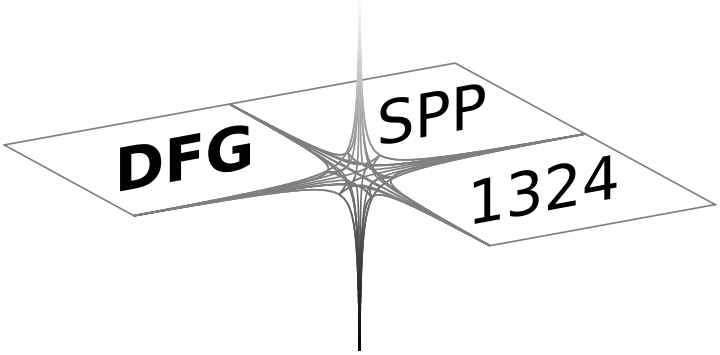
DFG-Schwerpunktprogramm 1324

„Extraktion quantifizierbarer Information aus komplexen Systemen”

On the Complexity of the Electronic Schrödinger Equation

H. Yserentant

Preprint 50



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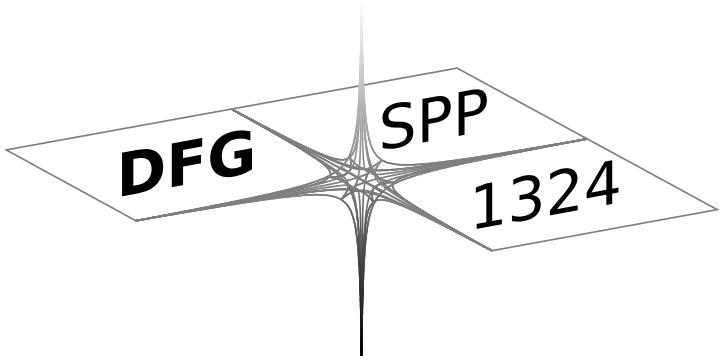

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On the complexity of the electronic Schrödinger equation

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The solutions of the electronic Schrödinger equation are high-dimensional objects depending on $3N$ variables, three for each of the N electrons under consideration. It is therefore rather surprising that simple expansions of the electronic wave functions can be constructed whose convergence rate, measured in terms of the number of determinants involved, is independent of the number of electrons and does not fall below that for a two- or even that for a one-electron system approximated in the same way. In this sense, the complexity of the electronic Schrödinger equation does not exceed that of an equation in three space dimensions. The purpose of this paper is to report on these developments and to explain the basic effects on which these results rely.

I. INTRODUCTION

Approximating the solutions of the electronic Schrödinger equation is without doubt one of the basic tasks of quantum chemistry. The electronic Schrödinger equation describes the motion of a finite set of electrons in the field of a given number of clamped nuclei. Its solutions are the eigenfunctions of the Hamilton operator

$$H \;=\; -\,\frac{1}{2}\sum_{i=1}^{N}\Delta_i \;+\; V_{ne} \;+\; \frac{1}{2}\sum_{\substack{i,j=1\\ i\neq j}}^{N}\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|} \qquad (1)$$

that is written down here in atomic units. It acts on functions with arguments $\mathbf{x}_1,\ldots,\mathbf{x}_N$ in the three-dimensional space, which are associated with the positions of the considered electrons. The external potential

$$V_{ne} \;=\; -\sum_{i=1}^{N}\sum_{\nu=1}^{K}\frac{Z_\nu}{|\mathbf{x}_i-\mathbf{a}_\nu|} \qquad (2)$$

covers the interaction of the electrons with the nuclei that are kept fixed at the positions $\mathbf{a}_1,\ldots,\mathbf{a}_K$. The Z_ν are the charges of the nuclei in multiples of the electron charge.

The problem with this equation is its high dimensionality which immediately rules out classical discretization methods for partial differential equations as they are used in engineering applications. To overcome this curse of dimensionality, procedures like the Hartree-Fock method and its many variants and successors or density functional theory based methods have been developed over the decades. While these methods are applied with much success, they suffer, however, either from modeling errors or from the fact that it is not clear how the accuracy can be systematically improved without the effort truly exploding for larger numbers of electrons.

It is therefore rather surprising that simple expansions of the electronic wave functions can be constructed whose convergence rate, measured in terms of the number of determinants involved, is independent of the number of electrons and does not fall below that for a two-electron system[1]. It is even possible to reach a convergence rate as for the case of a single electron adding a simple regularizing factor that depends explicitly on the interelectronic distances[2]. The purpose of the present paper is to report on these developments and to explain the basic effects behind these results. For details and rigorous proofs we refer to the mentioned mathematical literature.

II. A MODEL PROBLEM

The principle behind these constructions can best be understood by means of a model problem, the mean-square approximation of functions u of the variables $x_1,\ldots,x_d$ that are odd and 2π-periodic in every coordinate direction on the cube $Q=[0,\pi]^d$ by tensor products

$$\phi(\mathbf{k},\mathbf{x}) \;=\; \prod_{i=1}^{d}\phi_{k_i}(x_i) \qquad (3)$$

of the one-dimensional trigonometric polynomials

$$\phi_{k_i}(\xi) \;=\; \sqrt{\frac{2}{\pi}}\,\sin(k_i\xi) \qquad (4)$$

labeled by the components $k_i = 1,2,\ldots$ of the multi-indices $\mathbf{k}$. Functions of this kind that are square integrable over the cube Q can be expanded into a multivariate Fourier series

$$u(\mathbf{x}) \;=\; \sum_{\mathbf{k}}\widehat{u}(\mathbf{k})\phi(\mathbf{k},\mathbf{x}), \qquad (5)$$

where the expansion coefficients are given by

$$\widehat{u}(\mathbf{k}) \;=\; \int_Q u(\mathbf{x})\phi(\mathbf{k},\mathbf{x})\,\mathrm{d}\mathbf{x}. \qquad (6)$$

