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Wavelet approximation of correlated wavefunctions. II. Hyperbolic wavelets and adaptive approximation schemes

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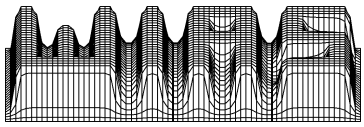

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Abstract

We have studied various aspects concerning the use of hyperbolic wavelets and adaptive approximation schemes for wavelet expansions of correlated wavefunctions. In order to analyze the consequences of reduced regularity of the wavefunction at the electron-electron cusp, we first considered a realistic exactly solvable many-particle model in one dimension. Convergence rates of wavelet expansions, with respect to L^2 and H^1 norms and the energy, were established for this model. We compare the performance of hyperbolic wavelets and their extensions through adaptive refinement in the cusp region, to a fully adaptive treatment based on the energy contribution of individual wavelets. Although hyperbolic wavelets show an inferior convergence behavior, they can be easily refined in the cusp region yielding an optimal convergence rate for the energy. Preliminary results for the helium atom are presented, which demonstrate the transferability of our observations to more realistic systems. We propose a contraction scheme for wavelets in the cusp region, which reduces the number of degrees of freedom and yields a favorable cost to benefit ratio for the evaluation of matrix elements.

1 Introduction

Within the last decade wavelets became a vivid part of applied mathematics. Most of the applications focused on signal and image processing [1], where wavelet transforms have been used as an alternative to the Fourier transformation. Beside some interesting formal relations between quantum theory and wavelet analysis [1], like Heisenberg's uncertainty principle, coherent states and the Wigner transform, there are more practical analogies, which provide the main motivation for an application to electronic structure theory. Image processing typically requires the resolution of structures ranging from very fine to coarse scales. Furthermore, fine structures often extend only over small regions, which are distributed across the whole picture. Wavelets enable a local and adaptive treatment of such kind of multiscale problems, leading to efficient schemes for data compression. More recently these schemes have been extended towards the sparse representation of various types of operators [2], resulting in the design of efficient solvers for elliptic partial differential equations.

The purpose of "data compression" is actually also a central motivation for recent developments in many-particle theory. It has been argued that the main achievement of density

functional theory (DFT), with respect to wavefunction based methods, is the reduction of relevant information from a many-particle wavefunction to a one-particle density or single-particle wavefunctions, respectively (see e.g. [3]). However, not only DFT but also wavefunction based methods can achieve a considerable reduction of complexity by selection of the correct degrees of freedom. This can be accomplished by means of a local treatment of electron correlations. Examples are the local ansatz of Stollhoff and Fulde [4, 5], the increment method of Stoll [6] and the local correlation methods of Pulay and Saebø [7], which have been further developed to linear scaling methods by Werner and collaborators [8, 9]. A common principle underlying all of these methods in practical calculations are so called atomic orbital basis sets. This term has mainly historical reasons, and in modern applications atomic orbitals have been replaced by atomic centered Gaussian type orbitals (GTO) [10]. In a first step the GTOs serve as a basis for a mean-field calculation, like Hartree-Fock (HF), generating a set of molecular orbitals (MO), which can be subject to further transformations for the purpose of localization. Projecting out the localized occupied MOs from the GTOs, produces a basis in the subspace of virtual orbitals, preserving the local character of the GTOs as far as possible. This serves as a starting point for the correlation treatment using various versions of Møller-Plesset perturbation theory or coupled cluster (CC) methods. Due to the local character of the transition amplitudes it is possible to achieve an improved scaling behavior with the size of the system.

A GTO basis fits perfectly the requirements of mean-field methods [11]. However, it is not well adapted to the description of electron correlations. Roughly speaking, within a tensor product basis of GTOs, electron correlations can be described by partial-wave expansions with respect to the atomic centers. At small inter-electronic distances, the convergence behavior of such kind of expansion is rather poor [12]. In the first paper of this series [13] (referenced as paper I in the sequel), we proposed a wavelet expansion of correlated wavefunctions. This ansatz enables an adaptive and local treatment of electron correlations, while retaining the tensor product structure of the wavefunction, which is advantageous from the computational point of view. Wavelets can be selected according to the length and energy scales of the physical processes under consideration, reflecting the local variations of the wavefunction on these scales. Guided by ideas from multi-scale analysis and image processing, we are aiming towards an approximation scheme, where wavelet tensor products are selected according to their contribution to the "exact" many-particle wavefunction. These so called nonlinear approximation schemes [14] are currently a very active area of research in applied mathematics. The term "nonlinear" here means that basis functions are selected according to their contribution to the function to be approximated. In other words the basis depends on the properties of the solution. Within this context wavelets are especially favorable and offer rigorous selection schemes based on local regularity requirements [15]. For correlated wavefunctions, regions of low regularity correspond mainly to inter-electron cusps, where a rather detailed knowledge of the analytic behavior is available [16]. This possibly bridges the gap between pure and applied mathematics.

Application of methods from multi-scale analysis for the approximation of correlated wavefunctions raises a multitude of questions concerning new numerical and physical aspects of this ansatz. Therefore it is desirable to keep the many-particle treatment as simple as possible. We have argued in paper I, that an appropriate starting point for our considerations is a product ansatz for the wavefunction

$$\Psi\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right) = \mathcal{F}\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right) \Phi\left(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N\right), \tag{1}$$

where the correlation factor $\mathcal{F}$, usually called Jastrow factor, is a symmetric function of the electron coordinates and Φ represents a mean-field solution or a linear combination of Slater determinants. The short-range behavior of the Jastrow factor $\mathcal{F}$ essentially reflects Kato's cusp condition [16] and its shape depends on the averaged electron density near the cusp.

Although the product ansatz (1) is in general only approximately valid for many-particle wavefunctions, it provides a good approximation for a large class of long- and short-range correlations [17]. In paper I, we were able to demonstrate the feasibility of our approach by presenting some preliminary results for the helium atom, which already required the full machinery for calculating one- and two-electron integrals. The integral evaluation by itself provides new numerical features concerning the development of fast algorithms in a wavelet representation.

