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Sparse grid spaces for the numerical solution of the electronic Schrödinger equation

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Abstract This article complements the author's recent work [Numer. Math. 98, 731–759 (2004)] on the regularity of the electronic Schrödinger equation in Hilbert spaces of mixed derivatives. It has been shown there that the solutions of this equation are surprisingly smooth and possess square integrable mixed weak derivatives of order up to $N+1$ with N the number of electrons across the singularities of the interaction potentials, and it has been claimed that this result can help to break the complexity barriers in computational quantum mechanics using correspondingly antisymmetrized sparse grid trial functions. A construction of this kind that can be interpreted as a sparse grid sampling theorem is sketched here.

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1 Introduction

Hundred grid points represent a fair resolution for two-point boundary value problems in one space dimension. To obtain the same resolution in three space dimensions, already a million grid points are needed. The number increases to unthinkable 10^{60} grid points for equations in 30 dimensions, such as the electronic Schrödinger equation for small molecules like water or ammonia. All the more surprising is the fact that the regularity properties of the admissible eigenfunctions of the electronic Schrödinger operator

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

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make it possible to approximate them by functions in comparatively simply built trial spaces, the dimension of which grows substantially slower in the number of electrons when increasing the accuracy, as is shown in this article. The construction of true numerical methods for computing the lowest eigenvalues and the corresponding eigenfunctions of the Schrödinger operator (1.1) not a priori based on strongly simplified physical models therefore comes into reach.

The Schrödinger operator (1.1) acts upon functions that depend on the coordinates $x_1, \ldots, x_N \in \mathbb{R}^3$ of given N electrons and are denoted as electronic wavefunctions. The eigenvalue problem for this Hamilton operator is of fundamental importance for our understanding of atoms and molecules. It describes the stationary states of N electrons in the field of K nuclei with fixed positions a_ν and charges Z_ν and more or less forms the basis of quantum chemistry. Of particular interest are the eigenfunctions to the minimum eigenvalue describing the ground state of the atom or molecule. For the background in quantum mechanics, see textbooks like [2] or [15]. The standard mathematical reference on Schrödinger operators like (1.1) is [16]. A nice discussion of the structure of the spectrum of such Schrödinger operators can also be found in [7]. See [11] and [19] for an actual review.

The most successful current methods for the calculation of electronic ground states are the many different variants of the Hartree-Fock method, that dates back to the beginnings of quantum mechanics, or are based on the more recent density functional theory. Both Hartree-Fock methods and density functional based methods reduce the Schrödinger equation to a simplified equation in three space dimensions. They heavily rely on physical arguments and are mathematically hard to justify. See [10] and [14] for an overview on the present state of the art in quantum chemistry.

Approximation properties as described above are only possible for functions, the smoothness of which strongly increases with the space dimension. The physically admissible eigenfunctions of the electronic Schrödinger operator (1.1) are surprisingly of such type as has recently been proved by the author [23]. For $s > 0$, let $H^{s,1}_{\mathrm{mix}}$ denote the completion of the Schwartz space $\mathcal{S}$ of the rapidly decreasing functions, the Fourier transforms

$$\widehat{u} : (\mathbb{R}^3)^N \to \mathbb{R} : (\omega_1, \ldots, \omega_N) \to u(\omega_1, \ldots, \omega_N) \tag{1.2}$$

of which then also belong to $\mathcal{S}$, under the norm given by the expression

$$|\!|\!| u |\!|\!|_s^2 \;=\; \int \Big(1 + \sum_{i=1}^{N} |\omega_i|^2\Big)\Big(\prod_{i=1}^{N} \big(1 + |\omega_i|^2\big)\Big)^s \, |\widehat{u}(\omega)|^2 d\omega. \tag{1.3}$$

For integer values of s, the space $H^{s,1}_{\mathrm{mix}}$ consists of square integrable functions with corresponding square integrable mixed weak derivatives of an order up to $sN+1$, that is, of functions that are much smoother than those in the original solution space H^1 or H^2 of the Schrödinger equation. The results proved in [23] then can be summarized as follows: For the physically admissible eigenfunctions u of the Hamilton operator (1.1),

$$u \in H^{1/2,1}_{\mathrm{mix}}, \quad u \in H^{1,1}_{\mathrm{mix}} \tag{1.4}$$

holds, depending on whether u is only partially antisymmetric with respect to the exchange of the electron coordinates in the way prescribed by the Pauli principle, or antisymmetric with respect to the exchange of all electron coordinates. Arbitrarily high regularity cannot be expected because of the singularities of the interaction potentials reflected in Kato's cusp conditions [13]; see [6] for the recent developments.

