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by

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Abstract

We suggest an alternative approach to electronic structure calculations based on numerical methods from multiscale analysis. By this we are aiming to achieve a better description of the various length- and energy-scales inherently connected with different types of electron correlations. Taking a product ansatz for the wavefunction $\Psi = \mathcal{F}\Phi$, where Φ corresponds to a given mean-field solution like Hartree-Fock or a linear combination of Slater determinants, we approximate the symmetric correlation factor $\mathcal{F}$ in terms of hyperbolic wavelets. Such kind of wavelets are especially adapted to high dimensional problems and allow for local refinement in the region of the electron-electron cusp. The variational treatment of the ansatz leads to a generalized eigenvalue problem for the coefficients of the wavelet expansion of $\mathcal{F}$. Several new numerical features arise from the calculation of the matrix elements. This includes the appearance of products of wavelets, which are not closed under multiplication. We present an approximation scheme for the accurate numerical treatment of these products. Furthermore the calculation of one- and two-electron integrals, involving the nonstandard representation of Coulomb matrix elements, is discussed in detail. No use has been made of specific analytic expressions for the wavelets, instead we employ exclusively the wavelet filter coefficients, which makes our method applicable to a wide class of different wavelet schemes. In order to illustrate the various features of the method, we present some preliminary results for the helium atom.

1 Introduction

1.1 Wavelets and electronic structure calculations

The fundamental difficulties of accurate electronic structure calculations are inherently connected with a simultaneous description of various physical processes on energy- and length-scales extending over several orders of magnitude [1]. Typical examples, ranging from high (short) to low (large) energy- (length-) scales, are processes inside atomic cores, chemical bonding varying from covalent bonding to van der Waals [2] and ionic interactions, collective excitations [3], and magnetic couplings [4]. Synergetic effects, caused by couplings between different scales, often prevent their separate treatment. Due to a lack of *a priori* knowledge on the strength of these couplings, it is important to perform the calculations *ab initio*, which means without *a priori* assumptions on specific system dependent quantities.

The development of *ab initio* methods is still one of the major tasks in quantum chemistry [5]. Currently there are two different lines of progress, based on the one side on density

functional theory [6] (DFT) and on the other side on wavefunction methods [7]. In DFT the many-particle problem is mapped onto a system of noninteracting particles, resulting in a significant computational simplification. The fundamental problem of this approach is that the mapping can be done only approximately and systematic ways for improvement are presently not known. Alternatively one can try to solve the original many-particle Schrödinger equation and calculate approximate eigenfunctions of the nonrelativistic Hamiltonian

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^{N}\Delta_i \; - \; \sum_{a=1}^{K}\sum_{i=1}^{N}\frac{Z_a}{|\mathbf{r}_i - \mathbf{R}_a|} \; + \; \sum_{i<j}^{N}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \; + \; \sum_{a<b}^{K}\frac{Z_a Z_b}{|\mathbf{R}_a - \mathbf{R}_b|}, \tag{1}$$

where Z_a, $\mathbf{R}_a$ are charges and positions of the nuclei, respectively. Atomic units have been used throughout this paper.

Common to all conventional wavefunction methods (for a review of these methods see e.g. Ref. [8]) is that one first has to determine an appropriate mean-field solution from Hartree-Fock (HF) or a generalized mean-field solution from multiconfigurational self-consistent field (MCSCF) type of equations, within a given finite single-particle basis set. The solution consists of a finite set of orbitals, which can be used to construct an orthogonal many-particle basis in terms of Slater determinants. Obviously, orbitals are just some kind of orthogonalization of the original single-particle basis set and can be subdivided into occupied and virtual orbitals, respectively, depending on whether or not they are included in the Slater determinant(s) which represent the (generalized) mean-field solution. Starting from the reference space spanned by the (generalized) mean-field solution, it is possible to construct a hierarchical decomposition of the many-particle space into subspaces characterized by the number of virtual orbitals contained in the Slater determinants belonging to it. This provides a natural setting for configuration-interaction (CI) and coupled-cluster (CC) methods. These methods are "exact" in a sense that they provide a hierarchy of approximate solutions, defined on these subspaces, which converge to the "exact" solution in the many-particle space defined with respect to the finite set of orbitals. Convergence to the exact eigenfunction of the Hamiltonian (1) requires in addition completeness with respect to the single-particle basis set.

Contrary to the large diversity of methods to approximate the high dimensional space of Slater determinants, essentially all of their realizations in quantum chemistry are based on single-particle basis sets constructed from atomic centred basis functions. Originally such kind of approach has been motivated by interpreting molecular orbitals as perturbed superpositions of atomic orbitals. Using Gaussian functions for the radial part of these atomic centred basis functions, the resulting so called Gaussian-type-orbitals (GTO) [9] have almost optimal approximation properties for mean-field solutions like HF [10]. In the context of many-particle theory, this corresponds to a partial-wave expansion of the wavefunction in the vicinity of a nucleus. A detailed analysis shows that partial-wave expansions are incapable to describe the wavefunction in those regions of configuration space where electrons are close together [11], leading to inferior convergence in the space of Slater determinants [12, 13]. Actually coalescence points of electrons are one of the rare cases where the analytic behavior of the wavefunction is known explicitly and became widely known as Kato's cusp condition [14, 15, 16]. The natural framework for the representation of the behavior of the wavefunction Ψ near the electron-electron cusp is a product decomposition [16]

$$\Psi\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right) = \mathcal{F}\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right) \Phi\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right) \tag{2}$$

where the symmetric part $\mathcal{F}$, usually called Jastrow factor, corrects for inadequacies of the antisymmetric mean-field solution Φ near the cusp. Jastrow factors are quite common in condensed matter and nuclear physics [17]. In this connection one has to mention the Gutzwiller wavefunction [1], Fermi hypernetted chain (FHNC) methods [18, 19, 20, 21, 22], and correlated

basis functions (CBF) [23]. For molecules, Jastrow factors have been used almost exclusively in combination with quantum Monte Carlo methods [24]. Within the framework of these methods, Jastrow factors depend explicitly on the interelectronic distances, hereby it becomes possible to meet Kato's cusp condition. Since interelectronic distances as coordinates are not compatible with the tensor product structure of the Slater determinants, their incorporation into conventional methods cause severe technical difficulties, which to overcome require considerable technical efforts [25]. Our approach differs in such a way that we avoid the use of explicit interelectronic coordinates, instead we use basis sets which are flexible enough to provide local adaptive refinements near the cusp.

Recently wavelets became a powerful tool in multiresolution analysis for solving partial differential equations (PDE) [26, 27]. Starting from a mother wavelet, a hierarchical basis set can be constructed using the operations of translation and dilation. Wavelet bases with a large variety of useful properties including compact support, (bi)orthogonality, and vanishing moments have been reported in the literature [28]. Not surprisingly wavelets attracted considerable attention in electronic structure theory [29, 30, 31, 32, 33, 34, 35, 36, 37]. Nevertheless all of these applications have been done in the context of DFT, where a coupled system of nonlinear three-dimensional PDEs has to be solved. We want address to the question whether wavelets can be advantageous for approximating many-particle wavefunctions of atoms, molecules and solids. An immediate objection against such kind of approach is the high dimensionality of the systems. So far wavelets have been mainly used for low dimensional problems [38]. However, due to the hierarchical structure of a wavelet basis it becomes possible to apply sparse grids techniques [39, 40, 41], keeping the size of the many-particle basis set within acceptable limits. It has been demonstrated that the resulting so called hyperbolic wavelets [42] have excellent approximation properties in high dimensional spaces. In the following we want to discuss some of the basic numerical algorithms, which are required for such kind of approach. With these algorithms at hand, we can attempt to tackle more fundamental problems of many-body theory. The product ansatz (2) seems to be an appropriate starting point, since it allows a unified view on apparently different methods like CC, FHNC and CBF [43]. The central topic for future research are approximation properties of wavelets with respect to the different energy- and length-scales of physical processes discussed above. Within the present work we want to give a preliminary discussion with respect to short-range correlations.

1.2 Multiresolution analysis in one dimension

The solution of Schrödinger's equation for many-particle systems is an intrinsically high dimensional problem. There are two principle approaches to construct wavelets in several dimensions (multivariate wavelets). In the first approach one tries to construct wavelets depending genuinly on several variables, whereas in the second approach one takes the tensor product of wavelets which depend on one variable (univariate wavelets) only. Traditionally most of the applications of wavelets appeared in signal and image processing [28, 38], where one has to deal with one- or two-dimensional problems. We decided to take the tensor product ansatz, where we start from a one-dimensional wavelet basis and construct successively higher dimensional basis functions. An obvious advantage of this approach is that we can benefit from the large variety of univariate wavelet constructions reported in the literature. Another more subtle point is that we have used tensor products to factorize some of the most expensive computational steps into one-dimensional subproblems, which will be discussed in more detail below.

In one dimension, multiresolution analysis provides a partition of the space of square integrable functions on the real line L^2 into an infinite sequence of ascending subspaces $\cdots \subset$

$V_{j-1} \subset V_j \subset V_{j+1} \subset \cdots$, where the index j runs over all integers. The union of these subspaces $\bigcup_j V_j$ is dense in L^2. There exists a scaling function $\varphi(x)$ which provides a basis set for V_j using the operations of dilation and translation. To be more explicit, the functions

$$\varphi_{j,a} := 2^{j/2}\varphi(2^j x - a) \tag{3}$$

span V_j where the dyadic dilation factor 2^j is kept fixed and a runs over all integers. The dilation factor scales the size of the basis functions $\varphi_{j,k}$, which means that with increasing j, the $\varphi_{j,k}$ provide a finer resolution in L^2. By definition, the scaling function $\varphi(x)$ has to fulfil the refinement relation

$$\varphi(x) = 2\sum_b h_b\,\varphi(2x - b), \tag{4}$$

which provides an explicit embedding of V_j into the larger space V_{j+1}. The scaling function also provides a resolution of the identity

$$1 = \sum_a \varphi(x - a). \tag{5}$$

As a consequence, the constant function can be exactly represented on each level j. For scaling functions with compact support the number of nonvanishing filter coefficients h_a in Eq. (4) remains finite. It should be emphasized that the choice of the filter coefficients uniquely specifies the scaling function $\varphi(x)$, which means that in principle no further information is required beyond these coefficients. In the present work, we follow this principle by avoiding any reference to analytic expressions, which in general might be quite implicit [26]. Therefore our approach becomes rather flexible with respect to the kind of wavelet construction to be employed in actual calculations. In view of the fact that it is presently not clear at all which kind of wavelets are the most appropriate for electronic structure calculations, this aspect has to be taken into account seriously.

Wavelets are introduced by taking a complement of V_j in V_{j+1}, which defines the wavelet space W_j. The corresponding wavelet basis for W_j is generated from a mother wavelet $\psi(x)$ analogous the Eq. (3)

$$\psi_{j,a} = 2^{j/2}\psi(2^j x - a). \tag{6}$$

A refinement relation similar to Eq. (4)

$$\psi(x) = 2\sum_b g_b\,\varphi(2x - b), \tag{7}$$

relates the mother wavelet to the scaling functions on the next finer level. From Eq. (7) we obtain an explicit embedding of W_j into V_{j+1}. Subdivisions $V_{j+1} = W_j \bigoplus V_j$ can be further extended in both directions of the sequence of spaces V_j using the reconstruction relation

$$\varphi(2x - a) = \sum_b \left[c_{ab}\,\varphi(x - b) + d_{ab}\,\psi(x - b)\right] \tag{8}$$

leading to a decomposition of $L^2 = \bigoplus_\ell W_\ell$ into wavelet subspaces W_ℓ [28]. We do not want to enter into a discussion concerning the relations between the filter coefficients h_a, g_a in Eqs. (4), (7) and the coefficients c_{ab}, d_{ab} in Eq. (8), instead we refer to the literature [26].

So far we have outlined some formal aspects of wavelet spaces. As we have already mentioned above, there exists a large variety of explicit wavelet constructions, which provide wavelet basis sets with different properties depending on the specific applications. There is a special class of wavelets forming biorthogonal basis sets, which seems to be especially appropriate for solving PDEs [26]. In a biorthogonal basis there exists a dual scaling function

$\tilde{\varphi}(x)$, which generates a sequence of spaces $\tilde{V}_j$ ($\tilde{W}_j$), where the corresponding scaling functions $\tilde{\varphi}_{j,a} := 2^{j/2}\tilde{\varphi}(2^j x - a)$ and wavelets $\tilde{\psi}_{j,a} := 2^{j/2}\tilde{\psi}(2^j x - a)$ satisfy the equations

$$\begin{aligned}
\int dx\ \varphi_{j,a}(x)\tilde{\varphi}_{j,b}(x) &= \delta_{a,b}, \\
\int dx\ \varphi_{j,a}(x)\tilde{\psi}_{\ell,b}(x) &= 0 \qquad\qquad \ell \geq j, \\
\int dx\ \psi_{j,a}(x)\tilde{\varphi}_{\ell,b}(x) &= 0 \qquad\qquad j \geq \ell, \\
\int dx\ \psi_{j,a}(x)\tilde{\psi}_{\ell,b}(x) &= \delta_{j,\ell}\,\delta_{a,b}.
\end{aligned} \tag{9}$$

This corresponds to the subspace relations $\tilde{W}_j \perp V_j$ and $\tilde{V}_j \perp W_j$. Given an arbitrary function $f(x) \in L^2$, we can take a wavelet decomposition of the Hilbert space $L^2 = V_{j_0} \bigoplus_{j \geq j_0} W_j$ and expand f in terms of the wavelet basis

$$f(x) = \sum_a u_{j_0,a}\,\varphi_{j_0,a}(x) + \sum_{j=j_0}^{\infty}\sum_a v_{j,a}\,\psi_{j,a}(x), \tag{10}$$

where the coefficients are given by

$$u_{j_0,a} = \int dx\ f(x)\,\tilde{\varphi}_{j_0,a}(x), \tag{11}$$

$$v_{j,a} = \int dx\ f(x)\,\tilde{\psi}_{j,a}(x), \tag{12}$$

according to Eqs. (9). It should be mentioned that an appropriate choice of j_0 is essential for an efficient expansion in (10), since the number of coefficients with absolute value above a certain threshold depends on it. Another property which is of great importance for wavelet expansions of smooth functions, is the number of vanishing moments n of the wavelet

$$\int dx\ x^\ell\,\psi(x) = 0 \quad \text{for} \quad \ell = 0, \ldots, n-1. \tag{13}$$

This property is closely related to the size of the wavelet [28]. Roughly speaking for wavelets with compact support the diameter $\approx 2n+1$. Therefore any specific choice of a wavelet basis for a particular application represents a compromise between the desired local character and the number of vanishing moments. In the following we will use vanishing moments to obtain sparse representations of certain matrices. Also closely related to the size is the regularity of the wavelet [28]. We benefit in certain steps of our method from a sufficiently high regularity of the wavelet basis.

