sum_{\alpha\in\mathscr{A}} \|\mathrm{e}^{\psi}\mathrm{D}^{\alpha}v\|_1^2 \lesssim |||\mathrm{e}^{\psi}v|||^2_{1,1}, \tag{7.2}$$

with constants that depend on the decay rate γ.

Proof This follows from the observation that for all multi-indices $\alpha \in \mathscr{A}$

$$\mathrm{D}^{\alpha}(\mathrm{e}^{\psi}v) = \sum_{\beta\leq\alpha} \gamma^{|\beta|} a_{\beta}\, \mathrm{e}^{\psi}\, \mathrm{D}^{\alpha-\beta}v,$$

where the bounded coefficient functions a_{β} are given by

$$a_{\beta}(x) = \prod_{i=1}^{N} \Big(\frac{x_i}{|x_i|}\Big)^{\beta_i}$$

and the relation $\beta \leq \alpha$ has to be understood componentwise. The reason is that the function $\mathrm{e}^{\psi}v$ is differentiated only once with respect to the components of every single x_i. Formally, the relation is obtained from the product rule, which can be justified in the sense of globally defined weak derivatives with an approximation argument as in the proof of Theorem 4.1. Differentiating the relation above once more, the proposition follows with help of the Hardy inequality (3.3), taking into account that $a_{\beta} = 1$ for $\beta = 0$, $\nabla_i a_{\beta} = 0$ if $\beta_i = 0$, and $|\nabla_i a_{\beta}| \leq 1/|x_i|$ otherwise. $\square$

A similar argument shows that the H^1-norm of the function $\mathrm{e}^{\Psi}u$ can be estimated by the L_2-norms of $\mathrm{e}^{\Psi}u$ and $\mathrm{e}^{\Psi}\nabla u$ and vice versa. The norm $|||\mathrm{e}^{\Psi}v|||_{1,1}$ measures therefore the exponentially weighted L_2-norms of the involved derivatives of v.

It is therefore reasonable to start from a sequence $T_n : H^1 \to H^1$, $n = 1,2,\ldots$, of linear approximation operators that are uniformly H^1-bounded and to require that

$$\|v - T_n v\|_1 \lesssim n^{-q}\, |||\mathrm{e}^{\Psi}v|||_{1,1} \tag{7.3}$$

for all functions $v \in H^1$ for which $\mathrm{e}^{\Psi}v \in H^{1,1}_{\mathrm{mix}}$. The constant $q > 0$ is an unspecified convergence rate also depending on what n means. These assumptions form a proper framework for sparse grid-like approximation methods, for example for the wavelet approximations studied in [18] or expansions into tensor products of Gaussians or other eigenfunctions of three-dimensional Schrödinger-like operators [16]. Another example is the expansion into tensor products of three-dimensional functions with given angular parts [16]. The range of the T_n is in this case infinite dimensional. The exponential factor is the tribute paid to the infinite extension of the domain.

Our assumptions imply the following error estimate for functions of reduced smoothness and in particular for the eigenfunctions of the operator (1.1).

Theorem 7.1 *For all functions $u \in H^1$ for which $\mathrm{e}^{\Psi}u \in H^{\vartheta,1}_{\mathrm{mix}}$ for some $0 < \vartheta < 1$,*

$$\|u - T_n u\|_1 \lesssim n^{-\vartheta q}\, |||\mathrm{e}^{\Psi}u|||_{\vartheta,1}. \tag{7.4}$$

Proof We use that $\|u\|_1 \lesssim \|\mathrm{e}^{\Psi}u\|_1$ for functions u for which $\mathrm{e}^{\Psi}u \in H^1$. The linearity of the T_n, their uniform boundedness, and (7.3) imply therefore the estimate

$$\|u - T_n u\|_1 \lesssim \|u - \mathrm{e}^{-\Psi}v\|_1 + \|\mathrm{e}^{-\Psi}v - T_n(\mathrm{e}^{-\Psi}v)\|_1 \lesssim \|\mathrm{e}^{\Psi}u - v\|_1 + n^{-q}\, |||v|||_{1,1}$$

for arbitrary such u and all $v \in X^1$. With that we can bound the approximation error

$$\|u - T_n u\|_1 \lesssim K(n^{-q}, \mathrm{e}^{\Psi}u)$$

in terms of the K-functional of $\mathrm{e}^{\Psi}u$. The proposition thus follows from (2.14). □