We measure the speed of convergence of this series in the sense of the L_2-norm whose square is

$$\|u\|_0^2 \;=\; \int_Q |u(\mathbf{x})|^2\,\mathrm{d}\mathbf{x} \qquad (7)$$

and reads in terms of the expansion coefficients

$$\|u\|_0^2 \;=\; \sum_{\mathbf{k}}|\widehat{u}(\mathbf{k})|^2. \qquad (8)$$

The speed of convergence of the series is therefore determined by the speed with which the expansion coefficients

decay. Assume that all partial derivatives of u of order s exist and are square integrable. This implies that

$$|\,u\,|_s^2 \;=\; \sum_{\mathbf{k}} |\,\mathbf{k}\,|^{2s}\,|\widehat{u}(\mathbf{k})|^2 \tag{9}$$

remains finite, where $|\,\mathbf{k}\,|$ is defined by

$$|\,\mathbf{k}\,|^2 \;=\; \sum_{i=1}^{d} k_i^2. \tag{10}$$

Consider now the finite part u_ε of the series (5) that extends over the multi-indices $\mathbf{k}$ inside the ball of radius $1/\varepsilon$ around the origin, that is, for which

$$|\,\mathbf{k}\,| \;<\; \frac{1}{\varepsilon}. \tag{11}$$

Due to the orthonormality of the functions (3), u_ε is the best approximation of u by a linear combination of the selected basis functions and satisfies the error estimate

$$\|u-u_\varepsilon\|_0^2 \;\le\; \varepsilon^{2s} \sum_{\mathbf{k}} |\,\mathbf{k}\,|^{2s}\,|\widehat{u}(\mathbf{k})|^2 \;=\; \varepsilon^{2s}\,|\,u\,|_s^2. \tag{12}$$

The number n of these basis functions grows like

$$n \;\sim\; \frac{1}{\varepsilon^d} \tag{13}$$

as ε goes to zero. The error thus decreases like

$$\sim\; \frac{1}{n^{s/d}} \tag{14}$$

in terms of the number n of the basis functions involved. For the order of differentiability s kept fixed, this is out of every reach for higher space dimensions d, the curse of dimensionality. It can only be broken if one restricts oneself to a class of functions whose smoothness increases sufficiently fast with the dimension d, for which s grows proportionally to d, for example.

The problem is that electronic wave functions are not especially smooth, generally not even differentiable at the singular points of the interaction potentials. The question is therefore how much the smoothness or regularity requirements can be relaxed without giving up the independence of the convergence rate from the space dimension. Assume that u possesses corresponding partial derivatives and that these are continuous and set

$$|\,u\,|_{1,\mathrm{mix}}^2 \;=\; \int_Q \Big|\,\frac{\partial^d u}{\partial x_1 \ldots \partial x_d}\,\Big|^2 \,\mathrm{d}\mathbf{x} \tag{15}$$

or, in terms of the expansion coefficients,

$$|\,u\,|_{1,\mathrm{mix}}^2 \;=\; \sum_{\mathbf{k}} \Big(\prod_{i=1}^{d} k_i\Big)^2\,|\widehat{u}(\mathbf{k})|^2. \tag{16}$$

Let u_ε^* be the function represented by the finite part of the series (5) that extends over the multi-indices $\mathbf{k}$ now not inside a ball (11) but inside the hyperboloid given by

$$\prod_{i=1}^{d} k_i \;<\; \frac{1}{\varepsilon}. \tag{17}$$

The L_2-error can then as above be estimated as

$$\|u-u_\varepsilon^*\|_0 \;\le\; \varepsilon\,|\,u\,|_{1,\mathrm{mix}} \tag{18}$$

and tends like $\mathcal{O}(\varepsilon)$ to zero. The difference is that the dimension n of the space spanned by the functions (3) for which (17) holds, now increases only like

$$n \;\sim\; |\log\varepsilon\,|^{d-1}\varepsilon^{-1}. \tag{19}$$

This shows that a comparatively slow growth of the smoothness can help to reduce the complexity substantially, an observation that forms the basis of the sparse grid or hyperbolic cross techniques that emerged from the Russian school of numerical analysis and approximation theory[3–5] and have since then been reinvented several times[6–8]. Since the work of Zenger[8], approaches of this kind have become increasingly popular in the numerical solution of partial differential equations[9]. Due to the presence of the logarithmic term, the applicability of such methods is, however, still limited to moderate space dimensions.

The rescue comes from the symmetry properties of the wave functions of a system of indistinguishable particles. They represent a possibility to escape from this dilemma without forcing up the smoothness requirements further, which has first been noted by Hackbusch[10]. Assume that the functions u to be approximated are antisymmetric with respect to the exchange of their variables, i.e., that

$$u(\mathbf{P}\mathbf{x}) \;=\; \mathrm{sign}(\mathbf{P})\,u(\mathbf{x}) \tag{20}$$

holds for all permutation matrices $\mathbf{P}$. It is not astonishing that symmetry properties such as the given one are immediately reflected in the expansion (5). Let

$$\widetilde{\phi}(\mathbf{k},\mathbf{x}) \;=\; \frac{1}{\sqrt{d!}} \sum_{\mathbf{P}} \mathrm{sign}(\mathbf{P})\,\phi(\mathbf{k},\mathbf{P}\mathbf{x}) \tag{21}$$

be the renormalized, antisymmetric parts of the functions (3), where the sums extend over the $d!$ permutation matrices $\mathbf{P}$ of order d. They can be written as determinants

$$\frac{1}{\sqrt{d!}} \begin{vmatrix} \phi_{k_1}(x_1) & \ldots & \phi_{k_d}(x_1) \\ \vdots & \ddots & \vdots \\ \phi_{k_1}(x_d) & \ldots & \phi_{k_d}(x_d) \end{vmatrix} \tag{22}$$

and easily evaluated in this way. For the functions u in the given symmetry class, many terms in the expansion (5) can be combined. It finally collapses into

$$u(\mathbf{x}) \;=\; \sum_{k_1>\ldots>k_d} \big(u,\widetilde{\phi}(\mathbf{k},\,\cdot\,)\big)\widetilde{\phi}(\mathbf{k},\mathbf{x}), \tag{23}$$

where the expansion coefficients are the L_2-inner products of u with the corresponding functions (21). The number of basis functions needed to reach a given accuracy is reduced by more than the factor $d!$, a very significant gain for larger dimensions d.