For further reference we define the approximation error of the wavelet expansion (10) of a function f up to level ℓ in the L^2 norm

$$E^{(\ell)}_{L^2}[f] = \left[\int dx\ \left(\sum_{j>\ell}\sum_a v_{j,a}\,\psi_{j,a}(x)\right)^2\right]^{\frac{1}{2}}. \tag{14}$$

Alternatively we can use the, from a computational point of view, more convenient expression

$$\bar{E}^{(\ell)}_{L^2}[f] = \left(\sum_{j>\ell}\sum_a |v_{j,a}|^2\right)^{\frac{1}{2}} \tag{15}$$

which is equivalent ($C_1\, E_{L^2}^{(\ell)} \leq \bar{E}_{L^2}^{(\ell)} \leq C_2\, E_{L^2}^{(\ell)}$) to the $E_{L^2}^{(\ell)}$ error for a biorthogonal wavelet basis [28].

In order to substantiate the following more formal discussions, we want to illustrate our method for a specific wavelet basis. We have taken a biorthogonal symmetric wavelet basis with compact support and six vanishing moments from Sweldens [44]. These wavelets are based on the interpolating scaling function of Deslauriers and Dubuc [45], where the dual basis with the same number of vanishing moments has been generated from a lifting scheme [44]. Scaling functions $\varphi, \tilde{\varphi}$ and wavelets $\psi, \tilde{\psi}$ together with their Fourier transforms

$$\hat{\varphi}(\omega) = \int_{-\infty}^{\infty} dx\ \exp(-i\omega x)\varphi(x), \tag{16}$$

are shown in Fig. 1. Additionally, the interpolating scaling function φ satisfies the vanishing moment property [44, 45]

$$\int dx\ x^{\ell}\, \varphi(x) = \delta_{\ell} \quad \text{for} \quad \ell = 0, \ldots, 5, \tag{17}$$

analogous to Eqs. (13) for the wavelet.

1.3 Multivariate wavelets and sparse grids

In order to pass from univariate to multivariate wavelets, we have employed two different construction schemes. Within the first approach, the multivariate wavelets belong to well defined levels j. This can be achieved by taking mixed tensor products of $\varphi_{j,a}$ and $\psi_{j,a}$ which corresponds in three dimensions to scaling functions

$$\beta_{j,\mathbf{a}}(\mathbf{r}) = \varphi_{j,a_x}(x)\ \varphi_{j,a_y}(y)\ \varphi_{j,a_z}(z) \tag{18}$$

and seven different types of wavelets

$$\begin{aligned}
\gamma_{j,\mathbf{a}}^{(1)}(\mathbf{r}) &= \psi_{j,a_x}(x)\ \varphi_{j,a_y}(y)\ \varphi_{j,a_z}(z), \\
&\vdots \\
\gamma_{j,\mathbf{a}}^{(4)}(\mathbf{r}) &= \psi_{j,a_x}(x)\ \psi_{j,a_y}(y)\ \varphi_{j,a_z}(z), \\
&\vdots \\
\gamma_{j,\mathbf{a}}^{(7)}(\mathbf{r}) &= \psi_{j,a_x}(x)\ \psi_{j,a_y}(y)\ \psi_{j,a_z}(z).
\end{aligned} \tag{19}$$

It is convenient to group the wavelets (19) into three classes, depending on the number of univariate wavelets in the tensor product.

Obviously such kind of construction scheme becomes impracticable for high dimensional problems, just because the number of basis functions increases too fast with dimension. In the following we will make use of it to define one-particle basis sets and as a basis for the evaluation of one- and two-electron integrals. Analogously to the univariate case, scaling functions and wavelets satisfy refinement relations

$$\beta_{j,\mathbf{a}}(\mathbf{r}) = 2^{3/2} \sum_{\mathbf{b}} H_{\mathbf{b}-2\mathbf{a}}\ \beta_{j+1,\mathbf{b}}(\mathbf{r}), \tag{20}$$

$$\gamma_{j,\mathbf{a}}^{(p)}(\mathbf{r}) = 2^{3/2} \sum_{\mathbf{b}} G_{\mathbf{b}-2\mathbf{a}}^{(p)}\ \beta_{j+1,\mathbf{b}}(\mathbf{r}), \tag{21}$$

where the multivariate filter coefficients are simple products of the univariate coefficients e.g. $H_{\mathbf{a}} = h_{a_x} h_{a_y} h_{a_z}$, $G_{\mathbf{a}}^{(1)} = g_{a_x} h_{a_y} h_{a_z}$.

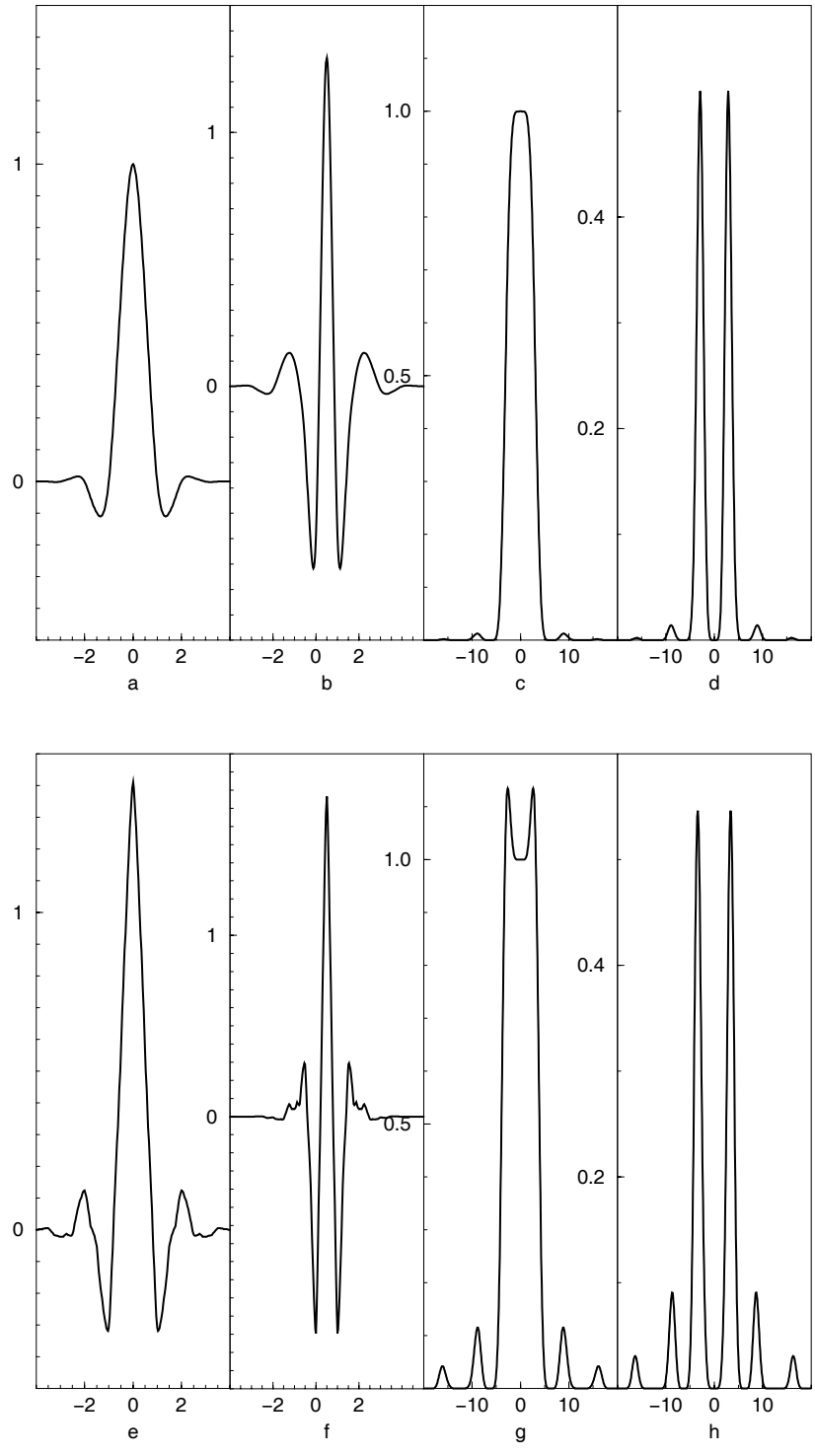

Figure 1: Biorthogonal wavelets with six vanishing moments from Sweldens [44] based on the interpolating scaling function of Deslauriers and Dubuc [45]. a) Scaling function $\varphi(x)$, b) wavelet $\psi(x)$ and their Fourier transforms c) $\hat{\varphi}(\omega)$, d) $|\hat{\psi}(\omega)|$, together with the corresponding pictures of the e) dual scaling function $\tilde{\varphi}(x)$, f) dual wavelet $\tilde{\psi}(x)$ and their Fourier transforms g) $\hat{\tilde{\varphi}}(\omega)$, h) $|\hat{\tilde{\psi}}(\omega)|$.

For the many-particle basis sets, we have taken tensor products just within this three-dimensional wavelet basis. The tensor product basis functions of general form

$$\gamma^{(p_1)}_{\ell_1,\mathbf{a}}(\mathbf{r}_1)\,\gamma^{(p_2)}_{\ell_2,\mathbf{b}}(\mathbf{r}_2)\,\cdots\,\gamma^{(p_N)}_{\ell_N,\mathbf{c}}(\mathbf{r}_N) \tag{22}$$

mix wavelets from different scales ℓ_i. Based on the fact that the wavelets (19) form a hierarchical basis, the sparse grids approximation [39, 40, 41] on the tensor products becomes applicable. In the wavelet literature, the resulting multivariate wavelet basis is known as hyperbolic wavelets [42]. The basic idea is to select a subset of the tensor products (22) which fulfils the additional requirement $\sum_{i=1}^{N}\ell_i \le Q$ for a given integer Q. This reduces the number of basis functions in the N particle case from $O(L^N)$ to $O(L\,log(L)^{N-1})$ where $L \sim 2^{3Q}$ is the number of single-particle basis functions. The actual loss of accuracy depends on the degree of regularity of the function to be approximated. For smooth functions there is almost no loss of accuracy compared to the full basis [42].

2 Hyperbolic wavelet approximation of the Jastrow factor

Fermionic wavefunctions have to meet Pauli's principle, which means that we have to impose a symmetry restriction on the tensor products by applying a symmetrization operator

$$\hat{\mathsf{S}} = \sum_{(i_1,i_2,\ldots,i_N)\in S_N} \hat{P}(i_1,i_2,\ldots,i_N) \tag{23}$$

acting on the electron coordinates $\mathbf{r}_i$, where the sum runs over all permutations $(i_1,i_2,\ldots,i_N)$ of the symmetric group S_N. Symmetrized wavelet tensor products

$$\begin{aligned}\mathcal{F}_{\mathbf{J},\mathbf{A}}\,(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N) &= \hat{\mathsf{S}}\,\gamma^{(p_1)}_{j_1,\mathbf{a}_1}(\mathbf{r}_1)\,\gamma^{(p_2)}_{j_2,\mathbf{a}_2}(\mathbf{r}_2)\,\cdots\,\gamma^{(p_N)}_{j_N,\mathbf{a}_N}(\mathbf{r}_N) \\ &= \sum_{(i_1,i_2,\ldots,i_N)\in S_N} \gamma^{(p_1)}_{j_1,\mathbf{a}_1}(\mathbf{r}_{i_1})\,\gamma^{(p_2)}_{j_2,\mathbf{a}_2}(\mathbf{r}_{i_2})\,\cdots\,\gamma^{(p_N)}_{j_N,\mathbf{a}_N}(\mathbf{r}_{i_N})\end{aligned} \tag{24}$$

serve as a basis for our expansion of the Jastrow factor, where $\mathbf{J} = (p_1,j_1,p_2,j_2,\ldots,p_N,j_N)$ and $\mathbf{A} = (\mathbf{a}_1,\mathbf{a}_2,\ldots,\mathbf{a}_N)$ are multi-indices specifying the types p_i, levels j_i and centers $\mathbf{a}_i$ of the wavelets involved in the product.

Depending on the physical problem under consideration, electron correlations have typical length- and energy-scales, which have their correspondence in a certain range of dilation parameters j of the wavelet basis. The long-range behavior of the Jastrow factor is determined by its cluster property [17], which means that for those regions of configuration space, where the electron coordinates can be subdivided into two subsets A and B with $\mid \mathbf{r}_a - \mathbf{r}_b \mid > \ell_{corr}\ \ \forall\,\mathbf{r}_a \in A,\ \mathbf{r}_b \in B$, the Jastrow factor factors into a product

$$\mathcal{F}\,(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N) = \mathcal{F}_A\,(\mathbf{r}_{a_1},\mathbf{r}_{a_2},\ldots)\ \mathcal{F}_B\,(\mathbf{r}_{b_1},\mathbf{r}_{b_2},\ldots) \tag{25}$$

of Jastrow factors $\mathcal{F}_A$ and $\mathcal{F}_B$ for the two subsets. Here we have introduced a characteristic length-scale ℓ_{corr} for electron correlations, which specifies the spatial range of the correlations to be described by the Jastrow factor. Obviously ℓ_{corr} depends on the system and the physical properties under consideration. Depending on their level j, wavelet subspaces W_j resolve different length- and energy-scales. We can therefore introduce a coarsest level j_0 in the wavelet expansion of $L^2 = V_{j_0}\bigoplus_{\ell\ge j_0} W_\ell$ corresponding to the characteristic length-scale ℓ_{corr}, where we take from V_{j_0} the constant function only. We formally define a "wavelet" standing for $\gamma_{j_0-1,\mathbf{0}} := 1$ on the next coarser level j_0-1, which represents the subspace spanned by the constant function in V_{j_0}. Furthermore we introduce an index p in the tensor products $\mathcal{F}^{(p)}_{\mathbf{J},\mathbf{A}}$,

where p specifies the number of wavelets in the product on levels $j \geq j_0$. In the following we obmit $\gamma_{j_0-1,\mathbf{0}}$ in our formulas. From this we obtain an additional hierarchy for the symmetrized tensor products (24) with respect to the index p

$$\begin{aligned}
\mathcal{F}^{(0)}\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right) &= 1, \\
\mathcal{F}^{(1)}_{j_1,\mathbf{a}_1}\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right) &= \gamma^{(q_1)}_{j_1,\mathbf{a}_1}(\mathbf{r}_1) + \gamma^{(q_1)}_{j_1,\mathbf{a}_1}(\mathbf{r}_2) + \cdots + \gamma^{(q_1)}_{j_1,\mathbf{a}_1}(\mathbf{r}_N), \\
\mathcal{F}^{(2)}_{\mathbf{J},\mathbf{A}}\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right) &= \gamma^{(q_1)}_{j_1,\mathbf{a}_1}(\mathbf{r}_1)\, \gamma^{(q_2)}_{j_2,\mathbf{a}_2}(\mathbf{r}_2) + \cdots + \gamma^{(q_1)}_{j_1,\mathbf{a}_1}(\mathbf{r}_{N-1})\, \gamma^{(q_2)}_{j_2,\mathbf{a}_2}(\mathbf{r}_N), \\
&\vdots
\end{aligned} \tag{26}$$

which resembles to single, double and higher excitations of the standard CI expansion.