The described regularity properties allow to approximate the eigenfunctions by infinitely extended sparse grid functions. Such constructions have a long tradition in approximation theory. They go back to the Russian literature [3], [20] and became very popular in numerical mathematics through the work of Zenger [25]; see [4] for a comprehensive survey on such techniques. Recent attempts to approximate electronic wavefunctions by sparse grid methods include [5], [8], [9], [12]. Here we discuss a conceptually very simple approach of this kind that can in some respect be understood as a sparse grid variant of the Whittaker-Shannon sampling theorem [17], [18], [21], [22]. Related constructions based on tensor products of three-dimensional wavelets with bounded support in position space should have a similar potential and may offer more flexibility.

To localize the approximations, the decay properties of the eigenfunctions have to be brought into play. They have been intensely studied in the seventies and eighties of the past century. The decisive source, also containing an extensive bibliography, is [1]. Furthermore we refer to the mentioned review articles [11] and [19] and, for a self-contained elementary exposition, to the lecture notes [24]. A typical result of this kind is that for all eigenfunctions u belonging to eigenvalues λ below the bottom Σ^* of the essential spectrum, and all Σ greater than λ and less than Σ^*, the function

$$x \;\to\; \mathrm{e}^{\,\delta|x|}\, u(x), \quad \delta = \sqrt{2\,(\Sigma-\lambda)}, \tag{1.5}$$

is square integrable, that is, that these eigenfunctions decay exponentially in the L_2-sense. Therefore only a small portion of the infinitely many sparse grid basis functions is needed to approximate such eigenfunctions. Taking further into account the symmetry properties with respect to the exchange of the electron coordinates as enforced by the Pauli principle [23], the dimension of the trial spaces should finally reduce to a tractable level.

2 The approximation by bandlimited functions

In the first step of our construction, the functions in $H^{s,\,1}_{\mathrm{mix}}$ are decomposed into a bandlimited part that will be treated separately and a remaining part that can be neglected. An obvious decomposition of this kind results directly from the definition (1.3) of the $H^{s,\,1}_{\mathrm{mix}}$-norm of a given function u in terms of its Fourier transform. For $L = 0, 1, 2, \ldots$, let

$$\Omega_L \;=\; \Big\{(\omega_1, \ldots, \omega_N) \in (\mathbb{R}^3)^N \;\Big|\; \prod_{i=1}^{N} \big(1 + |\omega_i|^2\big) \le 4^L \Big\}. \tag{2.1}$$

Let u_L be the corresponding projection

$$u_L(x) = \Big(\frac{1}{\sqrt{2\pi}}\Big)^{3N} \int_{\Omega_L} \widehat{u}(\omega) \exp(\mathrm{i}\,\omega\cdot x) d\omega \tag{2.2}$$

of $u \in H^{s,1}_{\mathrm{mix}}$ onto the space of bandlimited functions with Fourier transform vanishing outside the hyperbolic cross (2.1). Because of the representation

$$\|u\|_1^2 \;=\; \int \Big(1 + \sum_{i=1}^{N} |\omega_i|^2\Big)\, |\widehat{u}(\omega)|^2 d\omega \tag{2.3}$$

of the H^1-norm in terms of the Fourier transform, then the error estimate

$$\|u - u_L\|_1 \;\le\; \Big(\frac{1}{2^L}\Big)^s \,|\!|\!|u|\!|\!|_s \tag{2.4}$$

holds. Thus it suffices to approximate the part u_L instead of the function u itself. The problem, however, is that this decomposition is not directly compatible with the sparse grid construction or similar approaches. Therefore we replace the hyperbolic crosses (2.1) by the regions

$$\widetilde{\Omega}_L \;=\; \bigcup \big\{ B_{l_1} \times \cdots \times B_{l_N} \big|\, l_1 + \cdots + l_N \le L \big\} \tag{2.5}$$

that are composed of cartesian products of the three-dimensional balls

$$B_l \;=\; \big\{\, \xi \in \mathbb{R}^3 \;\big|\; |\xi| \le 2^{l+1} \big\}, \quad l = 0, 1, 2, \dots, \tag{2.6}$$

and correspondingly replace the projection (2.2) by

$$\widetilde{u}_L(x) \;=\; \Big(\frac{1}{\sqrt{2\pi}}\Big)^{3N} \int_{\widetilde{\Omega}_L} \widehat{u}(\omega) \exp(\mathrm{i}\,\omega\cdot x) d\omega. \tag{2.7}$$