The scheme thus exploits the smoothness of the functions even if the convergence rate decreases unsurprisingly with decreasing smoothness. In the case of the solutions u of the electronic Schrödinger equation studied in this paper, we can apply the estimate for the K-functional of $\mathrm{e}^{\Psi}u$ from Theorem 5.1 directly. It leads to an estimate

$$\|u - T_n u\|_1 \lesssim \ln(n)\, n^{-3/4\, q} \tag{7.5}$$

for the approximation error: the convergence rate comes arbitrarily close to $3/4\,q$. Essentially only the factor $3/4$ gets lost compared to the case of full mixed regularity.

8 From approximation order back to regularity

Under some additional assumptions one can show that this convergence order cannot be improved further. We start from an orthogonal or biorthogonal expansion

$$v = \sum\nolimits_\lambda (v, \phi'_\lambda)\, \phi_\lambda \tag{8.1}$$

of the square integrable functions into a series of functions $\phi_\lambda \in H^1$, where λ runs over a countable set of indices. The example that we have in mind is the expansion into wavelets from [18]. We introduce a new scale of discrete norms given by

$$|||[v]|||^2_{\vartheta,m} = \sum\nolimits_\lambda \kappa_0(\lambda)^m \kappa(\lambda)^\vartheta (v, \phi'_\lambda)^2, \tag{8.2}$$

where $\kappa_0(\lambda)$ and $\kappa(\lambda)$ are weight factors. The first one basically serves to measure the first order derivatives. The second one splits in Zeiser's construction into a part that is associated with the mixed derivatives and another one that is position dependent and associated with the decay of the functions under consideration. We assume in the sequel that, for the functions v for which $\mathrm{e}^\Psi v$ is contained in the space $H^{1,1}_{\mathrm{mix}}$,

$$|||v|||_{1,1} \lesssim |||[v]|||_{1,1} \lesssim |||\mathrm{e}^\Psi v|||_{1,1}, \tag{8.3}$$

and that for $\vartheta = 0$ and $m = 1$ the new norm is equivalent to the H^1-norm, that is, that

$$\|v\|_1 \lesssim |||[v]|||_{0,1} \lesssim \|v\|_1 \tag{8.4}$$

holds for all functions $v \in H^1$. The wavelet expansions from [18] fulfill these assumptions. Our approximation operators T_n are now defined by

$$T_n v = \sum\nolimits'_\lambda (v, \phi'_\lambda)\, \phi_\lambda, \tag{8.5}$$

where the dash indicates that the sum runs here only over the indices λ for which $\kappa(\lambda)$ is less than a bound that is monotonely increasing with n and tending to infinity as n goes to infinity, say less than n^{2q} to adapt the notation to that in the previous section. The T_n are then bounded as operators from H^1 to H^1. Furthermore,

$$\|v - T_n v\|_1 \lesssim n^{-q}\, |||\mathrm{e}^\Psi v|||_{1,1} \tag{8.6}$$

for the functions v for which $\mathrm{e}^\Psi v$ is contained in $H^{1,1}_{\mathrm{mix}}$. The operators thus fit into the framework considered before; in particular the error estimates (7.4) and (7.5) hold. The rest follows with help of a standard argument [3] from approximation theory:

Lemma 8.1 *Let u be a function in H^1 for which the error behaves like*

$$\|u - T_n u\|_1 = \mathscr{O}(n^{-\delta q}) \tag{8.7}$$

for n tending to infinity, where $0 < \delta < 1$. Then $u \in H^{\vartheta,1}_{\mathrm{mix}}$ for $\vartheta < \delta$.