It remains to count the number of the ordered sequences $k_1 > k_2 > \ldots > k_d$ of natural numbers that satisfy the condition (17) and with that also the number of basis function (21) needed to reach the accuracy $\mathcal{O}(\varepsilon)$. To study the asymptotic behavior of the number of these sequences in dependence of the dimension d and the accuracy ε, it suffices when we restrict ourselves to the case $\varepsilon = 1/2^L$, with positive integers L. That is, we have to give bounds for the number of sequences $k_1 > \ldots > k_d$ of natural numbers $k_i = 1, 2, \ldots$ for which

$$\prod_{i=1}^{d} k_i \;\leq\; 2^L. \tag{24}$$

The problem to estimate this number has to do with the prime factorization of integers. To simplify this problem, we group the numbers k_i into levels. Let

$$\ell(k_i) \;=\; \max\left\{\, \ell \in \mathbb{Z} \;\middle|\; 2^{\,\ell} \leq k_i \,\right\}. \tag{25}$$

An upper bound for the number of these sequences is then the number $a(d, L)$ of the strictly decreasing sequences $k_1 > k_2 > \ldots > k_d$ of natural numbers for which

$$\prod_{i=1}^{d} 2^{\,\ell(k_i)} \leq\; 2^L. \tag{26}$$

The numbers $a(d, L)$ can be calculated recursively[1]. If

$$d \;=\; \sum_{\ell=0}^{m} 2^{\,\ell} + j, \quad 0 \leq j < 2^{m+1}, \tag{27}$$

the minimum L for which $a(d, L) > 0$ is that for which the single levels ℓ are maximally filled, that is, since there are $2^{\,\ell}$ numbers k_i for which $\ell(k_i) = 2^{\,\ell}$,

$$L \;=\; \sum_{\ell=0}^{m} 2^{\,\ell}\,\ell + j\,(m+1). \tag{28}$$

Let $L(d)$ denote this minimum L assigned to the number d given by (27). The $L(d)$ increase very rapidly; for $d = 179$ already $L(d) > 1000$. A crude estimate yields $a(d, L) = 0$ if $L + 1 < d$. Thus

$$a^*(L) \;:=\; \max_{d \geq 1} a(d, L) \;=\; \max_{d \leq L+1} a(d, L). \tag{29}$$

Figure 1 shows, in logarithmic scale, how the $a(d, L)$ behave compared to their joint least upper bound $a^*(L)$. It becomes obvious from this picture that this common upper bound exceeds the actual dimensions for larger d by many orders of magnitude, the more the more the number d of variables increases.

The joint least upper bound that is independent of d for the number of the sequences $k_1 > \ldots > k_d$ of natural numbers k_i for which (24) holds grows at least like $\sim 2^L$. The reason for that is that already in the case $d = 1$, there are 2^L such "sequences", namely those with values

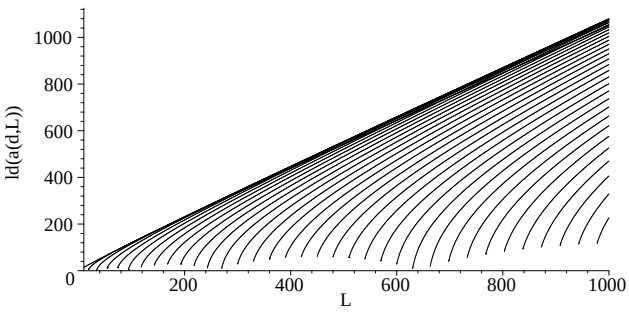

FIG. 1. The numbers $a(d, L)$ for $d = 10, 15, 20, \ldots, 175$

$k_1 = 1, \ldots, 2^L$. Figure 1 suggests conversely that the upper bound (29) for the number of these sequences does not grow much faster than $\sim 2^L$. This is in fact the case since the number of the decreasing infinite sequences $k_1 \geq k_2 \geq k_3 \geq \ldots$ of natural numbers for which

$$\prod_{i=1}^{\infty} 2^{\,\ell(k_i)} \leq\; 2^L, \tag{30}$$

with L a given nonnegative integer, is bounded by

$$\sum_{\ell=0}^{L} p(\ell)\, 2^{\,\ell}, \tag{31}$$

where $p(\ell)$ denotes the partition number of ℓ, the number of possibilities of representing ℓ as sum of nonnegative integers without regard to the order.

To show this, we observe that the number of these sequences is bounded from above by the number of sequences $k_1, k_2, k_3, \ldots$ of natural numbers for which at least their levels $\ell(k_1), \ell(k_2), \ldots$ decrease and that satisfy (30). We show that the expression (31) counts the number of these sequences. Let the integers $\ell_i = \ell(k_i)$ first be given. As there are $2^{\,\ell_i}$ natural numbers k_i for which $\ell(k_i) = \ell_i$, namely $k_i = 2^{\,\ell_i}, \ldots, 2^{\,\ell_i+1} - 1$, there are

$$\prod_{i=1}^{\infty} 2^{\,\ell_i} \;=\; 2^{\,\ell}, \quad \ell \;=\; \sum_{i=1}^{\infty} \ell_i, \tag{32}$$

sequences $k_1, k_2, k_3, \ldots$ for which the $\ell(k_i)$ attain the prescribed values ℓ_i. The problem thus reduces to the question how many decreasing sequences of nonnegative integers ℓ_i exist that sum up to values $\ell \leq L$, i.e., for which

$$\sum_{i=1}^{\infty} \ell_i \;=\; \ell. \tag{33}$$

This number is by definition the partition number $p(\ell)$ of the nonnegative integer ℓ.