We are aiming towards a synthesis of local correlation methods and nonlinear approximation schemes. The main objective of the present work was to develop adaptive approximation schemes for the Jastrow factor $\mathcal{F}$, resulting in data sparse representations of many-particle wavefunctions. In order to simplify numerical and analytical studies, we first considered an exactly solvable many-particle model in one dimension. For this model, we were able to study the convergence behavior of individual approximation schemes over several wavelet levels. Following that, we have studied the transferability of our findings for the model system to the helium atom. This can give us some hints of what we can expect for larger systems.

2 Exactly solvable many-particle model in one dimension

As a first application of our method, we want to discuss an exactly solvable many-particle model system in one dimension. A large class of such systems, whose exact ground-state wavefunctions are of product type (1), can be found in Ref. [18]. In particular this class includes systems with Hamiltonian [1]

$$\hat{H}_{\text{model}} = -\frac{1}{2}\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2} + \frac{1}{2}\sum_{i=1}^{N} x_i^2 + \sum_{i<j}\left(\delta(x_i - x_j) - \frac{1}{2}|x_i - x_j|\right), \tag{2}$$

whose exact ground-state wavefunction is of the form

$$\Psi_0(x_1, x_2, \ldots, x_N) = \mathcal{N}\prod_{i<j}\exp\left[\frac{1}{2}|x_i - x_j|\right]\prod_{i=1}^{N}\exp\left[-\frac{1}{2}x_i^2\right], \tag{3}$$

with normalization constant $\mathcal{N}$. The corresponding ground-state energy is given by

$$E_0 = \frac{1}{2}N - \frac{1}{24}(N-1)N(N+1). \tag{4}$$

Atomic units have been used throughout this paper. In the following we take

$$\mathcal{F}(x_1, x_2, \ldots, x_N) = \prod_{i<j}\exp\left[\frac{1}{2}|x_i - x_j|\right] \tag{5}$$

as the Jastrow factor. Consequently

$$\Phi(x_1, x_2, \ldots, x_N) = \prod_{i=1}^{N}\exp\left[-\frac{1}{2}x_i^2\right] \tag{6}$$

models the one-particle part in our approach. A Hamiltonian of the form (2) and the corresponding ground-state wavefunction can be also found in Ref. [19] and might be considered as a limit [20, 21] of the Hamiltonian discussed by Forrester [22].

[1] In order to show this, one first has to verify that $\varphi(x) = \frac{1}{2}\text{sgn}x$, $\tau(x) = -x$, $f(x) = -\frac{1}{12}$, $\lambda(x) = 0$ and $F(x) = \frac{1}{2}|x|$ meet the requirements (2.10) and (2.11) of Proposition 1 in Ref. [18]. The statement follows immediately after putting φ, τ, f, λ and F in (2.12) and (2.13) in Ref. [18]. Note that a factor 2 is missing in front of $\lambda(x)$ and $F(x)$ in the formulas (2.9), (2.12) and (2.13) in Ref. [18]. The correct results are obtained by replacing $\lambda(x)$ by $2\lambda(x)$ and $F(x)$ by $2F(x)$!

The Hamiltonian (2) describes a system of coupled harmonic oscillators interacting via repulsive short-range and long-range two-body potentials. Although the exact solution (3) corresponds to the bosonic ground state, its short-range behavior looks rather similar to the corresponding behavior of three-dimensional many-electron systems. Especially at the two-particle coalescence points it resembles closely Kato's cusp condition [23], in particular there is the same dominating linear term $|x_i - x_j|$ in the short-range expansion of $\mathcal{F}$. Such kind of behavior is a consequence of the δ-function in the interaction potential. For the construction of simplified one-dimensional models it is common practice to replace the three-dimensional Coulomb interaction by a δ-function [24, 25, 26]. An important argument for taking a δ-function potential in one dimension has been given by Herrick and Stillinger [27]. They showed that the δ-function potential arises in the one-dimensional scaling limit, with respect to the dimension, of the helium atom in dimensions greater than one. Herewith an interaction of the form $1/|\mathbf{x}_1 - \mathbf{x}_2|$ has been assumed in higher dimensions.

2.1 Approximation schemes for the two-particle model

We want to start our discussion with the simplest case of the two-particle model. For two particles, without spin dependent interactions, the bosonic and fermionic ground states coincide. The wavefunction (3) with $N = 2$ is therefore a realistic model for the helium atom, which in turn can serve as a benchmark for more general many-electron systems. Due to the low dimensionality of the problem, we were able to compare the performance of various approximation schemes, including a nonlinear scheme, which would have not been feasible otherwise. In particular it is possible to illustrate distinct features of these approximation schemes. Furthermore we have explicitly studied different kinds of convergence criteria for this model, which are otherwise difficult to access. These studies gave us some insights concerning realistic electronic structure calculations.

2.1.1 Wavelet expansion of the Jastrow factor

Following our approach outlined in paper I, we have first performed standard tensor product wavelet expansions, up to levels ℓ, for the Jastrow factor (5)

$$\begin{aligned} \mathcal{F}_\ell\,(x_1, x_2) &= f^{(0)} + \sum_{j_1=j_0}^{\ell} \sum_{a_1} f^{(1)}_{j_1,a_1} \mathcal{F}^{(1)}_{j_1,a_1}\,(x_1, x_2) \\ &+ \sum_{j_1 \le j_2} \sum_{a_1,a_2} f^{(2)}_{(j_1,j_2),(a_1,a_2)} \mathcal{F}^{(2)}_{(j_1,j_2),(a_1,a_2)}\,(x_1, x_2)\,, \end{aligned} \tag{7}$$

where we have used symmetric one- and two-particle terms

$$\begin{aligned} \mathcal{F}^{(1)}_{j_1,a_1}\,(x_1, x_2) &= \psi_{j_1,a_1}(x_1) + \psi_{j_1,a_1}(x_2), \\ \mathcal{F}^{(2)}_{(j_1,j_2),(a_1,a_2)}\,(x_1, x_2) &= \psi_{j_1,a_1}(x_1)\,\psi_{j_2,a_2}(x_2) + \psi_{j_2,a_2}(x_1)\,\psi_{j_1,a_1}(x_2), \end{aligned} \tag{8}$$

represented with respect to an univariate wavelet basis $\psi_{j,a}(x) = 2^{j/2}\psi(2^j x - a)$ with dilation levels j ranging between $j_0 \le j \le \ell$. For some elementary facts concerning wavelet analysis, required in the sequel, we refer to the introduction of paper I. In the wavelet expansion (7), we have assumed that a coarsest level j_0 exists, corresponding to the maximal length-scale of correlations, below which contributions can be neglected. This assumption is not completely obvious for the isolated Jastrow factor (5) of our model. However we are only concerned with the product $\mathcal{F}\Phi$, where the exponential decay of Φ confines the distance between the two particles.