Proof Let $\widetilde{T}_\ell = T_{2^\ell}$ for abbreviation. Then

$$|||[\widetilde{T}_n u]|||_{\vartheta,1} \,\leq\, |||[\widetilde{T}_1 u]|||_{\vartheta,1} + \sum_{\ell=1}^{n-1} (2^{\ell+1})^{\vartheta q}\, |||[\widetilde{T}_{\ell+1} u - \widetilde{T}_\ell u]|||_{0,1},$$

as follows from the triangle inequality and the inverse inequality

$$|||[v]|||_{\vartheta,1} \leq (2^{\ell+1})^{\vartheta q} |||[v]|||_{0,1}$$

for the functions v in the range of $\widetilde{T}_{\ell+1}$. By the given assumptions,

$$|||[\widetilde{T}_{\ell+1} u - \widetilde{T}_\ell u]|||_{0,1} \,\lesssim\, \|\widetilde{T}_{\ell+1} - u\|_1 + \|u - \widetilde{T}_\ell u\|_1 \,\lesssim\, (2^{\ell+1})^{-\delta q}.$$

That means that the discrete norm

$$|||[u]|||_{\vartheta,1} = \lim_{n\to\infty} |||[\widetilde{T}_n u]|||_{\vartheta,1}$$

of u remains finite for $0 < \vartheta < \delta$. This implies $u \in H^{\vartheta,1}_{\mathrm{mix}}$ since

$$|||v|||_{\vartheta,1} \,\lesssim\, |||[v]|||_{\vartheta,1},$$

which follows by means of interpolation from (8.3) and (8.4), expressing both norms as in Lemma 2.1 in terms of the corresponding K-functionals. □

We conclude that for the functions considered in the previous sections, and in particular for electronic wave functions, a convergence rate ϑq, $\vartheta > 3/4$, is in general not possible. The estimate (7.5) is thus optimal, at least up to the logarithmic factor. Nonlinear, adaptive methods might shift this bound but also encounter hard limits due to the location of the singularities on the diagonals [4,5].

References

1. Bachmayr, M.: Hyperbolic wavelet discretization of the two-electron Schrödinger equation in an explicitly correlated formulation. Preprint AICES-2010/06-2, RWTH Aachen (2010)
2. Bergh, J., Löfström, J.: Interpolation Spaces, *Die Grundlehren der mathematischen Wissenschaften in Einzeldarstellungen*, vol. 223. Springer, Berlin Heidelberg New York (1976)
3. Butzer, P.L., Scherer, K.: Approximationsprozesse und Interpolationsmethoden, *B.I.-Hochschultaschenbücher*, vol. 826/826a. Bibliographisches Institut, Mannheim (1968)
4. Flad, H.J., Hackbusch, W., Schneider, R.: Best N-term approximation in electronic structure calculations. I. One-electron reduced density matrix. M2AN **40**, 49–61 (2006)
5. Flad, H.J., Hackbusch, W., Schneider, R.: Best N-term approximation in electronic structure calculations. II. Jastrow factors. M2AN **41**, 261–279 (2007)
6. Fournais, S., Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T., Østergard Sørensen, T.: Sharp regularity estimates for Coulombic many-electron wave functions. Commun. Math. Phys. **255**, 183–227 (2005)
7. Fournais, S., Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T., Østergard Sørensen, T.: Analytic structure of many-body Coulombic wave functions. Commun. Math. Phys. **289**, 291–310 (2009)
8. Hamaekers, J.: Tensor Product Multiscale Many-Particle Spaces with Finite-Order Weights for the Electronic Schrödinger Equation. Doctoral thesis, Universität Bonn (2009)
9. Hoffmann-Ostenhof, M., Hoffmann-Ostenhof, T., Østergard Sørensen, T.: Electron wavefunctions and densities for atoms. Ann. Henri Poincaré **2**, 77–100 (2001)