Every sequence $k_1 > k_2 > \ldots > k_d$ of natural numbers for which (24) holds can obviously be expanded to an infinite, decreasing sequence $k_1 \geq k_2 \geq k_3 \geq \ldots$ of natural numbers that satisfies the condition (30) by setting all

$k_i = 1$ for $i > d$. The sum (31) represents therefore also an upper bound for the number of these sequences.

The partition number plays a big role in combinatorics and has first been studied by Euler. Hardy and Ramanujan[11] have shown it behaves asymptotically like

$$p(\ell) \;=\; \left(\frac{1}{4\sqrt{3}} + o(1)\right) \frac{\exp\left(\pi\,\sqrt{2\ell/3}\,\right)}{\ell} \tag{34}$$

as ℓ goes to infinity. They established also a somewhat weaker, nevertheless for our purposes sufficient estimate[1]

$$p(\ell) \;\le\; \frac{K}{\ell}\,\mathrm{e}^{\,2\sqrt{2\ell}}, \tag{35}$$

with K a constant independent of ℓ. We conclude that the upper bound (29) behaves like

$$a^*(L) = (2^L)^{1+\varepsilon(L)}, \quad 0 \le \varepsilon(L) \le cL^{-1/2}, \tag{36}$$

where c is a constant independent of L. Using the representation (29) and the recursively calculated values $a(d, L)$, the exponents $1+\varepsilon(L)$ can be calculated exactly. They decay for L ranging from 10 to 1000 monotonely from 1.406 to 1.079. For $L = 100$, $1 + \varepsilon(L) = 1.204$. In other words, the error decreases now faster than

$$\sim \frac{1}{n^{1-\vartheta}}, \tag{37}$$

with $\vartheta > 0$ chosen arbitrarily small, in terms of the number n of determinants involved. Not only does the convergence rate deteriorate neither with the dimension nor the number of variables, it behaves asymptotically almost as in the one-dimensional case. Similar results hold for partially antisymmetric functions as they occur in quantum mechanics and will be considered in the sequel.

III. WEAK DERIVATIVES AND WEAK SOLUTIONS

The essential condition that the above estimate for the convergence rate holds is that the expression (16) remains finite, which, however, does not conversely mean that the derivatives appearing in (15) must exist. The property that characterizes this condition is the existence of corresponding so-called weak derivatives, to which this section is devoted. We restrict ourselves hereby to functions that are defined on the whole $3N$-dimensional space.

The wave functions depend on the three-dimensional position vectors $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ of the electrons that split into the coordinates $x_{i,1}$, $x_{i,2}$, and $x_{i,3}$. Accordingly, we label partial derivatives doubly, that is, by multi-indices

$$\boldsymbol{\alpha} = (\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_N), \quad \boldsymbol{\alpha}_i = (\alpha_{i,1}, \alpha_{i,2}, \alpha_{i,3}), \tag{38}$$

with integer components $\alpha_{i,\nu} \ge 0$. The differentiation operator $\mathrm{D}^{\boldsymbol{\alpha}}$ of order $|\boldsymbol{\alpha}| = \sum_{i,\nu} \alpha_{i,\nu}$ reads in this notation

$$\mathrm{D}^{\boldsymbol{\alpha}} = \prod_{i=1}^{N} \prod_{\nu=1}^{3} \Big(\frac{\partial}{\partial x_{i,\nu}}\Big)^{\alpha_{i,\nu}}. \tag{39}$$

Correspondingly one defines the monomials

$$\mathbf{x}^{\boldsymbol{\alpha}} = \prod_{i=1}^{N} \prod_{\nu=1}^{3} x_{i,\nu}^{\alpha_{i,\nu}}. \tag{40}$$

Weak derivatives play an important role in the theory of partial differential equations and can be introduced in different ways. We start from the Fourier transform

$$\widehat{u}(\mathbf{k}) \;=\; \Big(\frac{1}{\sqrt{2\pi}}\Big)^{3N} \int u(\mathbf{x})\,\mathrm{e}^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\,\mathrm{d}\mathbf{k} \tag{41}$$

of infinitely differentiable functions u that vanish together with all their derivatives at infinity more rapidly than any polynomial increases. The Fourier transform of the derivative $\mathrm{D}^{\boldsymbol{\alpha}} u$ of such a function reads

$$(\widehat{\mathrm{D}^{\boldsymbol{\alpha}} u})(\mathbf{k}) \;=\; (\mathrm{i}\mathbf{k})^{\boldsymbol{\alpha}}\,\widehat{u}(\mathbf{k}). \tag{42}$$

Like $\mathrm{D}^{\boldsymbol{\alpha}} u$ itself, it is square integrable and

$$\int |(\widehat{\mathrm{D}^{\boldsymbol{\alpha}} u})(\mathbf{k})|^2\,\mathrm{d}\mathbf{k} \;=\; \int |(\mathrm{D}^{\boldsymbol{\alpha}} u)(\mathbf{x})|^2\,\mathrm{d}\mathbf{x}. \tag{43}$$

Fourier back transformation yields vice versa

$$(\mathrm{D}^{\boldsymbol{\alpha}} u)(\mathbf{x}) \;=\; \Big(\frac{1}{\sqrt{2\pi}}\Big)^{3N} \int (\mathrm{i}\mathbf{k})^{\boldsymbol{\alpha}}\,\widehat{u}(\mathbf{k})\,\mathrm{e}^{\,\mathrm{i}\mathbf{k}\cdot\mathbf{x}}\,\mathrm{d}\mathbf{k}. \tag{44}$$

Conversely we say that a square integrable function u possesses a square integrable weak derivative $\mathrm{D}^{\boldsymbol{\alpha}} u$ if the function $\mathbf{k} \to (\mathrm{i}\mathbf{k})^{\boldsymbol{\alpha}}\,\widehat{u}(\mathbf{k})$ is square integrable too. The weak derivative $\mathrm{D}^{\boldsymbol{\alpha}} u$ is then obtained from this function by Fourier back transformation. A weakly differentiable function does not need to be differentiable in the usual sense. The hydrogen ground state wave function

$$u(\mathbf{x}) \;=\; \frac{1}{\sqrt{\pi}}\,\mathrm{e}^{-|\mathbf{x}|} \tag{45}$$

represents such an example. Its Fourier transform is

$$\widehat{u}(\mathbf{k}) \;=\; \frac{\sqrt{2}}{\pi}\,\frac{2}{(1+|\mathbf{k}|^2)^2}. \tag{46}$$

It possesses therefore weak partial derivatives of orders one and two but is, of course, not differentiable at the origin. If we speak in the sequel of derivatives we will mean weak derivatives unless stated otherwise.