We have determined the variational parameters $f^{(0)}$, $f^{(1)}_{j_1,a_1}$, $f^{(2)}_{(j_1,j_2),(a_1,a_2)}$ by solving a generalized eigenvalue problem of the form

$$\mathbf{H}\,\mathbf{f} = E\,\mathbf{M}\,\mathbf{f}, \tag{9}$$

which arises from the Rayleigh-Ritz variational principal applied to the expectation value of the energy. The matrix elements with respect to the Hamiltonian (2) are given by

$$H_{(p,\mathbf{J},\mathbf{A})(q,\mathbf{L},\mathbf{B})} = \int\int dx_1 dx_2\; \mathcal{F}^{(p)}_{\mathbf{J},\mathbf{A}}\Phi\; \hat{H}_{\text{model}}\; \mathcal{F}^{(q)}_{\mathbf{L},\mathbf{B}}\Phi, \tag{10}$$

$$M_{(p,\mathbf{J},\mathbf{A})(q,\mathbf{L},\mathbf{B})} = \int\int dx_1 dx_2\; \mathcal{F}^{(p)}_{\mathbf{J},\mathbf{A}}\Phi\; \mathcal{F}^{(q)}_{\mathbf{L},\mathbf{B}}\Phi, \tag{11}$$

where the indices $\mathbf{J} = \{\}, \{j_1\}, \{j_1, j_2\}$, $\mathbf{A} = \{\}, \{a_1\}, \{a_1, a_2\}$ refer to multi indices depending on whether $\mathcal{F}^{(p)}_{\mathbf{J},\mathbf{A}}$ represents a constant, one- or two-particle term.

In order to solve the generalized eigenvalue problem (9) by means of a direct or iterative procedure, care has to be taken concerning almost linear dependencies among the $\mathcal{F}^{(p)}_{\mathbf{J},\mathbf{A}}$ containing wavelets on coarse levels. This is due to the fact that on sufficiently coarse levels the wavelets are almost constant on the whole domain of the system. Thereby they become nearly linear dependent within the domain of the system, giving rise to ill conditioned matrices (10) and (11). To overcome this problem, we first performed a singular value decomposition of the $\mathbf{M}$ matrix limited to the coarse levels, in order to generate a well conditioned basis on these levels. Due to the comparatively small number of basis functions on the coarse levels the additional computational effort is rather small.

Straightforward evaluation of the matrix elements (10) and (11) leads to one- and two-dimensional integrals, where products of Gaussians with wavelets appear in the integrands. To specify these products we introduce the functions

$$\phi(x) := \exp\left[-\frac{1}{2}x^2\right], \tag{12}$$

$$\zeta_{\mathbf{J},\mathbf{A}}(x) := \begin{cases} \phi(x) \\ \phi(x)\psi_{j,a}(x) \end{cases}, \tag{13}$$

$$\eta_{\mathbf{J},\mathbf{A}}(x) := \begin{cases} \phi^2(x) \\ \phi^2(x)\psi_{j_1,a_1}(x) \\ \phi^2(x)\psi_{j_1,a_1}(x)\psi_{j_2,a_2}(x) \end{cases}, \tag{14}$$

where $\mathbf{J}$, $\mathbf{A}$ again denote appropriately chosen multi indices characterizing the wavelets appearing in the functions (13) and (14). With these definitions at hand, we can write down the required integrals for the Laplacian

$$\int dx\; \zeta_{\mathbf{J},\mathbf{A}}(x)\; \Delta\; \zeta_{\mathbf{L},\mathbf{B}}(x), \tag{15}$$

the one-body potential $V(x) = \frac{1}{2}x^2$

$$\int dx\; x^2\; \eta_{\mathbf{J},\mathbf{A}}(x) \tag{16}$$

and for the two-body potentials $V_2(x_1 - x_2) = \delta(x_1 - x_2)$, $\frac{1}{2}|x_1 - x_2|$

$$\int\int dx_1 dx_2\; \eta_{\mathbf{J},\mathbf{A}}(x_1)\; V_2(x_1 - x_2)\; \eta_{\mathbf{L},\mathbf{B}}(x_2). \tag{17}$$

We have presented a detailed exposition of how to calculate such kind of integrals in paper I. In the first step, wavelet expansions of the functions ϕ, ζ, η have to be performed using the wavelet coupling coefficients defined in paper I. Due to the comparatively small number of contributing wavelets in one dimension, we can avoid the telescopic expansion underlying the nonstandard representation of operators. Instead we have transformed the wavelet expansion of the functions ϕ, ζ, η into a basis of scaling functions $\varphi_{\ell,a}(x) := 2^{\ell/2}\varphi(2^{\ell}x - a)$ on a sufficiently fine level ℓ, e.g.

$$\eta_{\mathbf{J},\mathbf{A}}(x) = \sum_{a} c_a \, \varphi_{\ell,a}(x). \tag{18}$$

Simple scaling relations can be used in order to reduce the integrals to so called elementary integrals

$$\int dx \; \varphi(x-a) \; \varphi(x), \tag{19}$$

$$\int dx \; \varphi(x-a) \; \Delta \; \varphi(x), \tag{20}$$

$$\int dx \; x^2 \; \varphi(x-a), \tag{21}$$

$$\int\int dx_1 dx_2 \; \varphi(x_1-a) \; |x_1 - x_2| \; \varphi(x_2), \tag{22}$$

with respect to the scaling function $\varphi(x-a)$. An iterative scheme according to Beylkin [28], Dahmen and Micchelli [29] can be applied to calculate these integrals. It only requires the filter coefficients and no closed analytic expression for the scaling function.