10. Kais, S., Herschbach, D.R., Levine, R.D.: Dimensional scaling as a symmetry operation. J. Chem. Phys. **91**, 7791–7796 (1989)
11. Kreusler, C.: Zur anisotropen Sobolev-Regularität der elektronischen Schrödinger-Gleichung. Doctoral thesis, Technische Universität Berlin (2011)
12. O'Connor, A.J.: Exponential decay of bound state wave functions. Commun. Math. Phys. **32**, 319–340 (1973)
13. Opic, B., Kufner, A.: Hardy-type inequalities, *Pitman Research Notes in Mathematics*, vol. 219. Longman Scientific & Technical, Harlow (1990)
14. Yserentant, H.: On the regularity of the electronic Schrödinger equation in Hilbert spaces of mixed derivatives. Numer. Math. **98**, 731–759 (2004)
15. Yserentant, H.: The hyperbolic cross space approximation of electronic wavefunctions. Numer. Math. **105**, 659–690 (2007)
16. Yserentant, H.: Regularity and Approximability of Electronic Wave Functions, *Lecture Notes in Mathematics*, vol. 2000. Springer, Heidelberg Dordrecht London New York (2010)
17. Yserentant, H.: The mixed regularity of electronic wave functions multiplied by explicit correlation factors. ESAIM: M2AN **45**, 803–824 (2011)
18. Zeiser, A.: Wavelet approximation in weighted Sobolev spaces of mixed order with applications to the electronic Schrödinger equation. Preprint 55, DFG-Schwerpunktprogramm 1324 (2010)

Preprint Series DFG-SPP 1324

http://www.dfg-spp1324.de

Reports

[1] R. Ramlau, G. Teschke, and M. Zhariy. A Compressive Landweber Iteration for Solving Ill-Posed Inverse Problems. Preprint 1, DFG-SPP 1324, September 2008.

[2] G. Plonka. The Easy Path Wavelet Transform: A New Adaptive Wavelet Transform for Sparse Representation of Two-dimensional Data. Preprint 2, DFG-SPP 1324, September 2008.

[3] E. Novak and H. Woźniakowski. Optimal Order of Convergence and (In-) Tractability of Multivariate Approximation of Smooth Functions. Preprint 3, DFG-SPP 1324, October 2008.

[4] M. Espig, L. Grasedyck, and W. Hackbusch. Black Box Low Tensor Rank Approximation Using Fibre-Crosses. Preprint 4, DFG-SPP 1324, October 2008.

[5] T. Bonesky, S. Dahlke, P. Maass, and T. Raasch. Adaptive Wavelet Methods and Sparsity Reconstruction for Inverse Heat Conduction Problems. Preprint 5, DFG-SPP 1324, January 2009.

[6] E. Novak and H. Woźniakowski. Approximation of Infinitely Differentiable Multivariate Functions Is Intractable. Preprint 6, DFG-SPP 1324, January 2009.

[7] J. Ma and G. Plonka. A Review of Curvelets and Recent Applications. Preprint 7, DFG-SPP 1324, February 2009.

[8] L. Denis, D. A. Lorenz, and D. Trede. Greedy Solution of Ill-Posed Problems: Error Bounds and Exact Inversion. Preprint 8, DFG-SPP 1324, April 2009.

[9] U. Friedrich. A Two Parameter Generalization of Lions' Nonoverlapping Domain Decomposition Method for Linear Elliptic PDEs. Preprint 9, DFG-SPP 1324, April 2009.

[10] K. Bredies and D. A. Lorenz. Minimization of Non-smooth, Non-convex Functionals by Iterative Thresholding. Preprint 10, DFG-SPP 1324, April 2009.

[11] K. Bredies and D. A. Lorenz. Regularization with Non-convex Separable Constraints. Preprint 11, DFG-SPP 1324, April 2009.

[12] M. Döhler, S. Kunis, and D. Potts. Nonequispaced Hyperbolic Cross Fast Fourier Transform. Preprint 12, DFG-SPP 1324, April 2009.

[13] C. Bender. Dual Pricing of Multi-Exercise Options under Volume Constraints. Preprint 13, DFG-SPP 1324, April 2009.