The concept of weak derivatives can be used to fix the behavior of the eigenfunctions at the singular points of the interaction potentials and at infinity and thus to state precisely what we mean by a solution of the electronic Schrödinger equation. The solution space of the electronic Schrödinger equation is the Hilbert space H^1 consisting of the square integrable functions of the electron positions with square integrable first-order weak derivatives or, in the language of physics, of the wave functions representing states of finite kinetic energy. It contains the normed functions u of finite total energy $a(u, u)$, where

$$a(u, v) \;=\; \int \Big\{\, \frac{1}{2} \sum_{i=1}^{N} \nabla_i u \cdot \nabla_i v \;+\; V u\, v \,\Big\}\,\mathrm{d}\mathbf{x} \tag{47}$$

denotes the associated bilinear form. The potential V is composed of the electron-electron interaction potential and the nucleus-electron interaction potential. To show this, one needs the three-dimensional Hardy inequality

$$\int \frac{1}{|\mathbf{x}|^2}\, v^2 \,\mathrm{d}\mathbf{x} \;\le\; 4 \int |\nabla v|^2 \,\mathrm{d}\mathbf{x} \tag{48}$$

that allows one to estimate the potential energy by the kinetic energy. Hardy-type inequalities play also an important role in the derivations and proofs of the results presented here. For infinitely differentiable functions u and v that vanish sufficiently fast at infinity, the bilinear form can be rewritten in terms of the Hamiltonian (1):

$$a(u,v) \;=\; \int Hu\, v \,\mathrm{d}\mathbf{x} \;=\; (Hu, v), \tag{49}$$

as is shown integrating by parts. The variational or weak form of the Schrödinger equation $Hu = \lambda u$ formally results from multiplying this equation with test functions v, integrating it and transforming the integrals on the left hand side integrating by parts. It reads as follows: Find functions $u \neq 0$ in H^1 and eigenvalues λ such that

$$a(u,v) \;=\; \lambda\,(u,v) \tag{50}$$

holds for all test functions v in this space, that is, find the stationary points of the Rayleigh quotient

$$\frac{a(u,u)}{(u,u)}. \tag{51}$$

Such weak solutions solve the electronic Schrödinger equation $Hu = \lambda u$ in the usual, classical sense outside the singular points of the interaction potentials. It should, however, be noted that only those solutions of the equation (50) are physically admissible that are antisymmetric with respect to the exchange of the positions of electrons of the same spin. This is a consequence of the Pauli principle and basic for our further considerations.

We are interested in eigenfunctions u for eigenvalues below the bottom of the essential spectrum, that is, in bound states. It is well-known that such eigenfunctions decay exponentially in the L_2-sense. That means there is a constant $\gamma > 0$ depending on the distance of the eigenvalue under consideration to the bottom of the essential spectrum such that the exponentially weighted function

$$\mathbf{x} \;\to\; \exp\left(\gamma \sum_{i=1}^{N} |\mathbf{x}_i|\right) u(\mathbf{x}) \tag{52}$$

is square integrable. That implies that all polynomial multiples of the eigenfunctions are square integrable.

IV. HIGHER ORDER DERIVATIVES

The aim is to transfer the techniques from the penultimate section from the simple model problem there to the solutions of the much more complicated Schrödinger equation (50). One may wonder that this can work considering all the singularities in the electron-electron interaction potential and the external potential (2). The deeper reason for that is that the terms of which these potentials are composed depend only on the coordinates of one or two electrons. This and the symmetry properties enforced by the Pauli principle suffice to show that the admissible solutions of the electronic Schrödinger equation fit into the indicated framework.

The key to a successful application of the mentioned techniques to the Schrödinger equation is the existence of high-order (weak) derivatives of the solutions representing bound states and, as the domain of definition is unbounded, the rapid decay of these derivatives. To describe the differentiability properties, let $\mathcal{A}$ be the set of the multi-indices $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_1, \ldots, \boldsymbol{\alpha}_N)$ for which

$$\alpha_{i,1} + \alpha_{i,2} + \alpha_{i,3} \;\le\; 1. \tag{53}$$

The maximum order that the assigned differentiation operators $\mathrm{D}^{\boldsymbol{\alpha}}$ can reach is N and grows therefore with the number of electrons; their order is, however, at most one in the components of the position vectors of the single electrons i. Subsets of this set of multi-indices are the set $\mathcal{A}_-$ consisting of the $\boldsymbol{\alpha}$ in $\mathcal{A}$ with components $\boldsymbol{\alpha}_i = \mathbf{0}$ for all electrons i with spin $+1/2$ and the correspondingly defined set $\mathcal{A}_+$ consisting of the $\boldsymbol{\alpha}$ in $\mathcal{A}$ with components $\boldsymbol{\alpha}_i = \mathbf{0}$ for the electrons i with spin $-1/2$. The corresponding operators $\mathrm{D}^{\boldsymbol{\alpha}}$ intermix only partial derivatives with respect to coordinates of electrons of the same spin. One of our main results[12,13] is that the weak derivatives