The key observation is that $\widetilde{\Omega}_L$ can be represented in the form

$$\widetilde{\Omega}_L \;=\; \Big\{ (\omega_1, \dots, \omega_N) \in (\mathbb{R}^3)^N \;\Big|\; \prod_{i=1}^{N} \eta(\omega_i) \le 2^L \Big\} \tag{2.8}$$

with help of the rotationally symmetric step function

$$\eta(\xi) \;=\; \min \{\, 2^l \mid \xi \in B_l,\; l = 0, 1, \dots \}. \tag{2.9}$$

Since this function satisfies the estimate

$$\eta(\xi)^2 \;\le\; 1 + |\xi|^2 \tag{2.10}$$

and $\widetilde{\Omega}_L$ thus covers Ω_L, $\widetilde{u}_L$ is an at least as good approximation of u as u_L.

Theorem 1 *For all $u \in H^{s,1}_{\mathrm{mix}}$,*

$$\|u - \widetilde{u}_L\|_1 \;\le\; \Big(\frac{1}{2^L}\Big)^s \,|\!|\!|u - \widetilde{u}_L|\!|\!|_s \;\le\; \Big(\frac{1}{2^L}\Big)^s \,|\!|\!|u|\!|\!|_s. \tag{2.11}$$

As the argumentation shows, the norm given by (1.3) on the right-hand side of the error estimate can even be replaced by the modified norm defined by

$$\|\!|u|\!\|_s^2 \;=\; \int \Big(1+\sum_{i=1}^{N}|\omega_i|^2\Big)\Big(\prod_{i=1}^{N}\eta(\omega_i)\Big)^{2s}\,|\widehat{u}(\omega)|^2 d\omega. \tag{2.12}$$

This norm is equivalent to the original norm on $H^{s,1}_{\mathrm{mix}}$, but can attain much smaller values for larger numbers N of electrons and comes much closer to the norms that have originally been considered in [23].

Let $\widehat{\chi} : \mathbb{R}^3 \to [0,1]$ now be a function with bounded support attaining the values $\widehat{\chi}(\xi) = 1$ for $|\xi| \le 1$ and $\widehat{\chi}(\xi) = 0$ for $|\xi| \ge 2$. The functions

$$\widehat{\chi}_0(\xi) = \widehat{\chi}\left(\frac{\xi}{2}\right), \quad \widehat{\chi}_l(\xi) = \widehat{\chi}\left(\frac{\xi}{2^{l+1}}\right) - \widehat{\chi}\left(\frac{\xi}{2^l}\right), \quad l = 1, 2, \ldots, \tag{2.13}$$

then form a locally finite partition of unity on the $\mathbb{R}^3$, and the products

$$\widehat{\chi}^{\,(l)}(\omega) \;=\; \prod_{i=1}^{N}\widehat{\chi}_{l_i}(\omega_i) \tag{2.14}$$

accordingly form a partition of unity on the $\mathbb{R}^{3N}$, where $l \in \mathbb{Z}_+^N$ now denotes a multiindex with nonnegative integer components l_i. Every square integrable function u therefore splits into the parts

$$u^{(l)}(x) \;=\; \left(\frac{1}{\sqrt{2\pi}}\right)^{3N}\int \widehat{\chi}^{\,(l)}(\omega)\widehat{u}(\omega)\exp(\mathrm{i}\,\omega\cdot x)d\omega. \tag{2.15}$$

that together form a multiscale decomposition of u. The levels $l_i = 0$ correspond to a lengthscale of order 1, that is, of the size of a single atom here. The levels $l_i > 0$ resolve finer details on lengthscales of order 2^{-l_i}.