[14] T. Müller-Gronbach and K. Ritter. Variable Subspace Sampling and Multi-level Algorithms. Preprint 14, DFG-SPP 1324, May 2009.

[15] G. Plonka, S. Tenorth, and A. Iske. Optimally Sparse Image Representation by the Easy Path Wavelet Transform. Preprint 15, DFG-SPP 1324, May 2009.

[16] S. Dahlke, E. Novak, and W. Sickel. Optimal Approximation of Elliptic Problems by Linear and Nonlinear Mappings IV: Errors in L_2 and Other Norms. Preprint 16, DFG-SPP 1324, June 2009.

[17] B. Jin, T. Khan, P. Maass, and M. Pidcock. Function Spaces and Optimal Currents in Impedance Tomography. Preprint 17, DFG-SPP 1324, June 2009.

[18] G. Plonka and J. Ma. Curvelet-Wavelet Regularized Split Bregman Iteration for Compressed Sensing. Preprint 18, DFG-SPP 1324, June 2009.

[19] G. Teschke and C. Borries. Accelerated Projected Steepest Descent Method for Nonlinear Inverse Problems with Sparsity Constraints. Preprint 19, DFG-SPP 1324, July 2009.

[20] L. Grasedyck. Hierarchical Singular Value Decomposition of Tensors. Preprint 20, DFG-SPP 1324, July 2009.

[21] D. Rudolf. Error Bounds for Computing the Expectation by Markov Chain Monte Carlo. Preprint 21, DFG-SPP 1324, July 2009.

[22] M. Hansen and W. Sickel. Best m-term Approximation and Lizorkin-Triebel Spaces. Preprint 22, DFG-SPP 1324, August 2009.

[23] F.J. Hickernell, T. Müller-Gronbach, B. Niu, and K. Ritter. Multi-level Monte Carlo Algorithms for Infinite-dimensional Integration on $\mathbb{R}^{\mathbb{N}}$. Preprint 23, DFG-SPP 1324, August 2009.

[24] S. Dereich and F. Heidenreich. A Multilevel Monte Carlo Algorithm for Lévy Driven Stochastic Differential Equations. Preprint 24, DFG-SPP 1324, August 2009.

[25] S. Dahlke, M. Fornasier, and T. Raasch. Multilevel Preconditioning for Adaptive Sparse Optimization. Preprint 25, DFG-SPP 1324, August 2009.

[26] S. Dereich. Multilevel Monte Carlo Algorithms for Lévy-driven SDEs with Gaussian Correction. Preprint 26, DFG-SPP 1324, August 2009.

[27] G. Plonka, S. Tenorth, and D. Roşca. A New Hybrid Method for Image Approximation using the Easy Path Wavelet Transform. Preprint 27, DFG-SPP 1324, October 2009.

[28] O. Koch and C. Lubich. Dynamical Low-rank Approximation of Tensors. Preprint 28, DFG-SPP 1324, November 2009.

[29] E. Faou, V. Gradinaru, and C. Lubich. Computing Semi-classical Quantum Dynamics with Hagedorn Wavepackets. Preprint 29, DFG-SPP 1324, November 2009.

[30] D. Conte and C. Lubich. An Error Analysis of the Multi-configuration Time-dependent Hartree Method of Quantum Dynamics. Preprint 30, DFG-SPP 1324, November 2009.

[31] C. E. Powell and E. Ullmann. Preconditioning Stochastic Galerkin Saddle Point Problems. Preprint 31, DFG-SPP 1324, November 2009.

[32] O. G. Ernst and E. Ullmann. Stochastic Galerkin Matrices. Preprint 32, DFG-SPP 1324, November 2009.

[33] F. Lindner and R. L. Schilling. Weak Order for the Discretization of the Stochastic Heat Equation Driven by Impulsive Noise. Preprint 33, DFG-SPP 1324, November 2009.

[34] L. Kämmerer and S. Kunis. On the Stability of the Hyperbolic Cross Discrete Fourier Transform. Preprint 34, DFG-SPP 1324, December 2009.