$$\mathrm{D}^{\boldsymbol{\alpha}} u, \;\; \frac{\partial}{\partial x_{i,\nu}} \mathrm{D}^{\boldsymbol{\alpha}} u \tag{54}$$

of the bound state solutions u of the electronic Schrödinger equation exist for all $\boldsymbol{\alpha}$ in $\mathcal{A}_-$ and in $\mathcal{A}_+$ and are square integrable. Moreover, they decay exponentially in the L_2-sense[1], that is, the functions

$$\exp\left(\gamma \sum_{i=1}^{N} |\mathbf{x}_i|\right) \mathrm{D}^{\boldsymbol{\alpha}} u, \;\; \left(\gamma \sum_{i=1}^{N} |\mathbf{x}_i|\right) \frac{\partial}{\partial x_{i,\nu}} \mathrm{D}^{\boldsymbol{\alpha}} u, \tag{55}$$

with the same coefficients $\gamma > 0$ as in (52), are square integrable. With that every polynomial multiple of the derivatives (54) is again square integrable too. The author's monograph mentioned in the introduction contains a thorough mathematical discussion of these results, including of some quantitative aspects.

V. REGULARIZING FACTORS

The proof of the results described in the previous sections utilizes that the physically admissible wave functions are by the Pauli principle antisymmetric under the exchange of electrons of same spin. Thus they vanish where such electrons meet, or avoid that they ever meet,

which counterbalances the singularities of the electron-electron interaction potential there. The singularities at the places where electrons of distinct spin meet are considerably stronger. This is the reason why it is not possible to show that the derivatives (54) and their exponentially weighted counterparts (55) are square integrable for all multi-indices $\boldsymbol{\alpha}$ in the set $\mathcal{A}$.

To overcome this problem, the electron correlation has to be taken into account explicitly, an approach that can be traced back to the work of Hylleraas[14] in the twenties of the last century. We partition the solutions u of the electronic Schrödinger equation into a regular part

$$u_0(\mathbf{x}) \,=\, \exp\left(-\sum_{i<j}\phi(\mathbf{x}_i-\mathbf{x}_j)\right)u(\mathbf{x}) \tag{56}$$

and a universal factor that covers the electron cusps already to a large extent. The function ϕ has to satisfy some technical conditions[2] that mainly concern the decay behavior of its first and second-order derivatives and its behavior at the origin. A possible example is

$$\phi(\mathbf{x}_i-\mathbf{x}_j) \,=\, \ln\Big(1+\frac{1}{2}\,|\mathbf{x}_i-\mathbf{x}_j|\Big), \tag{57}$$

or even simpler than this,

$$\phi(\mathbf{x}_i-\mathbf{x}_j) \,=\, \frac{1}{2}\,|\mathbf{x}_i-\mathbf{x}_j|. \tag{58}$$

The crucial point is that the weak derivatives

$$\mathrm{D}^{\boldsymbol{\alpha}}u_0,\quad \frac{\partial}{\partial x_{i,\nu}}\,\mathrm{D}^{\boldsymbol{\alpha}}u_0 \tag{59}$$

and even their exponentially weighted counterparts as in (55) are square integrable for all multi-indices $\boldsymbol{\alpha}$ in the set $\mathcal{A}$ introduced in the previous section, not only for the $\boldsymbol{\alpha}$ in $\mathcal{A}_-$ and $\mathcal{A}_+$. This reflects the fact that the regularizing factor largely compensates the singular behavior of the wave functions at the points where two or more electrons meet[2]. Approximations of the wave functions u can be found first approximating their regular parts (56) and then dividing the result by the given universal factor.

The same kind of results as for the regular parts (56) also hold if the regularizing factor is replaced by factor

$$\exp\left(2\sum_{i,\nu}Z_\nu\,\phi(\mathbf{x}_i-\mathbf{a}_\nu)\,-\sum_{i<j}\phi(\mathbf{x}_i-\mathbf{x}_j)\right) \tag{60}$$

that contains an additional term smoothing the singularities at the positions $\mathbf{a}_\nu$ of the nuclei. This additional term does not improve the mixed regularity of the wave functions and from this point of view is of little value. The crucial observation is that the eigenfunctions can be locally represented as the reciprocal of this factor times a real-analytic function plus a real-analytic function outside the points where more than two particles meet, provided that $\phi(\mathbf{x}) = \widetilde{\phi}(|\mathbf{x}|)$ and $\widetilde{\phi}(r)$ can be locally expanded into a power series. This can be deduced without much effort from the results in the literature[15]. The regularizing factor thus covers the singularities of the eigenfunctions in the neighborhood of such points completely. Approximation methods can clearly benefit from this although it is difficult to quantify this effect.

VI. THE RADIAL-ANGULAR DECOMPOSITION

As a first consequence of the existence and the decay of the weak derivatives of the solutions under consideration of the electronic Schrödinger equation, we discuss their decomposition into (tensor-)products of three-dimensional angular momentum eigenfunctions. Consider a complete L_2-orthonormal system

$$\phi_{n\ell m}(\mathbf{x}) \,=\, \frac{1}{r}\,f_{n\ell}(r)\,Y_\ell^m(\mathbf{x}),\quad r=|\mathbf{x}|, \tag{61}$$

of such functions, where the Y_ℓ^m are the spherical harmonics, n and ℓ are nonnegative integers, and m ranges from $-\ell$ to ℓ. The joint eigenfunctions of the harmonic oscillator and the angular momentum operators L^2 and L_3 form an example of such a system. Every square integrable function u of the electron positions $\mathbf{x}_1,\ldots,\mathbf{x}_N$ can then be expanded into an orthogonal series

$$u(\mathbf{x}) \,=\, \sum_{\mathbf{n},\boldsymbol{\ell},\mathbf{m}}\widehat{u}(\,\mathbf{n},\boldsymbol{\ell},\mathbf{m})\,\prod_{i=1}^{N}\phi_{\,n_i\ell_i m_i}(\mathbf{x}_i), \tag{62}$$