Further restrictions can be imposed on the wavelet expansion (7), like the hyperbolic wavelet approximation, which we have discussed in paper I. Together with adaptive refinement schemes near the cusp region, this offers the possibility to reduce the computational effort considerably. However, at first we have to establish the convergence behavior of the standard wavelet expansion (7) with respect to the levels ℓ. We have chosen for our calculations a biorthogonal symmetric wavelet basis with compact support and six vanishing moments from Sweldens [30]. These wavelets are based on the interpolating scaling function of Deslauriers and Dubuc [31], where the dual basis with the same number of vanishing moments has been generated from a lifting scheme [30].

In the first step we have to identify the coarsest level j_0 from which we start our wavelet expansions. This was done iteratively by choosing a coarse level j and saturating the wavelet basis $\psi_{j,a}$ on this level with respect to the energy. The saturating threshold on a level was set to 10^{-4} Hartree relative to the energy. In the next step, we have added wavelets from the next coarser level $j-1$ and checked whether they contribute to the energy. If this was the case, we have saturated the basis with respect to the wavelets $\psi_{j-1,a}$ and added wavelets from level $j-2$. This process has been continued until the coarsest level $j-n$ did not contribute to the energy any more, by definition we set $j_0 = j - n + 1$. Obviously our choice of j_0 is not necessarily strict and depends on the desired final accuracy one wants to achieve with such an expansion. By means of the exact solution Ψ_0, it can be seen that the size of the system is of the order of the characteristic scale at level $j = -2$. Starting the iterative scheme at $j = -2$, we actually observed a rather sharp cut in the contribution to the energy. By going to the next coarser level $j = -3$, we observed a gain in energy of $\approx 10^{-4}$ Hartree, which is below the accuracy aimed at in the present application. Noteworthy, the level $j = -2$ contributes 92% to the total defect energy ΔE defined by the energy difference [2]

$$\Delta E := \frac{\langle \Phi | \hat{H} | \Phi \rangle}{\langle \Phi | \Phi \rangle} - E_0. \tag{23}$$

[2]The defect energy ΔE differs from the correlation energy because Φ is not the HF solution of the model.

In analogy to this, we have defined the defect energy at level ℓ

$$\Delta E(\ell) := \frac{\langle \mathcal{F}_\ell \Phi | \hat{H} | \mathcal{F}_\ell \Phi \rangle}{\langle \mathcal{F}_\ell \Phi | \mathcal{F}_\ell \Phi \rangle} - E_0. \tag{24}$$

Once j_0 has been settled, we have extended the wavelet basis by adding successively finer levels. The corresponding defect energies ranging from level $\ell = -2$ to $\ell = 3$ are listed in Table 1. Starting already at level $\ell = -1$, the energy shows an asymptotic convergence rate of $O(2^{-\ell})$. To consider the energy alone does not give too much insight into the approximation properties of our wavelet expansion. Therefore, we have calculated the norm of the defect function

$$\delta\Psi_\ell(x_1, x_2) := \Psi_0(x_1, x_2) - \mathcal{F}_\ell \, \Phi(x_1, x_2) \tag{25}$$

of our approximate solution on various levels ℓ with respect to alternative function spaces.

In order to get a visual impression of the accuracy of the wavelet expansion (7), we have shown in Fig. 1 the exact solution Ψ_0 and the defect function $\delta\Psi_\ell$ on various levels ($\ell = -2, 0, 2$). A prominent feature in Fig. 1 is the two-particle cusp along the diagonal $x_1 = x_2$. Apart from the diagonal, we observed an increasingly fast decay of the approximation error by going to finer levels ℓ.

The standard Hilbert space used in quantum theory for bound states of Schrödinger's equation is L^2. Hence a natural measure for the approximation error on level ℓ is given by the L^2 norm of the defect function defined by

$$E_{L^2}(\ell) = \| \, \delta\Psi_\ell \, \|_{L^2} := \left(\int\int dx_1 dx_2 \; |\delta\Psi_\ell(x_1, x_2)|^2 \right)^{\frac{1}{2}}. \tag{26}$$

Calculating the integral in $E_{L^2}(\ell)$ over the square $[-2, 2]^2$ numerically, we observed an asymptotic convergence of $O(2^{-\ell})$, as can be seen from Table 1. A more sensitive measure for the accuracy of our wavelet expansion is the error in the norm of the Sobolev space $H^1(\mathbf{R}^2)$ [32] defined by

$$E_{H^1}(\ell) = \| \, \delta\Psi_\ell \, \|_{H^1} := \left[\int\int dx_1 dx_2 \left(|\delta\Psi_\ell(x_1, x_2)|^2 + \left| \frac{\partial \delta\Psi_\ell(x_1, x_2)}{\partial x_1} \right|^2 + \left| \frac{\partial \delta\Psi_\ell(x_1, x_2)}{\partial x_2} \right|^2 \right) \right]^{\frac{1}{2}}. \tag{27}$$

Here we also take into account the approximation error of the first derivatives of the wavefunction, which is the relevant quantity with respect to the convergence of the energy. As can be seen from Table 1, we observed an asymptotic convergence of $O(2^{-\ell/2})$ for the H^1 norm. Due to the variational nature of our approach one has to expect that the error in the energy is of $O([E_{H^1}(\ell)]^2)$, which is actually the case as can be seen from Table 1.