The decomposition into the parts (2.15) reflects the analytic behavior of the wavefunctions that is expressed by the regularity of the Schrödinger equation in Hilbert spaces of mixed derivatives. It forms the basis of many possible approximation procedures that differ mainly by the way how the partition of unity is actually chosen and how the parts are finally approximated by functions in finite dimensional spaces. Since

$$\sum_{l_1+\cdots+l_N\le L}\widehat{\chi}^{\,(l)}(\omega) \tag{2.16}$$

attains the value 1 for all ω in the region (2.5) and a value between 0 and 1 everywhere else, the corresponding part

$$u_L^* \;=\; \sum_{l_1+\cdots+l_N\le L} u^{(l)} \tag{2.17}$$

of u approximates u at least as well as the function $\widetilde{u}_L$ considered above.

Theorem 2 *For all* $u \in H^{s,1}_{\mathrm{mix}}$,

$$\|u - u_L^*\|_1 \;\le\; \left(\frac{1}{2^L}\right)^s \;|\!|\!|u - u_L^*|\!|\!|_s \;\le\; \left(\frac{1}{2^L}\right)^s \;|\!|\!|u|\!|\!|_s. \tag{2.18}$$

In the case that $\widehat{\chi}$ has minimum support and is the characteristic function of the unit ball, the approximations u_L^* and $\widetilde{u}_L$ coincide. The parts (2.15) then form an orthogonal decomposition of u. The same holds if $\widehat{\chi}$ is the characteristic function of any other region like a cube, for example. On the other hand, the $\widehat{\chi}^{\,(l)}$ become arbitrarily smooth if $\widehat{\chi}$ is chosen accordingly.

The number of the parts $u^{\,(l)}$ in (2.17) that are essentially different from each other depends on the symmetry properties of the wavefunction u with respect to the exchange of the electron coordinates. In the most extreme case of complete antisymmetry, only the multiindices l with $l_1 \ge \cdots \ge l_N$ are left. The number of these multindices is bounded independent of the number N of electrons, as Hackbusch noticed [9]. This is seen as follows. Let $c(k, L)$ denote the number of the monotonely decreasing infinite sequences $l_1, l_2, \ldots$ of nonnegative integers $l_i \le k$ that sum up to the value L. The number of the parts (2.15) in (2.17) that are essentially different from each other is then less equal the sum of the $c(k, k)$ for $k \le L$. The numbers $c(k, L)$ can be calculated recursively. The recursion starts with $c(k, 0) = 1$ for $L = 0$; only the zero sequence exists in that case. For $L \ge 1$,

$$c(k, L) \;=\; \sum_{l_1=1}^{\min(k,L)} c(l_1, L - l_1) \tag{2.19}$$

as every sequence starting with $l_1 \le k$ and necessarily $l_1 \le L$ can be followed by any of the $c(l_1, L - l_1)$ sequences $l_2, l_3, \ldots$ with $l_2 \le l_1$ summing up to $L - l_1$. Typical values are $c(10, 10) = 42$ and $c(30, 30) = 5604$. The argumentation for the general case of wavefunctions satisfying the symmetry conditions enforced by the Pauli principle is similar.

3 The sparse grid representation of the bandlimited part

In the second step, the parts (2.15) of the given function u are approximated by linear combinations of ansatz functions centered around the points of anisotropic rectangular grids. First, the functions (2.14) are represented as

$$\widehat{\chi}^{\,(l)}(\omega) \;=\; \big(\widehat{\phi}^{\,(l)}(\omega)\big)^2. \tag{3.1}$$

Setting $\widehat{v}^{\,(l)} = \widehat{\phi}^{\,(l)}\,\widehat{u}$, the parts (2.15) then can be written in the form

$$u^{\,(l)}(x) \;=\; \left(\frac{1}{\sqrt{2\pi}}\right)^{3N} \int \widehat{\phi}^{\,(l)}(\omega)\,\widehat{v}^{\,(l)}(\omega)\exp(\mathrm{i}\,\omega\cdot x)\,d\omega. \tag{3.2}$$