where $\mathbf{n}$, $\boldsymbol{\ell}$, and $\mathbf{m}$ are multi-indices here with components n_i, ℓ_i, and m_i. Define the orthogonal projections

$$\big(Q(\boldsymbol{\ell},\mathbf{m})u\big)(\mathbf{x}) \,=\, \sum_{\mathbf{n}}\widehat{u}(\,\mathbf{n},\boldsymbol{\ell},\mathbf{m})\,\prod_{i=1}^{N}\phi_{\,n_i\ell_i m_i}(\mathbf{x}_i) \tag{63}$$

in which the angular parts are kept fixed and the sum extends only over the corresponding radial parts. These projections can in fact be defined without recourse to the given expansion. They are not only L_2-orthogonal but also orthogonal with respect to many inner products involving derivatives, for example with respect to

$$(u,v)_1 \,=\, \int\big\{\nabla u\cdot\nabla v+uv\big\}\,\mathrm{d}\mathbf{x}, \tag{64}$$

the inner product that induces the H^1-norm given by

$$\|u\|_1^2 \,=\, \|u\|_0^2+\|\nabla u\|_0^2, \tag{65}$$

the norm in which the approximation error has to be measured. For functions in the solution space H^1,

$$\|u\|_1^2 \,=\, \sum_{\boldsymbol{\ell},\mathbf{m}}\|Q(\boldsymbol{\ell},\mathbf{m})u\|_1^2. \tag{66}$$

Let I_- and I_+ be the sets of the indices of the electrons with spin $-1/2$ respectively spin $+1/2$. The point is that the weighted norms defined by the expressions

$$|\!|\!|u|\!|\!|_\pm^2 \,=\, \sum_{\boldsymbol{\ell},\mathbf{m}}\Big\{\prod_{i\in I_\pm}\Big(1+\ell_i\,(\ell_i+1)\Big)\Big\}\|Q(\boldsymbol{\ell},\mathbf{m})u\|_1^2 \tag{67}$$

of the corresponding eigenfunctions remains finite. The proof is, roughly speaking, based on the fact that the projections $Q(\boldsymbol{\ell}, \mathbf{m})u$ are eigenfunctions of the products

$$\mathcal{L}_I \,=\, \prod_{i \in I} \mathrm{L}_i^2 \tag{68}$$

of the squares

$$\mathrm{L}_i^2 \,=\, -\,\frac{1}{2} \sum_{\substack{\nu,\mu=1 \\ \nu \neq \mu}}^{3} \left(x_{i,\nu}\, \frac{\partial}{\partial x_{i,\mu}} \,-\, x_{i,\mu}\, \frac{\partial}{\partial x_{i,\nu}} \right)^2 \tag{69}$$

of the angular momentum operators acting on the coordinates of the particles i for the eigenvalues

$$\prod_{i \in I} \ell_i \,(\ell_i + 1). \tag{70}$$

Distributing the derivatives by integration by parts to both sides and using the described results on the existence and the decay of the weak derivatives, the boundedness of the expressions $(u, \mathcal{L}_I u)_1$ for subsets I of the index sets I_- and I_+, and with that of the norms given by (67), can be shown. A mathematically rigorous form of this argument considering first functions u in a harmless dense subspace can again be found in the author's monograph cited in the introduction.

This observation means that, with given distribution of spins, the norm defined by

$$|\!|\!| u |\!|\!|^2 \,=\, |\!|\!| u |\!|\!|_-^2 \,+\, |\!|\!| u |\!|\!|_+^2 \tag{71}$$

of the corresponding eigenfunctions u of the electronic Hamilton operator remains finite. Thus only very few of the projections make a significant contribution to the eigenfunctions. To quantify this, let u_ε be that part of the expansion of u that is made up of the contributions assigned to the multi-indices $\boldsymbol{\ell}$ for which

$$\prod_{i \in I_-} \Big(1 + \ell_i \,(\ell_i + 1) \Big) + \prod_{i \in I_+} \Big(1 + \ell_i \,(\ell_i + 1) \Big) < \frac{1}{\varepsilon^2}, \tag{72}$$

where ε is again a parameter controlling the accuracy. Using the orthogonality properties of the decomposition,

$$\|u - u_\varepsilon\|_1 \,\leq\, \varepsilon\, |\!|\!| u - u_\varepsilon |\!|\!| \,\leq\, \varepsilon\, |\!|\!| u |\!|\!| \tag{73}$$

follows. The need to distinguish between the electrons with spin $-1/2$ and those with spin $+1/2$ disappears when one considers instead of the full eigenfunctions only their regular parts (56). Then the full expression

$$\sum_{\boldsymbol{\ell}, \mathbf{m}} \left\{ \prod_{i=1}^{N} \Big(1 + \ell_i \,(\ell_i + 1) \Big) \right\} \|Q(\boldsymbol{\ell}, \mathbf{m}) u_0\|_1^2 \tag{74}$$

remains finite and the contributions of the single parts to the total energy decrease like

$$\left\{ \prod_{i=1}^{N} \Big(1 + \ell_i \,(\ell_i + 1) \Big) \right\}^{-1} \tag{75}$$

with the angular momentum quantum numbers ℓ_i.