The convergence rates observed from our calculations are within the general estimates for the finite element method with piecewise linear basis functions. This clearly indicates that within the cusp region we can not benefit from the higher regularity of our wavelet basis. It is shown in Appendix A that the exact solution Ψ_0 belongs to the Sobolev space $H^{\frac{3}{2}-\varepsilon}$ for $\varepsilon \geq 0$ (for a definition of Sobolev spaces with real coefficients, see e.g. Ref. [32] and Appendix A). From this we can expect [32]

$$E_{H^1}(\ell) \leq C \, 2^{-\ell(\frac{1}{2}-\varepsilon)} \, \| \, \Psi_0 \, \|_{H^{\frac{3}{2}-\varepsilon}}, \tag{28}$$

which is in agreement with our numerical observations. Further extension of this estimate with respect to the $E_{L^2}(\ell)$ error requires that the exact solution belongs to the Sobolev space H^2, which is not the case for our model. At best we can obtain a not necessarily sharp estimate [32]

$$E_{L^2}(\ell) \leq E_{H^{1/2}}(\ell) \leq C \, 2^{-(\ell-\varepsilon)} \, \| \, \Psi_0 \, \|_{H^{\frac{3}{2}-\varepsilon}}, \tag{29}$$

which is in agreement with our calculations.

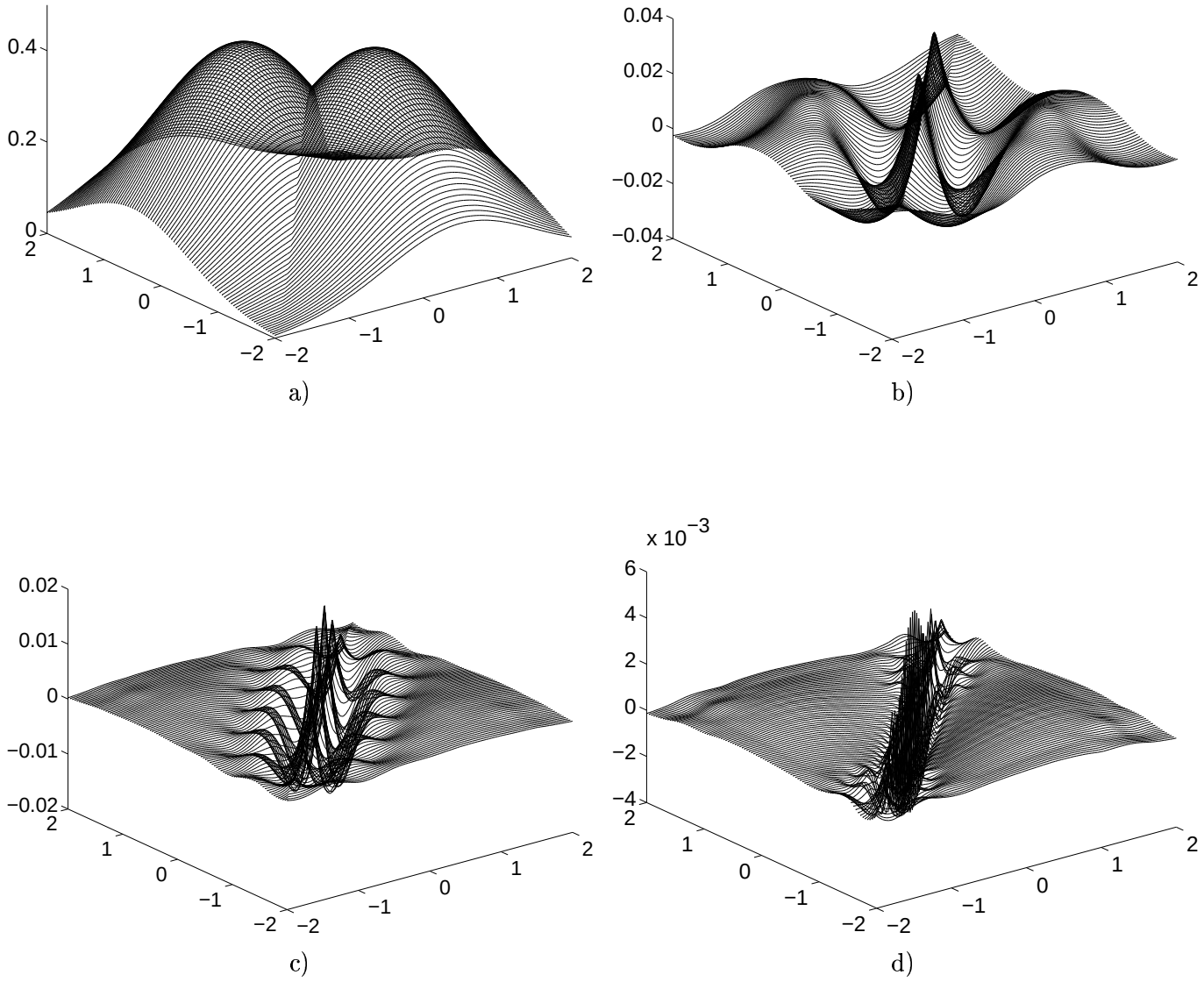

Figure 1: Standard tensor product wavelet expansion of $\mathcal{F}$ for the two-particle model. A wavelet with six vanishing moments has been taken from Sweldens [30]. a) exact solution Ψ_0. Defect functions $\delta\Psi_\ell$: b) $\ell = -2$, c) $\ell = 0$, d) $\ell = 2$. Different scalings of the vertical axes are used on the various levels according to the absolute size of the errors. The coefficients of the wavelet expansion have been obtained from the Rayleigh-Ritz variational principal applied to the expectation value of the energy.

Table 1: Approximation errors of standard tensor product wavelet expansion $\mathcal{F}_\ell$ for the two-particle model. A wavelet with six vanishing moments has been taken from Sweldens [30]. We have listed errors corresponding to the L^2 ($E_{L^2}(\ell)$) and H^1 ($E_{H^1}(\ell)$) norms as well as errors in the energy $\Delta E(\ell)$ (Hartree). The coefficients of the wavelet expansions have been obtained from the Rayleigh-Ritz variational principal applied the energy expectation value. For comparison, we have presented the L^2 error of the direct wavelet expansion of the total wavefunction Ψ_0 ($E_\Psi(\ell)$) according to Eqs. (30).