We can apply the hyperbolic wavelet approximation to the expansion of the Jastrow factor

$$\mathcal{F}\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right) = \sum_{p=0}^{N} \sum_{|\mathbf{J}| \leq Q} \sum_{\mathbf{A}} f^{(p)}_{\mathbf{J},\mathbf{A}}\ \mathcal{F}^{(p)}_{\mathbf{J},\mathbf{A}}\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right) \tag{27}$$

with variational parameters $f^{(p)}_{\mathbf{J},\mathbf{A}}$, where only those $\mathcal{F}^{(p)}_{\mathbf{J},\mathbf{A}}$ are admissible for which $|\mathbf{J}| := \sum_{i=1}^{N} j_i \leq Q$. As already mentioned above, such kind of approach is most efficient for smooth functions, where it achieves almost the same quality of approximation as a full tensor product basis. The many-electron wavefunction is smooth except at the electron-electron cusp [15]. Therefore, the hyperbolic wavelet approximation requires some modifications in the cusp region. Adaptive refinement schemes of the hyperbolic wavelet basis in the cusp region, based on analytic properties of many-electron wavefunctions, will be discussed below in further detail.

The question arises whether an ansatz of the form (27) satisfies a size-extensivity condition. This would require that the Jastrow factor factorizes according to the cluster property (25), given a system (A, B) composed of the noninteracting subsystems A and B. Applying the hyperbolic wavelet approximation with parameter Q to (A, B) produces terms $\mathcal{F}^{(p)}_{\mathbf{Q},\mathbf{A}}$ for A with $|\ \mathbf{Q}\ | = Q$, where all wavelets are located in A and vice versa for B. In order to factorize properly, this would require products of the type $\mathcal{F}^{(p)}_{\mathbf{Q},\mathbf{A}}\, \mathcal{F}^{(q)}_{\mathbf{Q},\mathbf{B}}$, which are not admissible within our approximation. Concerning size-extensivity, hyperbolic wavelets introduce some kind of ambiguity into the calculations. There are some similarities to truncated CI expansions, which also show such kind of behavior. In order to fully overcome this problem, we have to abandon the linear ansatz (27) and replace it by an exponential ansatz. This has been accomplished by the FHNC method [18, 19, 20, 21, 22], which provides a hierarchical system of equations in order to determine an optimal Jastrow factor and the corresponding energy. Due to the computational complexity of the exponential ansatz, it is necessary to introduce further approximations. The FHNC method just as the CC method is not strictly variational any more. In the present work we are primarily interested in numerical aspects of wavelet expansions of correlated wavefunctions, which are mostly independent of the many-particle method employed. Therefore, we restrict ourself to the linear ansatz (27), which enables a strictly variational treatment without any uncontrolled approximations, at least for small systems.

The Rayleigh-Ritz variational principal applied to the expectation value of the energy

$$E[\mathcal{F}] = \frac{\langle \mathcal{F}\Phi | \hat{H} | \mathcal{F}\Phi \rangle}{\langle \mathcal{F}\Phi | \mathcal{F}\Phi \rangle} \tag{28}$$

yields a generalized eigenvalue problem of the form

$$\mathbf{H}\ \mathbf{f} = E\ \mathbf{M}\ \mathbf{f}, \tag{29}$$

with matrix elements

$$H_{(p,\mathbf{J},\mathbf{A})(q,\mathbf{L},\mathbf{B})} = \int d^3r_1, \ldots, d^3r_N \; \mathcal{F}^{(p)}_{\mathbf{J},\mathbf{A}} \Phi \; \hat{H} \; \mathcal{F}^{(q)}_{\mathbf{L},\mathbf{B}} \Phi \tag{30}$$

$$M_{(p,\mathbf{J},\mathbf{A})(q,\mathbf{L},\mathbf{B})} = \int d^3r_1, \ldots, d^3r_N \; \mathcal{F}^{(p)}_{\mathbf{J},\mathbf{A}} \Phi \; \mathcal{F}^{(q)}_{\mathbf{L},\mathbf{B}} \Phi. \tag{31}$$

Hyperbolic wavelets keep the growth of dimension of the generalized eigenvalue problem (29), for an increasing number of electrons, within reasonable limits. However the computation of the matrix elements (30) and (31) becomes rather involved for large N. This difficulty is less severe due to the fact that for small Q, the products $\mathcal{F}^{(q)}_{\mathbf{J},\mathbf{A}} \Phi$ partially preserve the orthogonality relations between the orbitals. A more detailed analysis for the matrices $\mathbf{M}$ [46] reveals that for fixed Q and $N >> Q$ the computational complexity is of $O(N^3)$. In principle, the algorithm can be generalized for matrices $\mathbf{H}$, at the expense of an increasing order of complexity. It should be mentioned however, that for large systems the wavelet approach introduces some sparsity into $\mathbf{H}$ and $\mathbf{M}$ matrices. At the present state of the project, it seems to be premature to enter into a detailed discussion of this subject.

2.1 Elementary considerations for the homogeneous electron gas

In order to get an estimate for the convergence behavior of our expansion, we consider the homogeneous electron gas at various densities ρ. For a cubic volume element Ω, with periodic boundary conditions, containing $N = \rho\,\Omega$ electrons, we can formulate a many-electron wavefunction

$$\Psi\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right) = \prod_{i<j}^{N} h(|\mathbf{r}_i - \mathbf{r}_j|) \; \Phi\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right), \tag{32}$$

where $\mathcal{F}$ is approximated by a product of electron-pair Jastrow factors h and Φ is a Slater determinant of Bloch orbitals. In the case of extended systems, we have to distinguish between the approximation of isolated subsystems like electron-pairs and aggregations of subsystems. The latter is of almost exclusively combinatorial character and will be treated separately. First of all, we want to discuss the approximation of a single electron-pair described by the Jastrow factor $h(|\mathbf{r}_1 - \mathbf{r}_2|)$, which depends only on the interelectronic distance due to symmetry. The shape of the Jastrow factor strongly depends on the electron density ρ. In Fig. 2 we have plotted Jastrow factors h for various electron densities ranging from high density regions inside atomic cores up to low densities close to the van Waals radius of atoms and molecules. Electron densities are characterized by the dimensionless parameter $r_s = (\frac{3}{4\pi\rho})^{1/3}/r_B$, where r_s corresponds to the average distance between the electrons expressed in units of Bohr's radius r_B. We have used a scaled interelectronic distance $\bar{r}_{12} = |\mathbf{r}_1 - \mathbf{r}_2|/r_s$ in Fig. 2, in order to demonstrate that r_s is an appropriate scaling parameter, characterizing the range of the Jastrow factor. Furthermore it has been observed that the depth of the Jastrow factor at the cusp is almost proportional to r_s [47]. Such kind of behavior can be partially transferred to inhomogeneous systems [47]. For atoms, the density decreases exponentially with the distance from the nucleus. Typically r_s ranges over one to two orders of magnitude between core regions and the van der Waals radius ($r_s \approx 5$).

From a physical point of view, it is reasonable to assume that h is an analytic function with respect to the interelectronic distance $|\mathbf{r}_1 - \mathbf{r}_2|$. Therefore we can perform a Taylor expansion

$$h(|\mathbf{r}_1 - \mathbf{r}_2|) = \sum_{m=0}^{\infty} \frac{a_m}{m!} \; |\mathbf{r}_1 - \mathbf{r}_2|^m \tag{33}$$

and consider the wavelet representation of each term separately. Obviously $|\mathbf{r}_1 - \mathbf{r}_2|^m$ is smooth except at the cusp $\mathbf{r}_1 = \mathbf{r}_2$. We can therefore limit our discussion, on the fine scales,

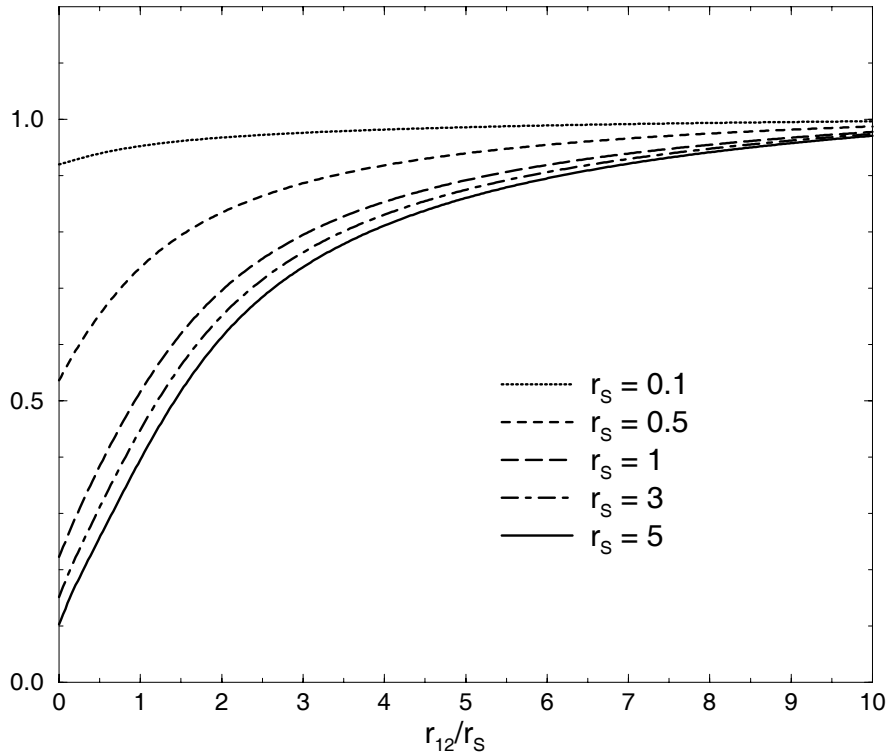

Figure 2: Jatrow factors of an electron pair for the homogeneous electron gas at various densities. $h(|\mathbf{r}_1 - \mathbf{r}_2|)$ is plotted versus the scaled interelectronic distance $\bar{r}_{12} = |\mathbf{r}_1 - \mathbf{r}_2|/r_s$ (Bohr), where the dimensionless parameter r_s corresponds to the average distance between the electrons expressed in units of Bohr's radius.

to tensor products (27) located on the diagonal $\mathbf{a}_1 = \mathbf{a}_2$. With respect to the levels j_1, j_2, it is sufficient to consider the diagonal case $j_1 = j_2$, since the coupling between different levels is of $O(2^{-3|j_1 - j_2|/2})$. A direct expansion in terms of a biorthogonal wavelet basis yields wavelet coefficients

$$\begin{aligned} h^{(m)}_{j,q_1,\mathbf{a},j,q_2,\mathbf{a}} &= \int d^3r_1 d^3r_2 \; |\mathbf{r}_1 - \mathbf{r}_2|^m \; \tilde{\gamma}^{(q_1)}_{j,\mathbf{a}}(\mathbf{r}_1) \; \tilde{\gamma}^{(q_2)}_{j,\mathbf{a}}(\mathbf{r}_2) \\ &= 2^{-(m+3)j} \int d^3r_1 d^3r_2 \; |\mathbf{r}_1 - \mathbf{r}_2|^m \; \tilde{\gamma}^{(q_1)}_{0,\mathbf{0}}(\mathbf{r}_1) \; \tilde{\gamma}^{(q_2)}_{0,\mathbf{0}}(\mathbf{r}_2) \\ &= 2^{-(m+3)j} \; h^{(m)}_{0,q_1,\mathbf{0},0,q_2,\mathbf{0}}, \end{aligned} \tag{34}$$

for which we obtain a scaling factor $2^{-(m+3)j}$ with respect to the levels j. The constant term $m = 0$ of the expansion (33) vanishes due to the vanishing moments property (13) of the wavelets, leaving us with the linear term $m = 1$ as the dominating contribution in the asymptotic limit. We can estimate the approximation error of our expansion for the L^2 norm (15) in the asymptotic limit

$$\bar{E}^{(\ell)}_{L^2}[h] = \left[\sum_{\max(j_1,j_2)>\ell} \sum_{q_1,q_2} \sum_{\mathbf{a}_1,\mathbf{a}_2} |h^{(1)}_{j_1,q_1,\mathbf{a}_1,j_2,q_2,\mathbf{a}_2}|^2 \right]^{\frac{1}{2}} \tag{35}$$

$$
\begin{aligned}
&\leq C \left[\sum_{j>\ell} \sum_{q_1,q_2} \sum_{\mathbf{a}} |h^{(1)}_{j,q_1,\mathbf{a},j,q_2,\mathbf{a}}|^2 \right]^{\frac{1}{2}} \\
&= C \left[\left(\sum_{q_1,q_2} |h^{(1)}_{0,q_1,\mathbf{0},0,q_2,\mathbf{0}}|^2 \right) \sum_{j>\ell} 2^{-5j} \right]^{\frac{1}{2}},
\end{aligned}
$$

where we have used in the last line of Eq. (35), the fact that the number of grid points on level ℓ belonging to Ω increases with $O(2^{3\ell})$. The constant $C = O(1)$ takes into account the neglect of off-diagonal contributions in the second line of Eq. (35). Hence it appears that $\bar{E}^{(\ell)}_{L^2}[h] = O(2^{-5\ell/2})$. In order to estimate convergence with respect to the energy, we require a stronger statement for the Sobolev space H^1 [48] concerning the approximation error of the wavelet expansion. The Sobolev space H^1 takes in addition into account convergence with respect to the first derivatives. This is necessary because of the dominance of the kinetic energy [12] in the energy expectation value.