[35] P. Cerejeiras, M. Ferreira, U. Kähler, and G. Teschke. Inversion of the noisy Radon transform on $SO(3)$ by Gabor frames and sparse recovery principles. Preprint 35, DFG-SPP 1324, January 2010.

[36] T. Jahnke and T. Udrescu. Solving Chemical Master Equations by Adaptive Wavelet Compression. Preprint 36, DFG-SPP 1324, January 2010.

[37] P. Kittipoom, G. Kutyniok, and W.-Q Lim. Irregular Shearlet Frames: Geometry and Approximation Properties. Preprint 37, DFG-SPP 1324, February 2010.

[38] G. Kutyniok and W.-Q Lim. Compactly Supported Shearlets are Optimally Sparse. Preprint 38, DFG-SPP 1324, February 2010.

[39] M. Hansen and W. Sickel. Best m-Term Approximation and Tensor Products of Sobolev and Besov Spaces – the Case of Non-compact Embeddings. Preprint 39, DFG-SPP 1324, March 2010.

[40] B. Niu, F.J. Hickernell, T. Müller-Gronbach, and K. Ritter. Deterministic Multi-level Algorithms for Infinite-dimensional Integration on $\mathbb{R}^{\mathbb{N}}$. Preprint 40, DFG-SPP 1324, March 2010.

[41] P. Kittipoom, G. Kutyniok, and W.-Q Lim. Construction of Compactly Supported Shearlet Frames. Preprint 41, DFG-SPP 1324, March 2010.

[42] C. Bender and J. Steiner. Error Criteria for Numerical Solutions of Backward SDEs. Preprint 42, DFG-SPP 1324, April 2010.

[43] L. Grasedyck. Polynomial Approximation in Hierarchical Tucker Format by Vector-Tensorization. Preprint 43, DFG-SPP 1324, April 2010.

[44] M. Hansen und W. Sickel. Best m-Term Approximation and Sobolev-Besov Spaces of Dominating Mixed Smoothness - the Case of Compact Embeddings. Preprint 44, DFG-SPP 1324, April 2010.

[45] P. Binev, W. Dahmen, and P. Lamby. Fast High-Dimensional Approximation with Sparse Occupancy Trees. Preprint 45, DFG-SPP 1324, May 2010.

[46] J. Ballani and L. Grasedyck. A Projection Method to Solve Linear Systems in Tensor Format. Preprint 46, DFG-SPP 1324, May 2010.

[47] P. Binev, A. Cohen, W. Dahmen, R. DeVore, G. Petrova, and P. Wojtaszczyk. Convergence Rates for Greedy Algorithms in Reduced Basis Methods. Preprint 47, DFG-SPP 1324, May 2010.

[48] S. Kestler and K. Urban. Adaptive Wavelet Methods on Unbounded Domains. Preprint 48, DFG-SPP 1324, June 2010.

[49] H. Yserentant. The Mixed Regularity of Electronic Wave Functions Multiplied by Explicit Correlation Factors. Preprint 49, DFG-SPP 1324, June 2010.

[50] H. Yserentant. On the Complexity of the Electronic Schrödinger Equation. Preprint 50, DFG-SPP 1324, June 2010.

[51] M. Guillemard and A. Iske. Curvature Analysis of Frequency Modulated Manifolds in Dimensionality Reduction. Preprint 51, DFG-SPP 1324, June 2010.

[52] E. Herrholz and G. Teschke. Compressive Sensing Principles and Iterative Sparse Recovery for Inverse and Ill-Posed Problems. Preprint 52, DFG-SPP 1324, July 2010.

[53] L. Kämmerer, S. Kunis, and D. Potts. Interpolation Lattices for Hyperbolic Cross Trigonometric Polynomials. Preprint 53, DFG-SPP 1324, July 2010.

[54] G. Kutyniok and W.-Q Lim. Shearlets on Bounded Domains. Preprint 54, DFG-SPP 1324, July 2010.