ℓ	$E_{L^2}(\ell)$	$E_\Psi(\ell)$	$E_{H^1}(\ell)$	$\Delta E(\ell)$
-2	0.0347	0.04183	0.1984	0.0191
-1	0.0229	0.00958	0.1679	0.0142
0	0.0103	0.00312	0.1236	0.0076
1	0.0044	0.00110	0.0885	0.0038
2	0.0021	0.00042	0.0647	0.0020
3	0.0015		0.0487	0.0011

2.1.2 Wavelet expansion of the total wavefunction

Alternatively we have considered another approach, to study the convergence in the L^2 norm, by means of a direct wavelet expansion of the total wavefunction

$$\begin{aligned}\Psi_0(x_1,x_2) = &\sum_{a,b} g^{(0)}_{j_0,(a,b)} \mathcal{G}^{(0)}_{j_0,(a,b)}(x_1,x_2) \\ &+ \sum_{j_0\le j_1}\sum_{a,b} g^{(1)}_{(j_0,j_1),(a,b)} \mathcal{G}^{(1)}_{(j_0,j_1),(a,b)}(x_1,x_2) \\ &+ \sum_{j_0\le j_1\le j_2}\sum_{a,b} g^{(2)}_{(j_1,j_2),(a,b)} \mathcal{G}^{(2)}_{(j_1,j_2),(a,b)}(x_1,x_2)\,,\end{aligned} \tag{30}$$

where we have introduced for $\mathcal{G}^{(0)}$ and $\mathcal{G}^{(1)}$ tensor products involving scaling functions on the coarsest level j_0

$$\begin{aligned}\mathcal{G}^{(0)}_{j_0,(a,b)}(x_1,x_2) &= \varphi_{j_0,a}(x_1)\varphi_{j_0,b}(x_2) + \varphi_{j_0,b}(x_1)\varphi_{j_0,a}(x_2), \\ \mathcal{G}^{(1)}_{(j_0,j_1),(a,b)}(x_1,x_2) &= \varphi_{j_0,a}(x_1)\psi_{j_1,b}(x_2) + \psi_{j_1,b}(x_1)\varphi_{j_0,a}(x_2), \\ \mathcal{G}^{(2)}_{(j_1,j_2),(a,b)}(x_1,x_2) &= \psi_{j_1,a}(x_1)\psi_{j_2,b}(x_2) + \psi_{j_2,b}(x_1)\psi_{j_1,a}(x_2).\end{aligned} \tag{31}$$

The wavelet coefficients g are given by scalar products with respect to the dual basis $\tilde\varphi_{j_0,a}, \tilde\psi_{j,a}$

$$\begin{aligned}g^{(0)}_{j_0,a,b} &= 2\int\int dx_1dx_2\ \Psi_0(x_1,x_2)\ \tilde\varphi_{j_0,a}(x_1)\ \tilde\varphi_{j_0,b}(x_2), \\ g^{(1)}_{j_0,j_1,a,b} &= 2\int\int dx_1dx_2\ \Psi_0(x_1,x_2)\ \tilde\varphi_{j_0,a}(x_1)\ \tilde\psi_{j_1,b}(x_2), \\ g^{(2)}_{j_1,j_2,a,b} &= 2\int\int dx_1dx_2\ \Psi_0(x_1,x_2)\ \tilde\psi_{j_1,a}(x_1)\ \tilde\psi_{j_2,b}(x_2).\end{aligned} \tag{32}$$

For computational simplicity, we have included scaling functions $\varphi_{j_0,a}$ in our expansion, which enables us to start at an arbitrary level j_0 without affecting the final accuracy. Please recall from paper I that we have excluded scaling functions from our expansion due to the finite range of electron correlations. This leads to considerable technical simplifications for the

calculation of matrix elements in the many-particle case [33], which however does not matter for the present purpose. It can be seen from Table 1 that the convergence rate in the L^2 norm (26) of the direct expansion ($E_\Psi(\ell)$) is of $O(2^{-3\ell/2})$, which is by a factor of $2^{-\ell/2}$ faster than what we found for the expansion based on the Rayleigh-Ritz variational principal applied to the energy expectation value. The latter is equivalent to minimizing the error in the H^1 norm, where the first derivatives dominate.

In order to elucidate the convergence behavior of the direct expansion, we can follow the same line of arguments given in paper I for the homogeneous electron gas. Obviously Ψ_0 is smooth except along the diagonal $x_1 = x_2$, where the first partial derivatives have discontinuities. We can therefore limit our discussion to diagonal matrix elements on fine levels $j >> j_0$. Performing a Taylor expansion of the Jastrow factor for such a matrix element and neglecting the variation of Φ within the supports of the wavelets

$$\begin{aligned} g^{(2)}_{j,j,a,a} &= \int\int dx_1 dx_2 \; \Psi_0(x_1,x_2)\tilde{\psi}_{j,a}(x_1)\; \tilde{\psi}_{j,a}(x_2) \\ &\approx \sum_{m=0}^{\infty} \frac{a_m}{m!} \int\int dx_1 dx_2 \; |x_1 - x_2|^m \, \tilde{\psi}_{j,a}(x_1)\; \tilde{\psi}_{j,a}(x_2) \\ &= \sum_{m=1}^{\infty} \frac{a_m}{m!} 2^{-(m+1)j} \int\int dx_1 dx_2 \; |x_1 - x_2|^m \tilde{\psi}(x_1)\tilde{\psi}(x_2), \end{aligned} \tag{33}$$

it is obvious that the linear term $|x_1 - x_2|$, corresponding to $m = 1$, governs the convergence behavior in the asymptotic limit. The matrix elements of this term decay with $O(2^{-2j})$, whereby their number increase with $O(2^j)$ along the diagonal. Here we take into account that Φ acts as a cutoff function, which confines the wavelet expansion to a finite interval on the diagonal. Wen can estimate the L^2 error in the asymptotic limit from the expression

$$\begin{aligned} (\bar{E}_{L^2}(\ell))^2 &= \sum_{j_1 \geq j_2 > \ell} \sum_{a,b} |g^{(2)}_{j_1,j_2,a,b}|^2 \\ &\approx \sum_{j>\ell} \sum_{a} |g^{(2)}_{j,j,a,a}|^2 \\ &\leq C \sum_{j>\ell} 2^{-3j}, \end{aligned} \tag{34}$$

which is equivalent ($C_1 \, E^{(\ell)}_{L^2} \leq \bar{E}^{(\ell)}_{L^2} \leq C_2 \, E^{(\ell)}_{L^2}$) to the $E^{(\ell)}_{L^2}$ error for a biorthogonal wavelet basis [34]. From this estimate we obtain a convergence of the direct expansion of $O(2^{-3\ell/2})$, which is in agreement with our numerical finding.