We can apply standard estimates for the finite element method in the case of piecewise linear basis functions. Higher order regularity of the basis functions do not contribute to the asymptotic convergence rate, due to the discontinous first derivatives of the exact wavefunction at the cusp. It is not difficult to see that an ansatz of the form (33) leads to a wavefunction which belongs to the Sobolev space $H^{\frac{5}{2}-\epsilon}(\Omega)$ for $\epsilon > 0$ [49]. Consequently we get the following two estimates [48] with respect to the level ℓ

$$
E^{(\ell)}_{L^2}[h] \leq C\, 2^{-\ell(\frac{5}{2}-\epsilon)} \parallel h \parallel_{H^{\frac{5}{2}-\epsilon}}, \tag{36}
$$

$$
E^{(\ell)}_{H^1}[h] \leq C\, 2^{-\ell(\frac{3}{2}-\epsilon)} \parallel h \parallel_{H^{\frac{5}{2}-\epsilon}}, \tag{37}
$$

for the solution of the eigenvalue problem (29). Here $\parallel h \parallel_{H^{\frac{5}{2}-\epsilon}}$ denotes the norm of h in $H^{\frac{5}{2}-\epsilon}(\Omega)$ [48] and $E^{(\ell)}_{H^1}[h]$ is the approximation error with respect to the H^1 norm. For the precise meaning of the various spaces and norms we refer to the literature [48], since these technical details are not essential for the following discussion. The error in the L^2 norm (36) agrees with the previous estimate (35) for the direct wavelet expansion, which has to be expected from the assumed regularity of the electron-pair Jastrow factor h. According to the estimate of the error in the H^1 norm (37) and taking into account that variation of the energy expectation value leads to an error in the energy which is quadratic with respect to the H^1 error of the wavefunction [48], we finally obtain an $O(2^{-3\ell})$ estimate for the convergence of the energy. This has to be brought in relation to the computational effort required for an adaptive refinement near the electron-electron cusp. For the homogeneous electron gas this needs a uniform refinement of the tensor products diagonal with respect to $\mathbf{a}$ in the domain Ω. The number of such tensor products increases with $O(2^{3\ell})$, which means that their straightforward incorporation into the wavelet expansion leads to a constant ratio between the number of degrees of freedom and the convergence rate. However due to translational symmetry the actual number of degrees of freedom increases only with $O(\ell)$, as can be seen from Eq. (34). Therefore it seems to be quite natural to use contracted tensor products on the diagonal

$$
\mathcal{F}^{(2)}_{\mathbf{J}}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \sum_{\mathbf{a}} \left[\gamma^{(q_1)}_{j,\mathbf{a}}(\mathbf{r}_1)\, \gamma^{(q_2)}_{j,\mathbf{a}}(\mathbf{r}_2) + \cdots + \gamma^{(q_1)}_{j,\mathbf{a}}(\mathbf{r}_{N-1})\, \gamma^{(q_2)}_{j,\mathbf{a}}(\mathbf{r}_N) \right] \tag{38}
$$

in the expansion (27). Here we have used equation (34) which shows that the wavelet expansion coefficients do not depend on the location $\mathbf{a}$ of the wavelets for the homogeneous electron gas. For inhomogeneous systems like molecules, we expect that the coefficients on the fine levels

ℓ vary smoothly with respect to the density. Therefore it should be possible to describe the variation of the coefficients by a small number of degrees of freedom, which is essentially independent of the level ℓ. It remains the problem to evaluate integrals with respect to contracted tensor products efficiently. Such kind of considerations will be subject for a further publication [49].

2.2 Nonstandard calculation of Coulomb matrix elements

Due to the tensor product ansatz for the Jastrow factor $\mathcal{F}$, the Coulomb interaction part of the **H** matrix elements factor into the standard one-electron

$$\langle \eta_{\mathbf{A}} | \frac{1}{r_{\mathbf{C}}} \rangle := \int d^3 r \; \frac{\eta_{\mathbf{A}}(\mathbf{r})}{\mid \mathbf{r} - \mathbf{C} \mid} \tag{39}$$

and two-electron Coulomb integrals

$$\langle \eta_{\mathbf{A}} | \frac{1}{r_{12}} | \eta_{\mathbf{B}} \rangle := \int d^3 r_1 d^3 r_2 \; \eta_{\mathbf{A}}(\mathbf{r}_1) \; \frac{1}{\mid \mathbf{r}_1 - \mathbf{r}_2 \mid} \; \eta_{\mathbf{B}}(\mathbf{r}_2). \tag{40}$$

These integrals have to be calculated for all existing combinations of products

$$\eta_{\mathbf{A}}(\mathbf{r}) = \begin{cases} \phi_i(\mathbf{r})\phi_j(\mathbf{r}) \\ \phi_i(\mathbf{r})\phi_j(\mathbf{r})\gamma^{(p)}_{m,\mathbf{a}}(\mathbf{r}) \\ \phi_i(\mathbf{r})\phi_j(\mathbf{r})\gamma^{(p)}_{m,\mathbf{a}}(\mathbf{r})\gamma^{(q)}_{n,\mathbf{b}}(\mathbf{r}) \end{cases}, \tag{41}$$

where we have used capital letters to represent multi-indices $\mathbf{A} := (i, j, m, n, p, q, \mathbf{a}, \mathbf{b})$ for convenience. A new numerical feature arises from the products of wavelets and orbitals which appear in the integrals (39) and (40). This makes an essential difference to most of the previous application of wavelets to PDEs like Poisson's equation and resembles to applications to nonlinear problems [50, 51]. The numerical treatment of these products is essential for an efficient calculation of these integrals.

Before we enter into a discussion of matrix element calculations, a few remarks are appropriate. As it has been oulined above, wavelets constitute a complete basis in L^2. For the wavelet expansion (27) of the Jastrow factor $\mathcal{F}$ we can chose an arbitrary subset according to our numerical and physical demands. In the following we have made extensive use of wavelet expansions for various kinds of functions. For that we have adopted the wavelet basis for each specific function in such a way that we take into account all wavelet contributions above a certain threshold, irrespective of our initial choice for the Jastrow factor. The threshold in turn depends on the further use of the expansion and enables us to keep control on the numerical accuracy of the matrix element calculations.

We made no attempt to solve the integrals (39) and (40) analytically. First of all, these integrals become rather complicated e.g. for wavelets given in terms of piecewise polynomial functions and the sheer number of these integrals prohibits the evaluation of any complicated analytic expressions. The same argument prevents the application of sophisticated numerical integration schemes. Instead we have exploited specific wavelet properties to derive an efficient and computationally simple integration scheme. To begin with, we calculate projections of the products (41) on the spaces $V_j \bigoplus W_j$

$$P_{V_j \bigoplus W_j} \, \eta_{\mathbf{A}}(\mathbf{r}) = \sum_p \sum_{\mathbf{a}} \langle \tilde{\gamma}^{(p)}_{j,\mathbf{a}} | \eta_{\mathbf{A}} \rangle \, \gamma^{(p)}_{j,\mathbf{a}}(\mathbf{r}) \; + \sum_{\mathbf{b}} \langle \tilde{\beta}_{j,\mathbf{b}} | \eta_{\mathbf{A}} \rangle \, \beta_{j,\mathbf{b}}(\mathbf{r}), \tag{42}$$

where $P_{V_j \bigoplus W_j}$ defines a projection operator on the subspace $V_j \bigoplus W_j$ according to Eq. (10). It should be mentioned that those products (41) containing wavelets have compact support,

which is typically of the size of the wavelet on the finest scale in the product. As a consequence, the wavelet expansions (42) become rather compact and well localized. For extended systems many of the $\eta_{\mathbf{A}}$ become zero due to vanishing overlap between the wavelets in the product.

The computational scheme we have used for the matrix elements (39) and (40) is based on the nonstandard representation of operators [52, 53]. The basic advantage of this approach is that it avoids couplings between different wavelet levels. For that we have to accept some overhead owing to the fact that we require for each level j not only the wavelet coefficients $\langle\tilde{\gamma}^{(p)}_{j,\mathbf{b}}|\eta_{\mathbf{A}}\rangle$ but also the coefficients with respect to the scaling functions $\langle\tilde{\beta}_{j,\mathbf{b}}|\eta_{\mathbf{A}}\rangle$. In an intermediate step we first expand the auxiliary function

$$\mathcal{R}(\mathbf{r_1}) := \int d^3r_2 \; \frac{1}{\mid \mathbf{r}_1 - \mathbf{r}_2 \mid} \; \eta_{\mathbf{B}}(\mathbf{r_2}) \tag{43}$$

in terms of wavelets and scaling functions on various levels. We start at an appropriately chosen finest level ℓ, where we approximate (43) within the dual space $\tilde{V}_\ell \bigoplus \tilde{W}_\ell$

$$\mathcal{R}(\mathbf{r}) \approx \sum_p \sum_{\mathbf{a}} \langle\gamma^{(p)}_{\ell,\mathbf{a}}|\mathcal{R}\rangle \, \tilde{\gamma}^{(p)}_{\ell,\mathbf{a}}(\mathbf{r}) + \sum_{\mathbf{b}} \langle\beta_{\ell,\mathbf{b}}|\mathcal{R}\rangle \, \tilde{\beta}_{\ell,\mathbf{b}}(\mathbf{r}) \tag{44}$$

inserting the wavelet expansion (42) with $j = \ell$ yields

$$\begin{aligned}
\mathcal{R}(\mathbf{r}) \;\; \approx \;\; & \sum_p \sum_{\mathbf{a}} \left(\sum_q \sum_{\mathbf{b}} \langle\gamma^{(p)}_{\ell,\mathbf{a}}| \frac{1}{r_{12}} |\gamma^{(q)}_{\ell,\mathbf{b}}\rangle \langle\tilde{\gamma}^{(q)}_{\ell,\mathbf{b}}|\eta_{\mathbf{B}}\rangle \right) \tilde{\gamma}^{(p)}_{\ell,\mathbf{a}}(\mathbf{r}) && (45) \\
+ \;\; & \sum_p \sum_{\mathbf{a}} \left(\sum_{\mathbf{b}} \langle\gamma^{(p)}_{\ell,\mathbf{a}}| \frac{1}{r_{12}} |\beta_{\ell,\mathbf{b}}\rangle \langle\tilde{\beta}_{\ell,\mathbf{b}}|\eta_{\mathbf{B}}\rangle \right) \tilde{\gamma}^{(p)}_{\ell,\mathbf{a}}(\mathbf{r}) && (46) \\
+ \;\; & \sum_{\mathbf{a}} \left(\sum_q \sum_{\mathbf{b}} \langle\beta_{\ell,\mathbf{a}}| \frac{1}{r_{12}} |\gamma^{(q)}_{\ell,\mathbf{b}}\rangle \langle\tilde{\gamma}^{(q)}_{\ell,\mathbf{b}}|\eta_{\mathbf{B}}\rangle \right) \tilde{\beta}_{\ell,\mathbf{a}}(\mathbf{r}) && (47) \\
+ \;\; & \sum_{\mathbf{a}} \left(\sum_{\mathbf{b}} \langle\beta_{\ell,\mathbf{a}}| \frac{1}{r_{12}} |\beta_{\ell,\mathbf{b}}\rangle \langle\tilde{\beta}_{\ell,\mathbf{b}}|\eta_{\mathbf{B}}\rangle \right) \tilde{\beta}_{\ell,\mathbf{a}}(\mathbf{r}), && (48)
\end{aligned}$$

where all the matrix elements and coefficients refer to the finest level ℓ only. In order to judge the computational efficiency of the expansion, we have to discuss the convergence properties of each of the sums separately. First of all, we notice that the wavelet Coulomb matrix elements in (45) and the mixed wavelet scaling function Coulomb matrix elements in (46) and (47) decay very fast with increasing distance $|\mathbf{a}-\mathbf{b}|$. The actual order of the decay depends on the number of vanishing moments n and on the wavelet type p envolved. A general discussion, including Coulomb interactions as a special case, can be found in Ref. [53]. We have shown some typical examples in Fig 3. As a consequence, the sums over the grid points $\mathbf{a}, \mathbf{b}$ in (45), (46) and (47) converge fast due to the fast decay of the Coulomb matrix elements and the typically local character of the products $\eta_{\mathbf{A}}$. However, the sum with respect to $\mathbf{a}$ in (48) converges rather slowly. This is due to the fact that for large distances $|\mathbf{a}-\mathbf{b}|$, the Coulomb matrix elements for scaling functions represent essentially point charge Coulomb interactions (Fig 3), which decay with $O(|\mathbf{a}-\mathbf{b}|^{-1})$. In order to circumvent this problem, we decompose $\tilde{V}_\ell = \tilde{V}_{\ell-1} \bigoplus \tilde{W}_{\ell-1}$. Inserting the identity

$$\sum_{\mathbf{a}} \mid \tilde{\beta}_{\ell,\mathbf{a}}\rangle\langle\beta_{\ell,\mathbf{a}} \mid = \sum_p \sum_{\mathbf{a}} \mid \tilde{\gamma}^{(p)}_{\ell-1,\mathbf{a}}\rangle\langle\gamma^{(p)}_{\ell-1,\mathbf{a}} \mid + \sum_{\mathbf{b}} \mid \tilde{\beta}_{\ell-1,\mathbf{b}}\rangle\langle\beta_{\ell-1,\mathbf{b}} \mid \tag{49}$$

into the sum (48) yields

$$\sum_{\mathbf{a}} \left(\sum_{\mathbf{b}} \langle\beta_{\ell,\mathbf{a}}| \frac{1}{r_{12}} |\beta_{\ell,\mathbf{b}}\rangle \langle\tilde{\beta}_{\ell,\mathbf{b}}|\eta_{\mathbf{B}}\rangle \right) \tilde{\beta}_{\ell,\mathbf{a}}(\mathbf{r})$$

$$= \sum_p \sum_{\mathbf{a}} \left(\sum_q \sum_{\mathbf{b}} \langle \gamma^{(p)}_{\ell-1,\mathbf{a}} | \frac{1}{r_{12}} | \gamma^{(q)}_{\ell-1,\mathbf{b}} \rangle \langle \tilde{\gamma}^{(q)}_{\ell-1,\mathbf{b}} | \eta_{\mathbf{B}} \rangle \right) \tilde{\gamma}^{(p)}_{\ell-1,\mathbf{a}}(\mathbf{r}) \tag{50}$$

$$+ \sum_p \sum_{\mathbf{a}} \left(\sum_{\mathbf{b}} \langle \gamma^{(p)}_{\ell-1,\mathbf{a}} | \frac{1}{r_{12}} | \beta_{\ell-1,\mathbf{b}} \rangle \langle \tilde{\beta}_{\ell-1,\mathbf{b}} | \eta_{\mathbf{B}} \rangle \right) \tilde{\gamma}^{(p)}_{\ell-1,\mathbf{a}}(\mathbf{r}) \tag{51}$$

$$+ \sum_{\mathbf{a}} \left(\sum_q \sum_{\mathbf{b}} \langle \beta_{\ell-1,\mathbf{a}} | \frac{1}{r_{12}} | \gamma^{(q)}_{\ell-1,\mathbf{b}} \rangle \langle \tilde{\gamma}^{(q)}_{\ell-1,\mathbf{b}} | \eta_{\mathbf{B}} \rangle \right) \tilde{\beta}_{\ell-1,\mathbf{a}}(\mathbf{r}) \tag{52}$$