VII. EIGENFUNCTION EXPANSIONS

The eigenspaces of the products (68) of the squares of the one-electron angular momentum operators are infinite dimensional so that the considerations from the previous section do not directly lead to an error estimate for the approximation of the electronic eigenfunctions by a finite set of ansatz functions or determinants. The technique applies, however, to corresponding products composed of three-dimensional Schrödinger type operators

$$H \,=\, -\,\frac{1}{2}\,\Delta + V \tag{76}$$

with polynomially growing confinement potentials $V \geq 0$ or, with rotationally symmetric potentials V, to the sum

$$H + \mathrm{L}^2 \tag{77}$$

of such operators and the square of the angular momentum operator, that have the same eigenfunctions. Operators of this type possess an L_2-complete, L_2-orthonormal system of eigenfunctions $\phi_1, \phi_2, \phi_3, \ldots$ for strictly positive eigenvalues $0 < \lambda_1 \leq \lambda_2 \leq \ldots$ of finite multiplicity. Every square integrable function u from $(\mathbb{R}^3)^N$ to $\mathbb{R}$ can therefore be represented as L_2-convergent series

$$u(\mathbf{x}) \,=\! \sum_{\mathbf{k}} \widehat{u}(\mathbf{k}) \prod_{i=1}^{N} \phi_{k_i}(\mathbf{x}_i) \tag{78}$$

with the expansion coefficients the L_2-inner products

$$\widehat{u}(\mathbf{k}) \,=\, \Big(u,\, \prod_{i=1}^{N} \phi_{k_i} \Big), \tag{79}$$

where the sum runs over the tensor products of the three-dimensional eigenfunctions that again form a complete orthonormal system.

Let I_- and I_+ again denote the indices of the electrons with spin $-1/2$ and spin $+1/2$. Using the technique that has been indicated and sketched in the previous section one can show that, for corresponding eigenfunctions u of the electronic Schrödinger operator, the expression

$$\sum_{\mathbf{k}} \Big(\sum_{i=1}^{N} \lambda_{k_i} \Big) \Big(\prod_{i \in I_-} \lambda_{k_i} + \prod_{i \in I_+} \lambda_{k_i} \Big)\, |\widehat{u}(\mathbf{k})|^2 \tag{80}$$

remains finite. Since the norm given by the expression

$$\|u\|^2 \,=\, \sum_{\mathbf{k}} \Big(\sum_{i=1}^{N} \lambda_{k_i} \Big)\, |\widehat{u}(\mathbf{k})|^2 \tag{81}$$

dominates the H^1-norm given by (65), one can proceed as above and select the correspondingly antisymmetrized tensor products of the three-dimensional eigenfunctions for which the associated eigenvalues satisfy the estimate

$$\prod_{i \in I_-} \lambda_{k_i} + \prod_{i \in I_+} \lambda_{k_i} < \frac{1}{\varepsilon^2} \tag{82}$$

to reach an H^1-error of order $\mathcal{O}(\varepsilon)$ in the approximation of the eigenfunctions u. The need to distinguish between the electrons with spin $-1/2$ and those with spin $+1/2$ disappears again when one approximates instead of the full eigenfunctions only their regular parts (56). Then

$$\sum_{\mathbf{k}} \Big(\sum_{i=1}^{N} \lambda_{k_i} \Big) \Big(\prod_{i=1}^{N} \lambda_{k_i} \Big) \, |\widehat{u}_0(\mathbf{k})|^2 \tag{83}$$

remains finite and the contributions of the individual summands to the total energy decrease like

$$\Big\{ \prod_{i=1}^{N} \lambda_{k_i} \Big\}^{-1}. \tag{84}$$

The dimension of the approximation spaces and with that the speed of convergence measured in terms of the number of determinants involved depends on the growth of the eigenvalues of the chosen three-dimensional operator (76) or (77). The faster the potential grows, the faster they tend to infinity. They increase like

$$\lambda_k \sim k^{s/3}, \tag{85}$$

with some exponent $s < 2$. Depending on the growth of the potential, this exponent can come arbitrarily close to the value $s = 2$ but cannot completely reach or surpass it. The eigenvalues of the harmonic oscillator increase like $\sim k^{1/3}$, and those of its modification (77) like $\sim k^{1/2}$. Starting from operators (76) with potentials V that grow faster than any polynomial but not too fast in comparison to the exponential decay of the wave function to be approximated, one can even reach a growth that is faster than that of any power k^s, $s < 2/3$, but has then to switch to a more complicated technique of proof[1]. In any case, the products of the eigenvalues become rapidly very large and behave as needed to apply sparse grid approximation techniques similar to those described in the second section. Thus we have reached our aim to transfer the technique there from our model problem to the electronic Schrödinger equation.

VIII. CONSEQUENCES AND CONCLUDING REMARKS

Our estimates demonstrate that the approximation error of the eigenfunctions for eigenvalues below the bottom of the essential spectrum decreases faster than

$$\sim \frac{1}{n^{1/6-\vartheta}}, \tag{86}$$

with $\vartheta > 0$ arbitrarily small, in the number n of the involved antisymmetrized tensor products or Slater determinants built up from properly chosen three-dimensional basis functions like eigenfunctions of corresponding three-dimensional Schrödinger operators or, what is also possible, certain wavelets. The six comes from the fact that the building blocks of which the approximating functions are composed are now three-dimensional and not one-dimensional as in our model problem, which already yields a three instead of a one, and the fact that not all partial derivatives $\mathrm{D}^{\boldsymbol{\alpha}} u$ of the eigenfunctions u for multi-indices $\boldsymbol{\alpha}$ in the set $\mathcal{A}$ from the fourth section can be estimated, but only those in its subsets $\mathcal{A}_-$ and $\mathcal{A}_+$, mixing only derivatives with respect to the coordinates of electrons of same spin, which yields another factor two. We observe that the convergence rate expressed in terms of the number of determinants involved astonishingly does not deteriorate with the space dimension $3N$ or the number N of electrons. It behaves almost as with the expansion of a two-electron wave function into products of basis functions of given type. The error of the best n-term approximation even decreases almost like

$$\sim \frac{1}{n^{1/3}} \tag{87}$$

if one takes the correlation effects explicitly into account and splits the singular part of the wave functions off. This is the convergence rate that is reached for a one-electron problem and corresponds to that of a first-order method applied to a three-dimensional partial differential equation. As usual, these rates double for the eigenvalues.

What all that means for the numerical solution of the Schrödinger equation is not clear so far. Probably one needs size consistent nonlinear schemes to break the dependence of the constants on the size of the atomic or molecular systems. But our considerations show at least that the complexity of the quantum-mechanical N-body problem is much lower than generally believed.

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