[55] A. Zeiser. Wavelet Approximation in Weighted Sobolev Spaces of Mixed Order with Applications to the Electronic Schrödinger Equation. Preprint 55, DFG-SPP 1324, July 2010.

[56] G. Kutyniok, J. Lemvig, and W.-Q Lim. Compactly Supported Shearlets. Preprint 56, DFG-SPP 1324, July 2010.

[57] A. Zeiser. On the Optimality of the Inexact Inverse Iteration Coupled with Adaptive Finite Element Methods. Preprint 57, DFG-SPP 1324, July 2010.

[58] S. Jokar. Sparse Recovery and Kronecker Products. Preprint 58, DFG-SPP 1324, August 2010.

[59] T. Aboiyar, E. H. Georgoulis, and A. Iske. Adaptive ADER Methods Using Kernel-Based Polyharmonic Spline WENO Reconstruction. Preprint 59, DFG-SPP 1324, August 2010.

[60] O. G. Ernst, A. Mugler, H.-J. Starkloff, and E. Ullmann. On the Convergence of Generalized Polynomial Chaos Expansions. Preprint 60, DFG-SPP 1324, August 2010.

[61] S. Holtz, T. Rohwedder, and R. Schneider. On Manifolds of Tensors of Fixed TT-Rank. Preprint 61, DFG-SPP 1324, September 2010.

[62] J. Ballani, L. Grasedyck, and M. Kluge. Black Box Approximation of Tensors in Hierarchical Tucker Format. Preprint 62, DFG-SPP 1324, October 2010.

[63] M. Hansen. On Tensor Products of Quasi-Banach Spaces. Preprint 63, DFG-SPP 1324, October 2010.

[64] S. Dahlke, G. Steidl, and G. Teschke. Shearlet Coorbit Spaces: Compactly Supported Analyzing Shearlets, Traces and Embeddings. Preprint 64, DFG-SPP 1324, October 2010.

[65] W. Hackbusch. Tensorisation of Vectors and their Efficient Convolution. Preprint 65, DFG-SPP 1324, November 2010.

[66] P. A. Cioica, S. Dahlke, S. Kinzel, F. Lindner, T. Raasch, K. Ritter, and R. L. Schilling. Spatial Besov Regularity for Stochastic Partial Differential Equations on Lipschitz Domains. Preprint 66, DFG-SPP 1324, November 2010.

[67] E. Novak and H. Woźniakowski. On the Power of Function Values for the Approximation Problem in Various Settings. Preprint 67, DFG-SPP 1324, November 2010.

[68] A. Hinrichs, E. Novak, and H. Woźniakowski. The Curse of Dimensionality for Monotone and Convex Functions of Many Variables. Preprint 68, DFG-SPP 1324, November 2010.

[69] G. Kutyniok and W.-Q Lim. Image Separation Using Shearlets. Preprint 69, DFG-SPP 1324, November 2010.

[70] B. Jin and P. Maass. An Analysis of Electrical Impedance Tomography with Applications to Tikhonov Regularization. Preprint 70, DFG-SPP 1324, December 2010.

[71] S. Holtz, T. Rohwedder, and R. Schneider. The Alternating Linear Scheme for Tensor Optimisation in the TT Format. Preprint 71, DFG-SPP 1324, December 2010.

[72] T. Müller-Gronbach and K. Ritter. A Local Refinement Strategy for Constructive Quantization of Scalar SDEs. Preprint 72, DFG-SPP 1324, December 2010.

[73] T. Rohwedder and R. Schneider. An Analysis for the DIIS Acceleration Method used in Quantum Chemistry Calculations. Preprint 73, DFG-SPP 1324, December 2010.

[74] C. Bender and J. Steiner. Least-Squares Monte Carlo for Backward SDEs. Preprint 74, DFG-SPP 1324, December 2010.

[75] C. Bender. Primal and Dual Pricing of Multiple Exercise Options in Continuous Time. Preprint 75, DFG-SPP 1324, December 2010.