$$+ \sum_{\mathbf{a}} \left(\sum_{\mathbf{b}} \langle \beta_{\ell-1,\mathbf{a}} | \frac{1}{r_{12}} | \beta_{\ell-1,\mathbf{b}} \rangle \langle \tilde{\beta}_{\ell-1,\mathbf{b}} | \eta_{\mathbf{B}} \rangle \right) \tilde{\beta}_{\ell-1,\mathbf{a}}(\mathbf{r}), \tag{53}$$

where we obtained an expression which looks very much like the sums (45), (46), (47) and (48), except that we have replaced ℓ by the next coarser level $\ell - 1$. Again all the sums converge fast except the persistent sum (53). However the number of grid points decreases on the coarser levels exponentially, which means that we have at least achieved a reduction in the computational effort. Performing further insertions of the form (49), we can shift the persistent sum to a coarse level ℓ_0, where the number of scaling functions is sufficiently small in order to perform the sum with acceptable computational effort. Such kind of telescopic expansions are standard in wavelet methods and enable us to exploit the local character and the regularity of the functions involved. Eventually we have obtained a mixed expansion

$$\mathcal{R}(\mathbf{r}) \approx \sum_{j=\ell_0}^{\ell} \left(\sum_p \sum_{\mathbf{a}} \mathcal{R}^{\gamma}_{j,p,\mathbf{a}} \tilde{\gamma}^{(p)}_{j,\mathbf{a}}(\mathbf{r}) + \sum_{\mathbf{b}} \mathcal{R}^{\beta}_{j,\mathbf{b}} \tilde{\beta}_{j,\mathbf{b}}(\mathbf{r}) \right) \tag{54}$$

in terms of wavelets and scaling functions on various levels j, where the coefficents are given by

$$\mathcal{R}^{\gamma}_{j,p,\mathbf{a}} = \sum_q \sum_{\mathbf{b}} \langle \gamma^{(p)}_{j,\mathbf{a}} | \frac{1}{r_{12}} | \gamma^{(q)}_{j,\mathbf{b}} \rangle \langle \tilde{\gamma}^{(q)}_{j,\mathbf{b}} | \eta_{\mathbf{B}} \rangle + \sum_{\mathbf{c}} \langle \gamma^{(p)}_{j,\mathbf{a}} | \frac{1}{r_{12}} | \beta_{j,\mathbf{c}} \rangle \langle \beta_{j,\mathbf{c}} | \eta_{\mathbf{B}} \rangle, \tag{55}$$

$$\mathcal{R}^{\beta}_{j,\mathbf{a}} = \begin{cases} \sum_q \sum_{\mathbf{b}} \langle \beta_{j,\mathbf{a}} | \frac{1}{r_{12}} | \gamma^{(q)}_{j,\mathbf{b}} \rangle \langle \tilde{\gamma}^{(q)}_{j,\mathbf{b}} | \eta_{\mathbf{B}} \rangle & j > \ell_0, \\ \sum_q \sum_{\mathbf{b}} \langle \beta_{\ell_0,\mathbf{a}} | \frac{1}{r_{12}} | \gamma^{(q)}_{\ell_0,\mathbf{b}} \rangle \langle \tilde{\gamma}^{(q)}_{\ell_0,\mathbf{b}} | \eta_{\mathbf{B}} \rangle + \sum_{\mathbf{c}} \langle \beta_{\ell_0,\mathbf{a}} | \frac{1}{r_{12}} | \beta_{\ell_0,\mathbf{c}} \rangle \langle \tilde{\beta}_{\ell_0,\mathbf{c}} | \eta_{\mathbf{B}} \rangle & j = \ell_0. \end{cases} \tag{56}$$

In principle we can express the scaling functions in terms of wavelets in order to obtain a standard wavelet espansion of $\mathcal{R}$. Actually this is not necessary for the evaluation of the two-electron Coulomb integrals (40)

$$\begin{aligned} \langle \eta_{\mathbf{A}} \mid \frac{1}{r_{12}} \mid \eta_{\mathbf{B}} \rangle &= \langle \eta_{\mathbf{A}} \mid \mathcal{R} \rangle \\ &= \sum_{j=\ell_0}^{\ell} \left(\sum_p \sum_{\mathbf{a}} \langle \eta_{\mathbf{A}} \mid \tilde{\gamma}^{(p)}_{j,\mathbf{a}} \rangle \mathcal{R}^{\gamma}_{j,p,\mathbf{a}} + \sum_{\mathbf{b}} \langle \eta_{\mathbf{A}} \mid \tilde{\beta}_{j,\mathbf{b}} \rangle \mathcal{R}^{\beta}_{j,\mathbf{b}} \right). \end{aligned} \tag{57}$$

The Coulomb integrals in the wavelet basis can be easily derived from the corresponding integrals for the scaling functions using the refinement relations (20) and (21), where we get e.g.

$$\langle \gamma^{(p)}_{j,\mathbf{a}} | \frac{1}{r_{12}} | \beta_{j,\mathbf{b}} \rangle = 2^3 \sum_{\mathbf{c},\mathbf{d}} G^{(p)}_{\mathbf{c}-2\mathbf{a}} \, H_{\mathbf{d}-2\mathbf{b}} \langle \beta_{j+1,\mathbf{c}} | \frac{1}{r_{12}} | \beta_{j+1,\mathbf{d}} \rangle. \tag{58}$$

Again these integrals satisfy a simple scaling relation

$$\begin{aligned} \langle \beta_{j,\mathbf{a}} | \frac{1}{r_{12}} | \beta_{j,\mathbf{b}} \rangle &= 2^{-2j} \langle \beta_{0,\mathbf{a}} | \frac{1}{r_{12}} | \beta_{0,\mathbf{b}} \rangle \\ &= 2^{-2j} \langle \beta_{0,\mathbf{a}-\mathbf{b}} | \frac{1}{r_{12}} | \beta_{0,\mathbf{0}} \rangle, \end{aligned} \tag{59}$$

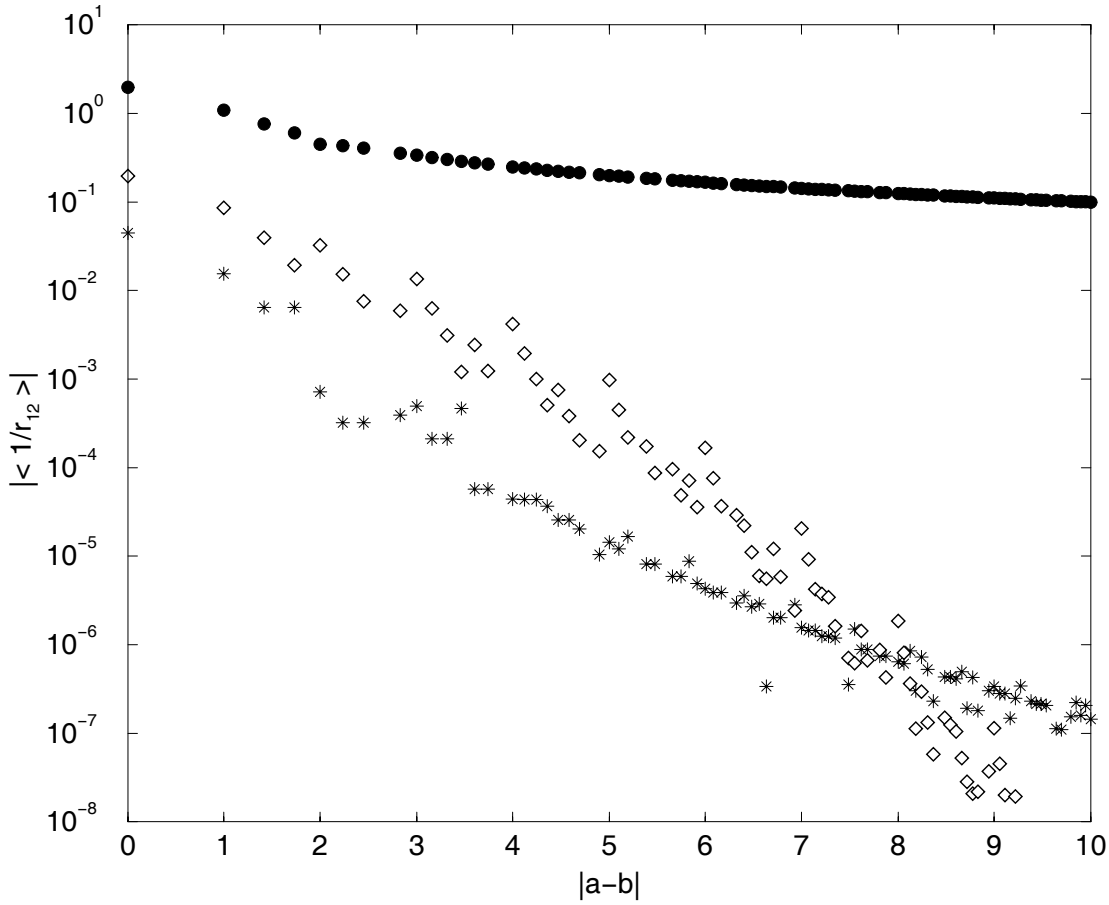

Figure 3: Sparse wavelet representation of Coulomb interactions. Matrix elements for three different combinations of wavelets $\gamma_{0,\mathbf{a}}^{(p)}$ and scaling functions $\beta_{0,\mathbf{a}}$ have been selected: ($\bullet$) $\langle\beta_{0,\mathbf{a}}|\frac{1}{r_{12}}|\beta_{0,\mathbf{b}}\rangle$, ($\star$) $\langle\beta_{0,\mathbf{a}}|\frac{1}{r_{12}}|\gamma_{0,\mathbf{b}}^{(1)}\rangle$, ($\diamond$) $\langle\gamma_{0,\mathbf{a}}^{(7)}|\frac{1}{r_{12}}|\gamma_{0,\mathbf{b}}^{(7)}\rangle$. Absolute values of the largest matrix elements at distance $|\mathbf{a}-\mathbf{b}|$ are plotted on a logarithmic scale. The three-dimensional wavelets and scaling functions were generated from the univariate wavelet with six vanishing moments of Sweldens [44] and the univariate scaling function of Deslauriers and Dubuc [45].

which relates Coulomb integrals on arbitrary levels j to level 0. In the second step of Eq. (59), we have used the translational symmetry of the scaling functions. Therefore it is sufficient to calculate Coulomb integrals for scaling functions at level $j = 0$, which are called elementary integrals in the sequel, all the other integrals can be obtained from relations (58) and (59). Furthermore it has to be mentioned that due to the compact supports of the scaling functions, the weak singularity of the integrand vanishes for sufficiently large distances $|\mathbf{a}-\mathbf{b}|$. As a consequence multipole expansions become applicable, which enable a simple and accurate computation of the elementary integrals in this case. Obviously elementary integrals do not depend on the specific system under consideration. Therefore we have to calculate these integrals only once for a certain type of scaling function and keep them, up to a given distance, in a library. Methods how to actually calculate elementary integrals are discussed in Appendix A.

Computation of the one-electron Coulomb integrals (39) follows the same line. We start with an expansion

$$\langle\eta_{\mathbf{A}}|\frac{1}{r_{\mathbf{C}}}\rangle \approx \sum_p \sum_{\mathbf{a}} \langle\gamma_{\ell,\mathbf{a}}^{(p)}|\frac{1}{r_{\mathbf{C}}}\rangle\langle\eta_{\mathbf{A}}|\tilde{\gamma}_{\ell,\mathbf{a}}^{(p)}\rangle + \sum_{\mathbf{b}} \langle\beta_{\ell,\mathbf{b}}|\frac{1}{r_{\mathbf{C}}}\rangle\langle\eta_{\mathbf{A}}|\tilde{\beta}_{\ell,\mathbf{b}}\rangle \tag{60}$$

on the finest level ℓ and perform a telescopic expansion analogous to Eqs. (45-48) until a sufficiently coarse level has been reached on which the persistent sum can be performed with acceptable effort.

2.3 Tensor product representation

The functions $\eta_{\mathbf{A}}$, we have to deal within the integral evaluation, require three-dimensional grids for their representation. To avoid extensive calculations on three-dimensional grids, we use tensor product expansions of these functions. For this, we just take the orbitals ϕ_i from a standard quantum chemistry program, where orbitals are represented as linear combinations of "Cartesian Gaussian" functions

$$\phi_i(\mathbf{r}) = \sum_a d_{i,a}\ (x - C_{a,x})^{\ell_a} (y - C_{a,y})^{m_a} (z - C_{a,z})^{n_a} \exp[-\alpha_a (\mathbf{r} - \mathbf{C}_a)^2]. \tag{61}$$

Such kind of expansion perfectly fits our requirements. The product formation can be performed in three consecutive steps, where in the first step all of the required one-dimensional "Cartesian Gaussian" functions have been expanded in the wavelet basis

$$\begin{aligned} \chi_{\mathbf{A}}(x) &:= (x - C)^{\ell} \exp[-\alpha (x - C)^2] \\ &= \sum_{j \geq j_0} \sum_a \langle \chi_{\mathbf{A}} | \tilde{\psi}_{j,a} \rangle\, \psi_{j,a}(x) + \sum_b \langle \chi_{\mathbf{A}} | \tilde{\varphi}_{j_0,b} \rangle\, \varphi_{j_0,b}(x). \end{aligned} \tag{62}$$

In the case of interpolating scaling functions like those of Deslauriers and Dubuc [45], the determination of expansion coefficients $\langle \chi_{\mathbf{A}} | \tilde{\psi}_{j,b} \rangle$, $\langle \chi_{\mathbf{A}} | \tilde{\varphi}_{j_0,b} \rangle$ is fairly straightforward. On a sufficiently fine level j, we simply take

$$\langle \chi_{\mathbf{A}} | \tilde{\varphi}_{j,a} \rangle = 2^{-j/2} \chi_{\mathbf{A}}(2^{-j} a) \tag{63}$$

and use the refinement relations (4) and (7) to get the coefficients on coarser levels. We want to refer to Appendix A.2 for the discussion of a method, which does not rely on the interpolation property.