3 Hyperbolic wavelets and adaptive refinement schemes

After we have established the convergence behavior of the wavelet expansion in the standard tensor product space, we want to discuss the hyperbolic wavelet approximation and related adaptive refinement schemes. Hyperbolic wavelets introduce a hierarchy on the set of standard tensor products according to the sum of their levels. A symmetrized tensor product

$$\sum_{(i_1,i_2,\ldots,i_N)\in S_N} \psi_{j_1,a_1}(x_{i_1})\; \psi_{j_2,a_2}(x_{i_2}) \ldots \psi_{j_N,a_N}(x_{i_N}) \tag{35}$$

is accessible for a hyperbolic wavelet approximation of level Q if

$$\sum_{i=1}^{N} j_i \leq Q. \tag{36}$$

Special regulations have to be taken for each of the n-particle terms $\mathcal{F}^{(n)}$, with $n < N$, of the Jastrow factor. Formally each n-particle term consists of tensor products of the form

$$\prod_{i=1}^{n} \psi_{j_i,a_i}(x_i) \prod_{k=n+1}^{N} \varphi_{j_0,a_k}(x_k). \tag{37}$$

Due to the finite range of electron correlations, we can replace the $\varphi_{j_0,a}$ by constant functions. For the hyperbolic wavelet approximation, however, we have to take the level j_0 of the scaling functions into account and use the condition

$$\sum_{i=1}^{n} j_i + (N-n)(j_0 - 1) \leq Q \tag{38}$$

instead [3]. In order to derive a notation which does not rely too much on arbitrary re-scalings of the wavelet variable, we introduce a shifted hyperbolic wavelet level

$$\tilde{Q} = Q - N(j_0 - 1). \tag{39}$$

It has been shown by DeVore et al. [35] that the approximation properties of hyperbolic wavelets for a given function depend on the size of the L^2 norm of its mixed derivatives. For our two-particle model, it can be easily seen that already the first mixed derivative of the wavefunction does not belong to L^2, actually we get

$$\partial^2 |x_1 - x_2| / \partial x_1 \partial x_2 = -2\delta(x_1 - x_2). \tag{40}$$

Numerical results of the hyperbolic wavelet approximation for the two-particle model are listed in Table 2, from which we derive a convergence rate on the coarse levels of $O(2^{-\tilde{Q}/4})$. By comparison with the standard tensor product expansion, one expects asymptotically a convergence rate of at least $O(2^{-\tilde{Q}/2})$, which can actually be observed at the finest level only. In Fig. 2 we have shown the grid points of the hyperbolic wavelet approximation at level $\tilde{Q} = 4$.

For obvious reasons one can expect that it should be possible to improve the convergence by adding wavelet products on fine levels along the diagonal. In order to make this statement more precise, we have considered a fully adaptive wavelet scheme, which is similar to a best N-term approximation [14], i.e. to find the set of N basis functions which yields the lowest energy. Starting from the coarsest level, we have systematically enlarged our wavelet basis by selecting tensor products according to their contribution to the energy. For this we went through the whole set of remaining standard tensor products and searched for the tensor product wavelet which gave the largest contribution to the energy. This was included into the expansion and the whole procedure was repeated again until the largest contribution was below a certain threshold. Following our notation for the standard tensor products, all tensor products with $j_1, j_2 \leq \ell$ were accessible for the fully adaptive scheme at level ℓ. Actually, we found that the energies on the various levels of the fully adaptive wavelet scheme are in good agreement with the standard tensor product expansion, as can be seen from Table 2. A comparison of the corresponding grids with those of the hyperbolic wavelet approximation shows that on the coarse levels (Fig. 2 and 3a) both grids appear rather similar. The underlying sparse grids of the hyperbolic wavelet approximation can be even further thinned out by removing points far from the diagonal. On the fine levels, we observed a pronounced concentration of grid points along the diagonal. The coupling between the fine levels is rather week and does not extend over the nearest levels.

[3] The scaling functions on level j_0 actually represent the wavelet spaces on levels $j < j_0$.

Table 2: Error in the energy $\Delta E(\ell)$ (Hartree) at level ℓ for the hyperbolic wavelet approximation (*hyperbolic*) and adaptive refinement schemes for the two-particle model. A wavelet with six vanishing moments has been taken from Sweldens [30]. Two adaptive schemes have been considered for hyperbolic wavelets: Adaptive refinement along the diagonal (*diagonal*) and its contracted version (*contracted*). Results are also shown for the fully adaptive treatment with respect to the energy (*adaptive*). For comparison, the standard tensor product expansion (*standard*) has been included. The number of tensor product basis functions n is shown for each case.

	standard		*adaptive*			*hyperbolic*		*diagonal*		*contracted*	
ℓ	n	$\Delta E(\ell)$	n	$\Delta E(\ell)$	$\tilde{Q}$	n	$\Delta E(\ell)$	n	$\Delta E(\ell)$	n	$\Delta E(\ell)$
-2	15	0.0191	14	0.0191	1	5	0.1566	9	0.0333	6	0.0398
-1	45	0.0140	28	0.0142	2	19	0.0188	23	0.0142	20	0.0150
0	153	0.0075	55	0.0076	3	43	0.0156	55	0.0076	45	0.0077
1	276	0.0038	52	0.0039	4	91	0.0127	105	0.0038	93	0.0038
2	496	0.0019	66	0.0020	5	155	0.0110	177	0.0020	158	0.0020
3	1128	0.0010	80	0.0011	6	260	0.0075	293	0.0011	266	0.0011

Obviously, our fully adaptive wavelet scheme is not applicable in realistic calculations. However it can give us some hints for the construction of an optimal scheme. A good candidate seems to be a combination of hyperbolic wavelets and diagonal refinements on the fine levels. Such a scheme is numerically in good agreement with the standard tensor products (see Table 2) and requires only a comparatively small number of additional basis functions. The number of degrees of freedom can be even further reduced by contracting the wavelet tensor products on the diagonal for each level j to a single basis function

$$\mathcal{F}_j^c(x_1, x_2) = \sum_a \psi_{j,a}(x_1)\psi_{j,a}(x_2). \tag{41}$$

In the case of our two-particle model this does not even introduce a further approximation, which can be seen from the exact solution (3) and Table 2. Contraction schemes have been already discussed in paper I, where we pointed to potentially interesting applications for inhomogeneous three-dimensional systems like molecules. In Section 5 we present the necessary generalizations and propose a numerical scheme for the efficient evaluation of integrals involving contracted tensor products.