The essential idea is to expand the $\widehat{v}^{\,(l)}$ locally into Fourier series

$$\widehat{v}^{\,(l)}(\omega) \;=\; \left(\frac{1}{\sqrt{8}}\right)^{3N+|\,l\,|} \sum_{k\in\mathbb{Z}^{3N}} c_k^{(l)} \exp(\mathrm{i}\,D_l^{-1}k\cdot\omega) \tag{3.3}$$

where $|\,l\,| = l_1 + \cdots + l_N$ and the linear transformation

$$D_l\omega \;=\; \frac{4}{\pi}\left(2^{l_1}\omega_1,\;\ldots\,,2^{l_N}\omega_N\right) \tag{3.4}$$

maps $[-\pi,\pi]^{3N}$ onto a region covering the support of $\widehat{\phi}^{\,(l)}$. Then

$$\sum_k |c_k^{(l)}|^2 \;=\; \int \widehat{\chi}^{\,(l)}(\omega)|\widehat{u}(\omega)|^2 d\omega. \tag{3.5}$$

Inserting (3.3) into (3.2), one recognizes that the part $u^{\,(l)}$ of u can be approximated arbitrarily well by the functions in the space

$$\mathcal{V}_l \;=\; \text{span}\left\{\,\phi^{\,(l)}(\,\cdot\,-D_l^{-1}k)\,\middle|\,k\in\mathbb{Z}^{3N}\right\} \tag{3.6}$$

with respect to every given Sobolev norm where

$$\phi^{\,(l)}(x) \;=\; \left(\frac{1}{\sqrt{2\pi}}\right)^{3N}\int \widehat{\phi}^{\,(l)}(\omega)\exp(\mathrm{i}\,\omega\cdot x)d\omega \tag{3.7}$$

splits in an obvious way into a product of three-dimensional functions of two distinct types tending faster to zero the smoother the $\widehat{\phi}^{\,(l)}$ are. We thus have arrived in the sparse grid representation of the bandlimited part:

Theorem 3 *The bandlimited parts (2.17) of square integrable functions u are contained in the closed linear hull of the spaces*

$$\mathcal{V}_l,\quad l_1+\cdots+l_N\le L, \tag{3.8}$$

spanned by the translates of the functions (3.7) centered around the points

$$D_l^{-1}k,\quad k\in\mathbb{Z}^{3N}, \tag{3.9}$$

in position space together forming an infinitely extended sparse grid.

4 The role of exponential decay

Theorems 2 and 3 outline the kind of approximation properties that can be expected for functions with L_2-bounded mixed derivatives. To localize the approximations, the decay behavior of the wavefunctions or equivalently the smoothness of their Fourier transforms has to be brought into play. We refer to [1] for a very comprehensive study of the decay behavior of eigenfunctions of second order elliptic operators like the electronic Schrödinger operator (1.1). A typical result of this kind has already been indicated in the introduction: For all eigenfunctions u belonging to eigenvalues λ below the bottom Σ^* of the essential spectrum or, in the language of physics, all bound states, and all Σ strictly between λ and Σ^*, the functions

$$x\;\;\rightarrow\;\;w(x)u(x),\;\;w(x)(\nabla u)(x),\;\;w(x)(\Delta u)(x), \tag{4.1}$$

with w the exponentially increasing weight function

$$w(x) = \exp\left(\sqrt{2\,(\Sigma-\lambda)}\,|\,x\,|\right) \tag{4.2}$$

are square integrable. That is, these eigenfunctions and their first and second order weak partial derivatives decay exponentially in the L_2-sense; the decay rate cannot be further improved. By the relations between a function and its Fourier transform, this not only means that the Fourier transforms of such wavefunctions are infinitely differentiable, but also that the integrals

$$\int \left(1 + |\omega|^2\right)^2 |(D^\alpha \widehat{u})(\omega)|^2 d\omega \tag{4.3}$$

can be controlled and in particular all remain finite. This fact allows to approximate the parts (2.15) of the wavefunction representing the different resolution levels very efficiently.

At this point, also the smoothness of the functions $\widehat{\chi}^{(l)}$ or $\widehat{\phi}^{(l)}$ enters. In the extreme case, the $\widehat{v}^{(l)}$ are as smooth as $\widehat{u}$ itself. The smoothness of the Fourier transform is then fully exploited and a very fast convergence is achieved in (3.3). The contributions of the translates then decrease very rapidly with increasing distance of their centers to the origin. Constructions like the one presented in this article therefore have the potential to break the current complexity barriers in quantum mechanical calculations.

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