From this point on, all the calculations are based exclusively on the wavelet expansions (62) of the Gaussians. In a second step, we generate all the required products of "Cartesian Gaussian" functions with univariate wavelets

$$\begin{aligned} \chi_{\mathbf{B}}(x) &= \chi_{\mathbf{A}}(x)\, \psi_{\ell,b}(x) \\ &= \sum_{j \geq j_0} \sum_a \langle \chi_{\mathbf{A}} | \tilde{\psi}_{j,a} \rangle\, \psi_{j,a}(x) \psi_{\ell,b}(x) + \sum_c \langle \chi_{\mathbf{A}} | \tilde{\varphi}_{j_0,c} \rangle\, \varphi_{j_0,c}(x) \psi_{\ell,b}(x) \\ &= \sum_{j \geq j_0} \sum_b \langle \chi_{\mathbf{B}} | \tilde{\psi}_{j,b} \rangle\, \psi_{j,b}(x) + \sum_c \langle \chi_{\mathbf{B}} | \tilde{\varphi}_{j_0,c} \rangle\, \varphi_{j_0,c}(x) \end{aligned} \tag{64}$$

and scaling functions $\varphi_{j,a}$, respectively, where $\mathbf{A}, \mathbf{B}$ represent appropriately chosen multi-indices in order to characterize the functions (62) and (64). The numerical evaluation of expansion coefficients of products $\langle \chi_{\mathbf{B}} | \tilde{\psi}_{j,b} \rangle$, $\langle \chi_{\mathbf{B}} | \tilde{\varphi}_{j,b} \rangle$ is discussed in Section 3. Finally we have to form products $\chi_{\mathbf{A}} = \chi_{\mathbf{B}} \chi_{\mathbf{C}}$, which are required for the functions $\eta_{\mathbf{A}}$. In Fig. 4 we have shown wavelet expansions of a Gaussian $\exp(-x^2)$ and its wavelet product $\exp(-x^2)\, \psi_{1,1}(x)$. As expected, the largest contribution to the product expansion comes from level $j = 1$ and neighboring levels, where the coefficients of the finer levels decay rapidly.

In order to represent the functions $\eta_{\mathbf{A}}(\mathbf{r})$ on a three-dimensional grid it is convenient to store the expansion coefficients of the functions $\chi_{\mathbf{A}}$ in the nonstandard representation, which means that for each function not only the wavelet but also the scaling function coefficients on each level j have to be stored. Although these are redundant informations, it is convenient

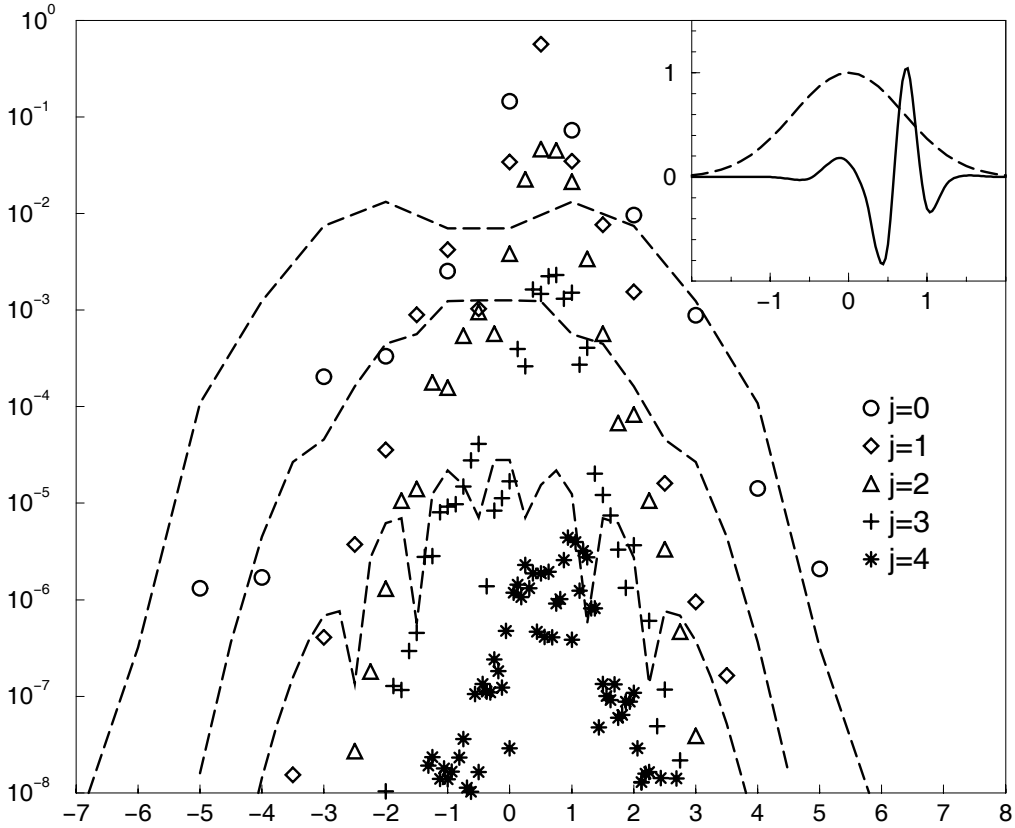

Figure 4: Wavelet expansions of a Gaussian $\exp(-x^2)$ and its wavelet product $\exp(-x^2)\,\psi_{1,1}(x)$. The wavelet with six vanishing moments has been taken from Sweldens [44]. Absolute values of the wavelet coefficients for the product at various levels j are plotted on a logarithmic scale. Dashed lines indicate the distribution of the wavelet coefficients for the Gaussian function alone. For comparison both functions are shown on the inlay.

in view of the tensor product structure of the wavelet basis (19). We can calculate the wavelet coefficients of simple products $\kappa(\mathbf{r}) = \chi_{\mathbf{A}}(x)\chi_{\mathbf{B}}(y)\chi_{\mathbf{C}}(z)$ using the coefficients of the nonstandard representations of their factors

$$\begin{bmatrix} \vdots \\ \langle \kappa \mid \tilde{\gamma}^{(p)}_{j,\mathbf{a}} \rangle \\ \langle \kappa \mid \tilde{\beta}_{j,\mathbf{a}} \rangle \\ \vdots \\ \langle \kappa \mid \tilde{\beta}_{j_0,\mathbf{a}} \rangle \end{bmatrix} = \begin{bmatrix} \vdots \\ \begin{pmatrix} \langle \chi_{\mathbf{A}} \mid \tilde{\psi}_{j,a_x} \rangle \\ \langle \chi_{\mathbf{A}} \mid \tilde{\varphi}_{j,a_x} \rangle \end{pmatrix} \times \begin{pmatrix} \langle \chi_{\mathbf{B}} \mid \tilde{\psi}_{j,a_y} \rangle \\ \langle \chi_{\mathbf{B}} \mid \tilde{\varphi}_{j,a_y} \rangle \end{pmatrix} \times \begin{pmatrix} \langle \chi_{\mathbf{C}} \mid \tilde{\psi}_{j,a_z} \rangle \\ \langle \chi_{\mathbf{C}} \mid \tilde{\varphi}_{j,a_z} \rangle \end{pmatrix} \\ \vdots \\ \langle \chi_{\mathbf{A}} \mid \tilde{\varphi}_{j_0,a_x} \rangle \times \langle \chi_{\mathbf{B}} \mid \tilde{\varphi}_{j_0,a_y} \rangle \times \langle \chi_{\mathbf{C}} \mid \tilde{\varphi}_{j_0,a_z} \rangle \end{bmatrix}. \qquad (65)$$

From this we easily get the expansion coefficients of the functions $\eta_{\mathbf{A}}$ by summing over the expansion coefficients of the orbitals (61). It should be emphasized that the storage requirements for the three-dimensional coefficients on the left side of Eq. (65) are of $O(M^3)$, where M is the number of coefficients in the expansions (62). Consequently, we calculate the three-dimensional coefficients from Eq. (65) just when they are needed in the course of the evaluation of the one- and two-electron Coulomb integrals as outlined above.

2.4 Kinetic energy and overlap integrals

It is evident from the tensor product representation (65) that the remaining integrals for the functions

$$\zeta_{\mathbf{A}}(\mathbf{r}) = \begin{cases} \phi_i(\mathbf{r}) \\ \phi_i(\mathbf{r})\gamma^{(p)}_{m,\mathbf{a}}(\mathbf{r}) \end{cases}, \tag{66}$$

with respect to the one-body operators $\hat{O} = 1,\ \Delta$

$$\langle \zeta_{\mathbf{A}} | \hat{O} | \zeta_{\mathbf{B}} \rangle := \int d^3r\ \zeta_{\mathbf{A}}(\mathbf{r})\ \hat{O}\ \zeta_{\mathbf{B}}(\mathbf{r}) \tag{67}$$

can be expressed in terms of one-dimensional integrals. These integrals can be obtained from the elementary integrals

$$\langle \varphi_{0,a} | \varphi_{0,0} \rangle = \int dx\ \varphi(x-a)\varphi(x), \tag{68}$$

$$\langle \varphi_{0,a} | \Delta | \varphi_{0,0} \rangle = \int dx\ \varphi(x-a)\Delta\varphi(x), \tag{69}$$

using the refinement relations (4), (7) and scaling relations analogous to Eq. (59).

3 Products of wavelets

Evaluation of the integrals (39) and (40) requires wavelet expansions of products of wavelets with orbitals. We have outlined in Section 2.3 how to factorize the products with respect to x, y, z. This considerably simplifies the wavelet expansion of products, due to the restriction to products of univariate functions. As a starting point, we consider the product $f(x)\,g(x)$ of two arbitrary functions $f(x) = \sum_{j,a} v_{j,a}\psi_{j,a}(x)$, $g(x) = \sum_{j,a} w_{j,a}\psi_{j,a}(x)$ both represented in terms of their pure wavelet expansions. We have chosen a pure wavelet expansion for f, g in order to simplify our notation. In actual applications, we have used expansions of the form (10), where scaling functions represent contributions from coarse levels below j_0. Except of the appearance of some additional terms, where wavelets have to be replaced by scaling functions, this does not affect the method outlined below. Obviously such kind of products can be traced back to products of wavelets

$$\psi_{j,a}(x)\,\psi_{\ell,b}(x) = \sum_m \sum_c \int dt\ \psi_{j,a}(t)\,\psi_{\ell,b}(t)\,\tilde{\psi}_{m,c}(t)\ \ \psi_{m,c}(x), \tag{70}$$

which themselve can be expressed in terms of the wavelet basis. We introduce the wavelet coupling coefficients

$$\begin{pmatrix} j & \ell & m \\ a & b & c \end{pmatrix} := \int dt\ \psi_{j,a}(t)\,\psi_{\ell,b}(t)\,\tilde{\psi}_{m,c}(t), \tag{71}$$

which represent the basic quantities for the product evaluation. The coupling coefficients can be easily calculated using the method of Beylkin, Dahmen and Micchelli outlined in Appendix A. Due to translation and dilation symmetry, the storage of only a small number of coupling coefficients is required. For example in the case $j \le \ell, m$ we have the simple relation

$$\begin{pmatrix} j & \ell & m \\ a & b & c \end{pmatrix} = 2^{j/2} \begin{pmatrix} 0 & \ell - j & m - j \\ 0 & b - 2^{\ell-j}a & c - 2^{m-j}a \end{pmatrix}, \tag{72}$$

which shows that we only have to deal with coupling elements of the form

$$\begin{pmatrix} 0 & \ell & m \\ 0 & b & c \end{pmatrix}_{(j \le \ell, m)}, \quad \begin{pmatrix} j & \ell & 0 \\ a & b & 0 \end{pmatrix}_{(j, \ell > m)}. \tag{73}$$

The coupling coefficients (73) for wavelets with compact support differ from zero only for a finite number of grid points b, c and a, b, respectively. Depending on the specific choice of the wavelet basis, the coupling coefficients show a characteristic decay for $j \leq \ell << m$ and $\ell >> j, m$, respectively. A sufficiently fast decay with respect to the level m is essential for an efficient approximation of products.

The product expansion

$$f(x)g(x) = \sum_m \sum_c \underbrace{\left[\sum_{j,\ell} \sum_{a,b} \begin{pmatrix} j & \ell & m \\ a & b & c \end{pmatrix} v_{j,a} w_{\ell,b} \right]}_{=u_{m,c}} \psi_{m,c}(x). \tag{74}$$

resembles to the coupling of angular momenta, where we couple two wavelet levels j, ℓ to a level m. However, contrary to angular momenta, the range of m is not strictly finite. In Appendix B we derive a rigorous upper bound for the coupling coefficients (71). The following useful estimate

$$\|\mathbf{u}_m\|_\infty \leq C^m_{j,\ell} \, \|\mathbf{v}_j\|_\infty \, \|\mathbf{w}_\ell\|_\infty \tag{75}$$

with

$$C^m_{j,\ell} = 2^{j/2} \max_{c \in \{0,\ldots,2^{m-j}-1\}} \left\{ \sum_{a,b} \left| \begin{pmatrix} 0 & \ell - j & m - j \\ 0 & b - 2^{\ell - j} a & c - 2^{m-j} a \end{pmatrix} \right| \right\} \tag{76}$$

based on the maximum norm $\|\mathbf{v}_j\|_\infty := \max_a \{|v_{j,a}|\}$ gives an upper bound on $|u_{m,c}|$. We show the constants $C^m_{j,\ell}$ for the case $j \leq \ell, m$ in Fig. 5.

4 Some preliminary results for the helium atom

We want to demonstrate the feasibility of our method by applying it to the helium atom. Actually this is a standard model for electron correlations, which already shows many characteristic features of large systems. By means of the helium atom, we can study the approximation properties of hyperbolic wavelets and develop strategies for adaptive refinements in the cusp region. Aggregates of noninteracting helium atoms can serve as a basis to study the size-extensivity error. These topics will be the subject of a forthcoming publication [49]. In the present work we focus on more elementary features of our method and want to demonstrate that the techniques discussed in the preceding sections are feasible for realistic applications.

Taking a multivariate wavelet basis $\gamma^{(p)}_{j,\mathbf{a}}$ for the wavelet expansion of $\mathcal{F}$, we have generated all possible symmetric one-body factors $\mathcal{F}^{(1)}_{j,\mathbf{a}}$ as well as two-body factors $\mathcal{F}^{(2)}_{\mathbf{J},\mathbf{A}}$, irrespective of the sparse grids condition. The mean-field part Φ corresponds to the closed shell HF wavefunction, where the $1s$ orbitals have been expanded by Gaussian's with exponents taken from Dunnings VQZ basis set [54]. In order to get a sufficiently accurate description near the electron-nuclear cusp, exponents are ranging up to $\alpha = 528.5$, which requires wavelets up to level $j = 5$ in the expansion (62).