[76] H. Harbrecht, M. Peters, and R. Schneider. On the Low-rank Approximation by the Pivoted Cholesky Decomposition. Preprint 76, DFG-SPP 1324, December 2010.

[77] P. A. Cioica, S. Dahlke, N. Döhring, S. Kinzel, F. Lindner, T. Raasch, K. Ritter, and R. L. Schilling. Adaptive Wavelet Methods for Elliptic Stochastic Partial Differential Equations. Preprint 77, DFG-SPP 1324, January 2011.

[78] G. Plonka, S. Tenorth, and A. Iske. Optimal Representation of Piecewise Hölder Smooth Bivariate Functions by the Easy Path Wavelet Transform. Preprint 78, DFG-SPP 1324, January 2011.

[79] A. Mugler and H.-J. Starkloff. On Elliptic Partial Differential Equations with Random Coefficients. Preprint 79, DFG-SPP 1324, January 2011.

[80] T. Müller-Gronbach, K. Ritter, and L. Yaroslavtseva. A Derandomization of the Euler Scheme for Scalar Stochastic Differential Equations. Preprint 80, DFG-SPP 1324, January 2011.

[81] W. Dahmen, C. Huang, C. Schwab, and G. Welper. Adaptive Petrov-Galerkin methods for first order transport equations. Preprint 81, DFG-SPP 1324, January 2011.

[82] K. Grella and C. Schwab. Sparse Tensor Spherical Harmonics Approximation in Radiative Transfer. Preprint 82, DFG-SPP 1324, January 2011.

[83] D.A. Lorenz, S. Schiffler, and D. Trede. Beyond Convergence Rates: Exact Inversion With Tikhonov Regularization With Sparsity Constraints. Preprint 83, DFG-SPP 1324, January 2011.

[84] S. Dereich, M. Scheutzow, and R. Schottstedt. Constructive quantization: Approximation by empirical measures. Preprint 84, DFG-SPP 1324, January 2011.

[85] S. Dahlke and W. Sickel. On Besov Regularity of Solutions to Nonlinear Elliptic Partial Differential Equations. Preprint 85, DFG-SPP 1324, January 2011.

[86] S. Dahlke, U. Friedrich, P. Maass, T. Raasch, and R.A. Ressel. An adaptive wavelet method for parameter identification problems in parabolic partial differential equations. Preprint 86, DFG-SPP 1324, January 2011.

[87] A. Cohen, W. Dahmen, and G. Welper. Adaptivity and Variational Stabilization for Convection-Diffusion Equations. Preprint 87, DFG-SPP 1324, January 2011.

[88] T. Jahnke. On Reduced Models for the Chemical Master Equation. Preprint 88, DFG-SPP 1324, January 2011.

[89] P. Binev, W. Dahmen, R. DeVore, P. Lamby, D. Savu, and R. Sharpley. Compressed Sensing and Electron Microscopy. Preprint 89, DFG-SPP 1324, March 2011.

[90] P. Binev, F. Blanco-Silva, D. Blom, W. Dahmen, P. Lamby, R. Sharpley, and T. Vogt. High Quality Image Formation by Nonlocal Means Applied to High-Angle Annular Dark Field Scanning Transmission Electron Microscopy (HAADF-STEM). Preprint 90, DFG-SPP 1324, March 2011.

[91] R. A. Ressel. A Parameter Identification Problem for a Nonlinear Parabolic Differential Equation. Preprint 91, DFG-SPP 1324, May 2011.

[92] G. Kutyniok. Data Separation by Sparse Representations. Preprint 92, DFG-SPP 1324, May 2011.

[93] M. A. Davenport, M. F. Duarte, Y. C. Eldar, and G. Kutyniok. Introduction to Compressed Sensing. Preprint 93, DFG-SPP 1324, May 2011.

[94] H.-C. Kreusler and H. Yserentant. The Mixed Regularity of Electronic Wave Functions in Fractional Order and Weighted Sobolev Spaces. Preprint 94, DFG-SPP 1324, June 2011.