Our results listed in Table 1 are only of preliminary character due to the incompleteness of our multivariate wavelet basis $\gamma^{(p)}_{j,\mathbf{a}}$ in the subspaces W_j under consideration. On each level j, only the nearest neighbor wavelets of each type p, with respect to the nucleus, have been taken into account. The contributions to the energy of type p wavelets decrease on all levels in the order $p = (1,2,3) >> (4,5,6) > 7$. This has to be expected due to the different number of univariate wavelets in the tensor products (19). It can be seen that the dominant contribution comes from the level $j = -2$, which allready recovers 83% of the correlation energy. Compared with it, the contribution of the next coarser level $j = -3$ is almost negligible ($< 10^{-4}$ Hatree), clearly demonstrating that the assumption of a lower bound on the coarse

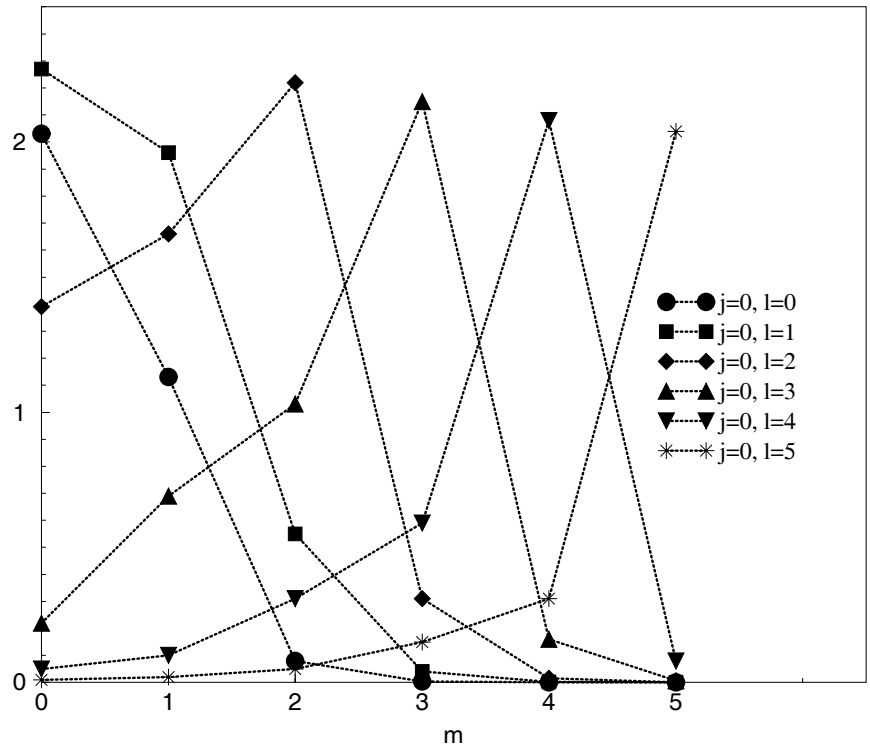

Figure 5: Constants $C^m_{j,\ell}$ of upper bounds for the wavelet coefficients of products. Dotted lines connect the cases where the levels j, ℓ are kept fixed. The constants refer to Sweldens biorthogonal wavelet basis [44] with six vanishing moments for ψ and $\tilde{\psi}$.

levels in the expansion (27) is reasonable. In the direction of finer scales, contributions to the correlation energy decrease quite fast. A definite statement concerning the asymptotic convergence behavior, however, cannot be drawn from our results. Nevertheless our results show that rather accurate energies can be achieved already with a rather small number of wavelets. This is encouraging in view of the fact that we have used regular Cartesian grids, which were not especially adopted to atomic symmetries, except that we have placed the nucleus in the origin.

5 Conclusions

We have outlined a wavelet based method for the description of electron correlations within the many-electron Schrödinger equation. Such kind of approach enables a multiscale treatment of electron correlations, which means that the specific length- and energy-scales of the various underlying physical processes can be explicitly represented by the wavelet basis. The high dimensionality of many-electron problems can be dealt with by means of the hyperbolic wavelet approximation. For an accurate description of short-range correlations, however, local refinements in the inter-electronic cusp regions are required.

Apart from physical aspects of our method, we have discussed various technical peculiarities. This includes the efficient calculation of one- and two-electron integrals, where we

Table 1: Full tensor product wavelet expansion of $\mathcal{F}$ for the helium atom. Wavelets in the expansion (27) range from the coarsest level $j_0 = -2$ up to the finest level $j_{\max}$. No restriction on the tensor products has been imposed ($Q = 2j_{\max}$). An analytic evaluation of the integrals in the Gaussian basis set yields a Hartree-Fock reference energy of -2.861514 Hartree. Three-dimensional wavelets were generated from the univariate wavelet with six vanishing moments of Sweldens [44] and the univariate scaling function of Deslauriers and Dubuc [45].

	Wavelet type p								
$j_{\max}$	1^a	2	3	4	5	6	7	n^b	Energy (Hartree)
-	-	-	-	-	-	-	-	0	-2.861525
-2	2	2	2	-	-	-	-	28	-2.894232
-1	2	2	2	-	-	-	-	91	-2.899038
0	2	2	2	-	-	-	-	190	-2.900613
-2	2	2	2	4	4	4	-	190	-2.896436
-1	2	2	2	4	4	4	-	703	-2.901015
0	2	2	2	4	4	4	-	1540	-2.902738
1	2	2	2	4	4	4	-	2701	-2.903004
-2	2	2	2	4	4	4	8	378	-2.896523
-1	2	2	2	4	4	4	8	1431	-2.901269
								exact	-2.903724

[a] Number of three-dimensional wavelets of type p (19) on each level $j_0 \leq j \leq j_{\max}$.
[b] Number of symmetrized tensor products.

have used the sparsity of Coulomb integrals within the nonstandard representation, in order to get an efficient scheme for the calculation of more complicated integrals. Moreover we have discussed the numerical calculation of elementary Coulomb integrals solely based on the knowledge of the filter coefficients. We also presented a detailed treatment of products of wavelets. Their appearance represents a key feature of our method.

To ilustrate the feasibility of our approach we applied it to the helium atom. Our results indicate that already with a comparatively small number of wavelets reasonable accuracies can be achieved.

Appendices

A Elementary integrals for scaling functions

We have seen in Section 2.2 that all the required integrals can be reduced to elementary integrals involving scaling functions $\beta_{0,\mathbf{a}}$ only. In this Appendix we want to discuss methods how to actually calculate these integrals. In principle there are two different ways to tackle this problem. One possible approach would be to use an analytic representation for the scaling

function e.g. in terms of piecewise polynomials and to calculate integrals analytically or by convenient quadrature formulas. However, closed analytic expressions are not always available for scaling functions and an approximate treatment seems to be problematic in view of their occasionally rather complicated structure. Another approach is to avoid any reference to analytic expressions for wavelets at all and to use filter coefficients only. We follow the latter approach, which makes our method more flexible with respect to the choice of the wavelet basis. The general procedure to compute integrals along this line depends on whether or not the integrals satisfy scaling relations of the form (59) with respect to the levels j. If this is the case we can use the very elegant and simple method of Beylkin [52], Dahmen and Micchelli [55]. Otherwise we have used the Gaussian transform method discussed below, which requires the Fourier transform of the scaling function. The Fourier transform can be easily calculated from the filter coefficients using a product formula.

A.1 Integral calculation according to Beylkin, Dahmen and Micchelli

The basic idea is to use a scaling relation of the form (59), which relates an integral for scaling functions on level $j+1$ to the same type of integral for scaling functions on level j. To illustrate this method, we want to discuss the simple case of overlap integrals in some detail. Inserting the refinement relation of the scaling functions (4) into the overlap integral

$$\begin{aligned}
\langle\varphi_{0,a}|\varphi_{0,0}\rangle &= \int dx\ \varphi(x-a)\varphi(x) \\
&= 2^2 \sum_{b,c} h_b h_c \int dx\ \varphi(2x-2a-b)\varphi(2x-c) \\
&= 2 \sum_{b,c} h_b h_c \int dx\ \varphi(x-2a-b+c)\varphi(x) \\
&= 2 \sum_{b} \left(\sum_{c} h_c h_{b-2a+c} \right) \langle\varphi_{0,b}|\varphi_{0,0}\rangle, \qquad (77)
\end{aligned}$$

we end up with a linear system of equations for these integrals. Alternatively, Eq. (77) can be viewed as an eigenvalue problem for the eigenvalue 1. Eqs. (77) do not completely specify the overlap integrals, the additional condition [52]

$$\sum_{a} \langle\varphi_{0,a}|\varphi_{0,0}\rangle = 1 \qquad (78)$$

is required in order to get a unique solution of Eqs. (77), which corresponds to the overlap integrals. The condition (78) is a simple consequence of Eq. (5) and the normalization property $1 = \int dx\varphi(x)$.

An iterative scheme can be applied for solving Eqs. (77) [52, 55]. For this we have to find an initial guess for the integrals $\langle\varphi_{0,a}|\varphi_{0,0}\rangle_{(0)}$ which satisfies condition (78) e.g.

$$\langle\varphi_{0,a}|\varphi_{0,0}\rangle_{(0)} = \delta_{0,a}. \qquad (79)$$

From this initial guess we obtain applying Eqs. (77) in a first iteration

$$\langle\varphi_{0,a}|\varphi_{0,0}\rangle_{(1)} = 2 \sum_{b} \left(\sum_{c} h_c h_{b-2a+c} \right) \langle\varphi_{0,b}|\varphi_{0,0}\rangle_{(0)}. \qquad (80)$$

This process continues until convergence has been achieved. Due to the structure of Eqs. (77), condition (78) is preserved in each iteration.

The wavelet coupling coefficients (71) can be traced back to integrals

$$\langle \varphi_{0,a} \varphi_{0,b} | \tilde{\varphi}_{0,0} \rangle := \int dx \; \varphi(x-a) \varphi(x-b) \tilde{\varphi}(x) \tag{81}$$

using the refinement relations (4) and (7). Analogous to the previous case, these integrals can be related to a linear system of equations

$$\langle \varphi_{0,a} \varphi_{0,b} | \tilde{\varphi}_{0,0} \rangle = 2^2 \sum_{c,d} \left(\sum_e \tilde{h}_e h_{c-2a+e} h_{d-2b+e} \right) \langle \varphi_{0,c} \varphi_{0,d} | \tilde{\varphi}_{0,0} \rangle, \tag{82}$$

supplemented by the additional condition

$$\sum_{a,b} \langle \varphi_{0,a} \varphi_{0,b} | \tilde{\varphi}_{0,0} \rangle = 1. \tag{83}$$

Together, Eqs. (82) and (83) uniquely specify the integrals (81).

The same technique applies to the kinetic energy integrals as well. The system of equations

$$\langle \varphi_{0,a} | \Delta | \varphi_{0,0} \rangle = 2^3 \sum_b \left(\sum_c h_c h_{b-2a+c} \right) \; \langle \varphi_{0,b} | \Delta | \varphi_{0,0} \rangle \tag{84}$$

has to be completed by the condition [52]

$$\sum_a a^2 \langle \varphi_{0,a} | \Delta | \varphi_{0,0} \rangle = 2 \tag{85}$$

in order to get the kinetic energy integrals. For the Deslauriers and Dubuc interpolating scaling functions, Eq. (85) is a simple consequence of $x^2 = \sum_a a^2 \varphi(x-a)$, which can be easily derived from Eqs. (5) and (17).

A slight modification of this method can be applied to elementary two-electron Coulomb integrals (59). This just requires the values of the integrals at large distances greater than the diameter L of the scaling function, where the supports of the scaling functions do not overlap any more. In such a case numerical quadrature formulas for wavelets [56] become applicable, which greatly simplifies the computation of these integrals. The scaling function of Deslauriers and Dubuc [44, 45] satisfies the vanishing moment property (17). For our present purposes it was therefore already sufficient to use the point charge approximation for the Coulomb integrals

$$\langle \beta_{0,\mathbf{a}} | \frac{1}{r_{12}} | \beta_{0,\mathbf{0}} \rangle \approx \frac{1}{|\mathbf{a}|} \tag{86}$$

at large distances $|\mathbf{a}| > L$. Keeping the integrals for $|\mathbf{a}| > L$ fixed, we have used equation

$$\langle \beta_{0,\mathbf{a}} | \frac{1}{r_{12}} | \beta_{0,\mathbf{0}} \rangle = 2 \sum_{\mathbf{b}} \left(\sum_{\mathbf{c}} H_{\mathbf{c}} H_{\mathbf{b}-2\mathbf{a}+\mathbf{c}} \right) \; \langle \beta_{0,\mathbf{b}} | \frac{1}{r_{12}} | \beta_{0,\mathbf{0}} \rangle \tag{87}$$

to calculate the integrals for $|\mathbf{a}| \leq L$ iteratively. No additional condition is required in this case. For our initial guess of the integrals $|\mathbf{a}| \leq L$, we simply used the point charge approximation, except at the origin, where some finite value has to be chosen. The accuracy of this scheme is just limited by the numerical error inherent to the integrals at large distances, which are kept fixed. We observed a fast convergence rate of $O(2^{-2k})$ with respect to the number of iterations k.

Iterative schemes cannot be applied to one-electron Coulomb integrals (39) for arbitrary positions $\mathbf{C}$ of the nucleus. However it is possible for the special case, where a nucleus is

located on a grid point. First we want to consider the case $\mathbf{C} = \mathbf{0}$. Obviously these integrals satisfy the equation

$$\langle \beta_{0,\mathbf{a}} | \frac{1}{r} \rangle = 2 \sum_{\mathbf{b}} H_{\mathbf{b}-2\mathbf{a}} \, \langle \beta_{0,\mathbf{b}} | \frac{1}{r} \rangle, \tag{88}$$

which means that we can apply the same technique as for the two-electron Coulomb integrals. In order to make the method applicable for general molecules, we notice that $\mathbf{C}$ can be approximated with arbitrary accuracy by an expansion of the form $\mathbf{C} = \sum_{i=0}^{m} 2^{-i} \mathbf{b}_i$, where the $\mathbf{b}_i$ are vectors with integer components. Using such kind of expansion, we can express an integral for a scaling function on level j by applying the multivariate refinement relation (20) n times ($H^n_{\mathbf{p}} = \sum_{\mathbf{b}} H^{n-1}_{\mathbf{b}} H_{\mathbf{p}-2\mathbf{b}}$)

$$\begin{aligned} \langle \beta_{j,\mathbf{a}} | \frac{1}{r_{\mathbf{C}}} \rangle &= 2^{3(n+j/2)} \sum_{\mathbf{p}} H^n_{\mathbf{p}} \int d^3 r \, \frac{\beta(2^{j+n}\mathbf{r} - 2^n \mathbf{a} - \mathbf{p})}{\mid \mathbf{r} - \mathbf{C} \mid} \\ &= 2^{3(n+j/2)} \sum_{\mathbf{p}} H^n_{\mathbf{p}} \int d^3 r \, \frac{\beta(2^{j+n}\mathbf{r} + \sum_{i=0}^{m} 2^{j+n-i} \mathbf{b}_i - 2^n \mathbf{a} - \mathbf{p})}{\mid \mathbf{r} \mid} \\ &= 2^{3n/2} \sum_{\mathbf{p}} H^n_{\mathbf{p}-2^n \mathbf{a} + \sum_{i=0}^{m} 2^{j+n-i} \mathbf{b}_i} \, \langle \beta_{j+n,\mathbf{p}} | \frac{1}{r} \rangle \end{aligned} \tag{89}$$

in terms of integrals of scaling functions with $\mathbf{C} = 0$ on level $j+n$, with $j+n \geq m$. Although such kind of procedure is always possible, it might become rather troublesome for large n. Therefore it seems to be reasonble to consider a different approach which avoids expansions over a large number of levels.

A.2 Gaussian transform method for Coulomb integrals

Typically quantum chemistry requires the computation of three- and six-dimensional integrals, where the integrands can be factorized except of functions depending on $|\mathbf{r}|$ and $|\mathbf{r_1} - \mathbf{r_2}|$, respectively. In some cases it is possible to apply the Gaussian transform method, which has been introduced into quantum chemistry by Boys and Shavitt [57]. The Coulomb potential can be expressed in terms of an integral over a Gaussian function

$$\frac{1}{|\mathbf{r} - \mathbf{C}|} = \frac{2}{\sqrt{\pi}} \int_0^{\infty} dt \, \exp(-|\mathbf{r} - \mathbf{C}|^2 t^2), \tag{90}$$

which enables a factorization of the three-dimensional integral

$$\langle \beta_{0,\mathbf{a}} | \frac{1}{r_{\mathbf{C}}} \rangle = \int d^3 r \, \frac{\varphi(x - a_x)\varphi(y - a_y)\varphi(z - a_z)}{\mid \mathbf{r} - \mathbf{C} \mid} \tag{91}$$

$$= \frac{1}{(2\pi)^2} \int_0^{\infty} dt \, G(a_x, t, C_x) \, G(a_y, t, C_y) \, G(a_z, t, C_z) \tag{92}$$

into a product of one-dimensional integrals [1]

$$G(a, t, C) = 2\pi^{1/2} \int_{-\infty}^{\infty} dx \, \exp[-(x + a - C)^2 t^2] \, \varphi(x), \tag{93}$$

at the expense of calculating an additional integral with respect to the auxiliary variable t. The function $G(a, t, C)$ is smooth with respect to t, due to the compact support of the scaling function φ. Provided that $G(a, t, C)$ shows a well behaved asymptotic behavior for

[1] We want to mention that such kind of integrals for dual scaling functions also appear in the wavelet expansion coefficients of Gaussians (62). As a byproduct, the method outlined below can be used for the calculation of these coefficients.

$\lim t \to \infty$ we can calculate the integral (92) numerically. For this we have determined Chebyshev approximations [58] for each $G(a,t,C)$ on a sequence of finite intervals, until it has approached its asymptotic expansion with given accuracy. This requires the evaluation of $G(a,t,C)$ for a certain number of grid points as well as the determination of the coefficients of the asymptotic expansion, both can be done rather efficiently by using the inverse fast Fourier transform (FFT). To see how this works, we insert the inverse Fourier transform of the scaling function $\varphi(x) = (2\pi)^{-1} \int d\omega \, \exp(i\omega x)\hat{\varphi}(\omega)$ into Eq. (93)

$$\begin{aligned} G(a,t,C) &= \pi^{-1/2} \int_{-\infty}^{\infty} dx \, \exp[-(x+a-C)^2 t^2] \int_{-\infty}^{\infty} d\omega \, \hat{\varphi}(\omega) \exp(i\omega x) \\ &= t^{-1} \int_{-\infty}^{\infty} d\omega \, \exp[-w^2/(4t^2)] \, \exp[i\omega(a+C)] \, \hat{\varphi}(\omega) \end{aligned} \tag{94}$$

and use the fact that the Fourier transform of a Gaussian is a Gaussian again.

The function $G(a,t,C)$ depends on the Fourier transform of the scaling function $\hat{\varphi}$, which can be obtained from the product formula [28]

$$\hat{\varphi}(\omega) = \prod_{j=1}^{\infty} h(2^{-j}\omega), \tag{95}$$

where $h(\omega) = \sum h_k \exp(-ik\omega)$ is a finite Fourier series with respect to the filter coefficients h_k. An advantage of this approach is that it does not require any specific knowledge of the scaling function φ beyond its filter coefficients, which characterize φ uniquely [28].

For the numerical treatment of the function $G(a,t,C)$, we first have to discuss its behavior with respect to small and large t values. It immediately follows from (93) that in the $\lim t \to 0$ the function $G(a,t,C)$ approaches the value

$$G(a,0,C) = 2\sqrt{\pi}\hat{\varphi}(0), \tag{96}$$

irrespective of the values of the parameters a, C. Within the intermediate regime of not too large values of t, the integrand (94) is dominated by the Gaussian, which guarantees an exponential slope. However, in the asymptotic regime, the slope of the Fourier transform of the scaling function becomes essential. We performed a Taylor expansion of the Gaussian function in order to obtain the asymptotic expansion in powers of t^{2n+1}

$$\lim_{t\to\infty} G(a,t,C) \approx \sum_{n\geq 0} \frac{G_n(a,C)}{t^{2n+1}} \tag{97}$$

$$G_n(a,C) = \frac{(-1)^n}{4^n n!} \int_{-\infty}^{\infty} d\omega \, \exp[i\omega(a+C)]\omega^{2n} \, \hat{\varphi}(\omega). \tag{98}$$

The leading order constant becomes

$$G_0(a,C) = 2\pi\varphi(a+C), \tag{99}$$

which gives for $C = 0$ and interpolating scaling functions $G_0(a,0) = 2\pi\delta_{0,a}$. At this point the regularity of the scaling function enters, which has to be sufficiently large in order to guarantee existence of at least the leading order term of the asymptotic expansion (97).

In order to use the inverse FFT for the calculation of the function $G(a,t,C)$, we replace the unbounded integral (94) by an integral over the interval $[0, 2\pi]$

$$G(a,t,C) = (-1)^a \int_0^{2\pi} d\omega \, \exp(ia\omega) \, g(\omega,t,C). \tag{100}$$

For this we have to perform a resummation of the integrand in terms of the complex valued function

$$g(\omega,t,C)=\sum_{\ell=odd} t^{-1}\exp[-(\omega+\ell\pi)^2/(4t^2)]\,\hat{\varphi}(\omega+\ell\pi)\,\exp[i(\omega+\ell\pi)C], \tag{101}$$

which is periodic on intervals of length 2π with respect to ω and satisfies the symmetry relation

$$g(\omega+\pi,t,C)=g^*(-\omega+\pi,t,C) \tag{102}$$

on the interval $[0,2\pi]$. For not too large values of t this sum converges fast due to the Gaussian factor and we can apply the inverse FFT to the integrals (94) in order to determine $G(a,t,C)$ for all required a simultaneously. The function $G(a,t,0)$ for the interpolating scaling function of Deslauriers and Dubuc [45] is shown in Fig. 6 for various values a. A differing asymptotic behavior for $a=0$ and $a\neq 0$ can be clearly recognized. Correspondingly, we can calculate the asymptotic coefficients

$$G_n(a,C)\approx\frac{(-1)^{a+n}}{4^n n!}\int_0^{2\pi} d\omega\,\exp(ia\omega)\,g_n(\omega,C) \tag{103}$$

with integrand

$$g_n(\omega,C)=\sum_{\ell=odd}(\omega+\ell\pi)^{2n}\,\hat{\varphi}(\omega+\ell\pi)\,\exp[i(\omega+\ell\pi)C], \tag{104}$$

where the convergence of the sum strongly depends on the regularity of the scaling function. A sufficiently high regularity of the scaling function is therefore desirable, in order to keep control on the asymptotic behavior of the integrand in Eq. (92).

The Gaussian transform method can also be applied to two-electron Coulomb integrals. It requires only some slight modifications with respect to the one-electron Coulomb integrals. For this we have used an identity analogous to (90) and obtained

$$\langle\beta_{0,\mathbf{a}}|\frac{1}{r_{12}}|\beta_{0,\mathbf{0}}\rangle=\frac{1}{(2\pi)^2}\int_0^\infty dt\,G(a_x,t)\,G(a_y,t)\,G(a_z,t) \tag{105}$$

where $G(a,t)$ is now given by

$$\begin{aligned} G(a,t) &= 2\pi^{1/2}\int_{-\infty}^{\infty} dx_1dx_2\,\exp[-(x_1-x_2)^2t^2]\,\varphi(x_1-a)\varphi(x_2) \\ &= t^{-1}\int_{-\infty}^{\infty} d\omega\,\exp[-w^2/(4t^2)]\,\exp(i\omega a)\,|\hat{\varphi}(\omega)|^2 \end{aligned} \tag{106}$$

which corresponds to (94) except that we have to replace the Fourier transform $\hat{\varphi}$ by $|\hat{\varphi}|^2$. Consequently, the numerical treatment of $G(a,t)$ can be done in the same way as for the one-electron Coulomb integrals.

B Rigorous estimates for wavelet coupling coefficients

We want to start our considerations of wavelet coupling coefficients with a convenient definition of the regularity of wavelets [59]. Instead of using pointwise regularity, it is favorable to use a definition based on Sobolev spaces H^s with real coefficients s. A univariate wavelet $\psi_{j,a}$ belongs to the Sobolev spaces H^s if and only if the integral

$$\|\,\psi_{j,a}\,\|_s^2:=\int_{-\infty}^{\infty} d\omega\,\left(1+\omega^2\right)^s\,\left|\hat{\psi}_{j,a}(\omega)\right|^2 \tag{107}$$

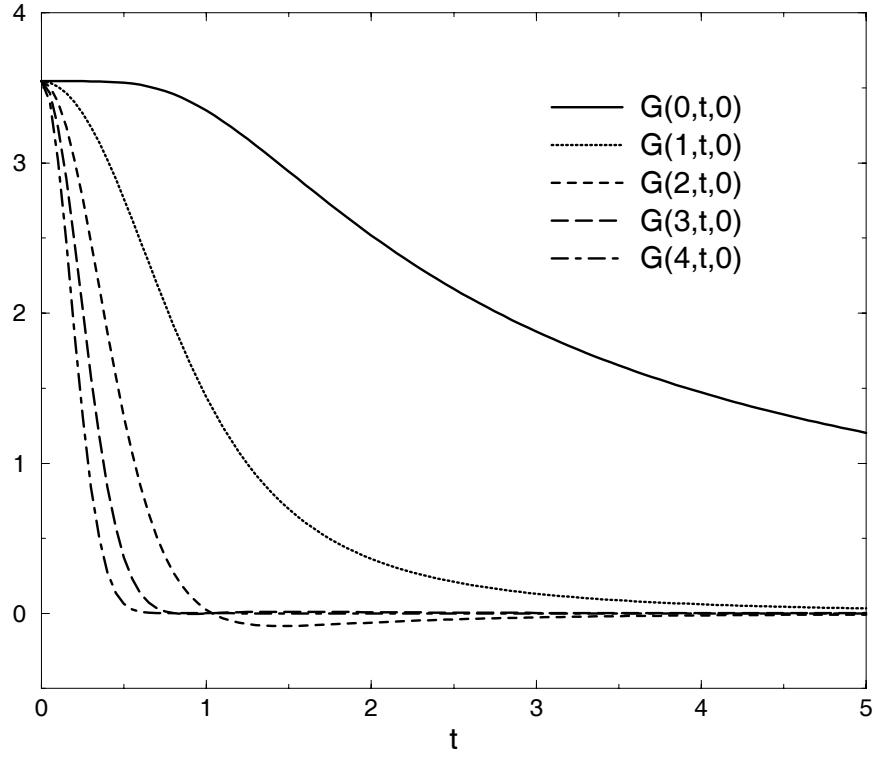

Figure 6: Function $G(a,t,0)$ of the interpolating scaling function φ of Deslauriers and Dubuc [45] for various values a.

exists. The regularity t of the wavelet is defined by the least upper bound on the set of parameters s for which the integral (107) exists

$$t := \sup\{s : \psi_{j,a} \in H^s\}. \tag{108}$$

In the following we asume that the regularity $\tilde{t}$ of dual wavelets $\tilde{\psi}_{j,a}$ satisfy $-\tilde{t} < t$. Actually this is a rather mild assumption on the regularity of dual wavelets and is e.g. satisfied for our choice of the wavelet basis.

In order to derive upper bounds on wavelet coupling coefficients, we have to refer to several estimates on wavelet norms. The first estimate concerns the L^∞ norm. For continuous wavelets with compact support this norm corresponds to $\| \psi_{j,a} \|_{L^\infty} = \sup_x\{|\psi_{j,a}(x)|\}$. The estimate

$$\| \psi_{j,a} \|_{L^\infty} \leq c\, 2^{j/2}. \tag{109}$$

is an immediate consequence of the definition (6). Here and in the following c refers to unspecified constants. The approximation property of wavelets gives the following two estimates for $0 \leq s < \min\{t, n\}$

$$\| \tilde{\psi}_{m,c} \|_{-s} \leq c\, 2^{-sm} \tag{110}$$

$$\| \psi_{j,a} \|_{s} \leq c\, 2^{sj} \tag{111}$$

where n corresponds to the number of vanishing moments of the wavelet. We refer to the literature [60, 61] for further details.

With these etimates at hand, we can derive upper bounds. We assume that $j, \ell \leq m$ and apply the Cauchy-Schwarz inequality to the wavelet coupling coefficients (71)

$$\left| \begin{pmatrix} j & \ell & m \\ a & b & c \end{pmatrix} \right| \leq \| \tilde{\psi}_{m,c} \|_{-s} \| \psi_{j,a} \psi_{\ell,b} \|_s \, . \tag{112}$$

In a second step we use Moser's estimate [62] for the wavelet product

$$\| \psi_{j,a} \psi_{\ell,b} \|_s \leq c \left[\| \psi_{j,a} \|_s \| \psi_{\ell,b} \|_{L^\infty} + \| \psi_{j,a} \|_{L^\infty} \| \psi_{\ell,b} \|_s \right], \tag{113}$$

again we refer to the literature for further details. Together with the estimates (109), (110) and (111) this yields an upper bound in terms of the wavelet levels j, ℓ, m

$$\left| \begin{pmatrix} j & \ell & m \\ a & b & c \end{pmatrix} \right| \leq c \, 2^{-sm} \left(2^{sj+\ell/2} + 2^{s\ell+j/2} \right). \tag{114}$$

For an efficient approximation of products, it is essential that wavelet coupling coefficients show a sufficiently fast decay with respect to m for $j, \ell << m$. According to the estimate (114) we get a decay rate of $O(2^{-tm})$ with respect to m. This again shows the peculiar role of the regularity of wavelets in our method.

It is in general a non trivial task to determine the regularity of a wavelet due to the lack of closed analytic expressions. We have tried to determine the regularity by means of a numerical evaluation of the integral (103). In the case of Sweldens wavelet with six vanishing moments [44] we obtained the bound $3 \leq t < 4$ on its regularity. This is in agreement with Fig. 5, where we observed a decay corresponding to $t \approx 4$.

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