3.1 Extension to many-particle models

The two-particle model provides a simplified, nevertheless realistic description of a two-electron system like the helium atom. For more than two-particles there is a discrepancy with respect to many-electron systems due to the fact that the model does not meet Pauli's principle. The wavefunction (3) is symmetric and describes the bosonic ground state of the model Hamiltonian (2). Since we are solely interested in the numerical aspects of the model, it makes sense to consider also cases with more than two particles. Actually these cases are more complicated than they would be for a fermionic system, because of an increased importance of the many-particle cusps. Electronic wavefunctions vanish in the coalescence points of more than two electrons. This is not the case for the model wavefunctions, in contrast the product of Gaussians, appearing in the exact solution (3), actually favors such coalescing arrangements.

In order to make the many-particle models tractable for our approach, we have used the hyperbolic wavelet approximation in combination with adaptive refinement along the

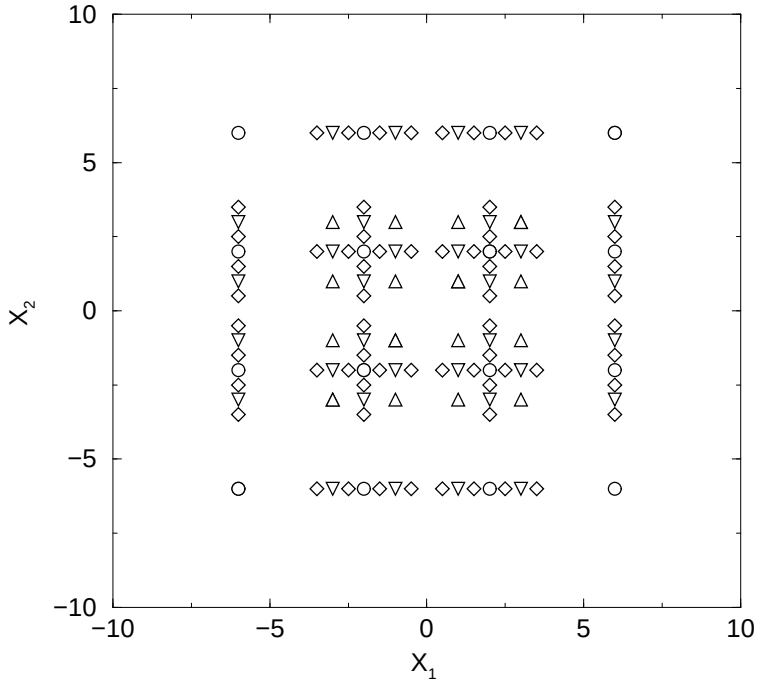

Figure 2: Grid points of the hyperbolic wavelet approximation up to $\tilde{Q} = 4$ for the two-particle model. Indicated are tensor products $\psi_{j_1,a_1}(x_1)\ \psi_{j_2,a_2}(x_2)$ at levels (j_1, j_2): $\tilde{Q} = 2$, $\bigcirc$ (-2,-2); $\tilde{Q} = 3$, $\bigtriangledown$ (-2,-1); $\tilde{Q} = 4$, $\diamondsuit$ (-2,0), $\bigtriangleup$ (-1,-1).

diagonals. By definition, simple diagonal n-particle tensor products

$$\chi_{\ell,a}(x_{i_1}, \ldots, x_{i_n}) := \psi_{\ell,a}(x_{i_1})\ \ldots \psi_{\ell,a}(x_{i_n}) \qquad \ell \leq \tilde{Q} + j_0 - 1 \tag{42}$$

or their contracted analogues

$$\chi_{\ell}(x_{i_1}, \ldots, x_{i_n}) := \sum_a \psi_{\ell,a}(x_{i_1})\ \ldots \psi_{\ell,a}(x_{i_n}) \qquad \ell \leq \tilde{Q} + j_0 - 1 \tag{43}$$

did not contribute to the hyperbolic wavelet level $\tilde{Q}$. They could be combined with other wavelets $\psi_{j,a}$ in an arbitrary manner. Symmetrized tensor products

$$\mathcal{F}^{(p)}_{\mathbf{J},\mathbf{A}} = \sum_{(i_1,i_2,\ldots,i_N)\in S_N} \psi_{j_1,a_1}(x_{i_1}) \ldots \psi_{j_q,a_q}(x_{i_q})\ \chi_k(x_{i_{q+1}}, \ldots, x_{i_p}) \tag{44}$$

were therefore accessible, if they satisfied the condition $\sum_{i=1}^{q} j_i - q(j_0 - 1) \leq \tilde{Q}$. Results for three-, four- and five-particle systems are listed in Tables 3, 4 and 5.

The hyperbolic wavelet approximation converges rather fast with $O(2^{-\tilde{Q}})$ on the coarse levels but slows down considerably when going to the finer levels, approaching an $O(2^{-\tilde{Q}/2})$ behavior. With increasing number of particles, the transition in the convergence behavior takes place at larger values of $\tilde{Q}$, indicating an increasing importance of off-diagonal tensor products on coarse scales. In contrast to this, the convergence for the adaptively refined schemes is of $O(2^{-\ell})$ throughout. Even on the coarse levels, we observed considerable improvements by means of diagonal refinement. Although the convergence rate is the same in the contracted and un-contracted case, we obtained smaller total errors in the energy for the latter. This can be understood by looking at the Taylor expansion of the Jastrow factor. The leading order

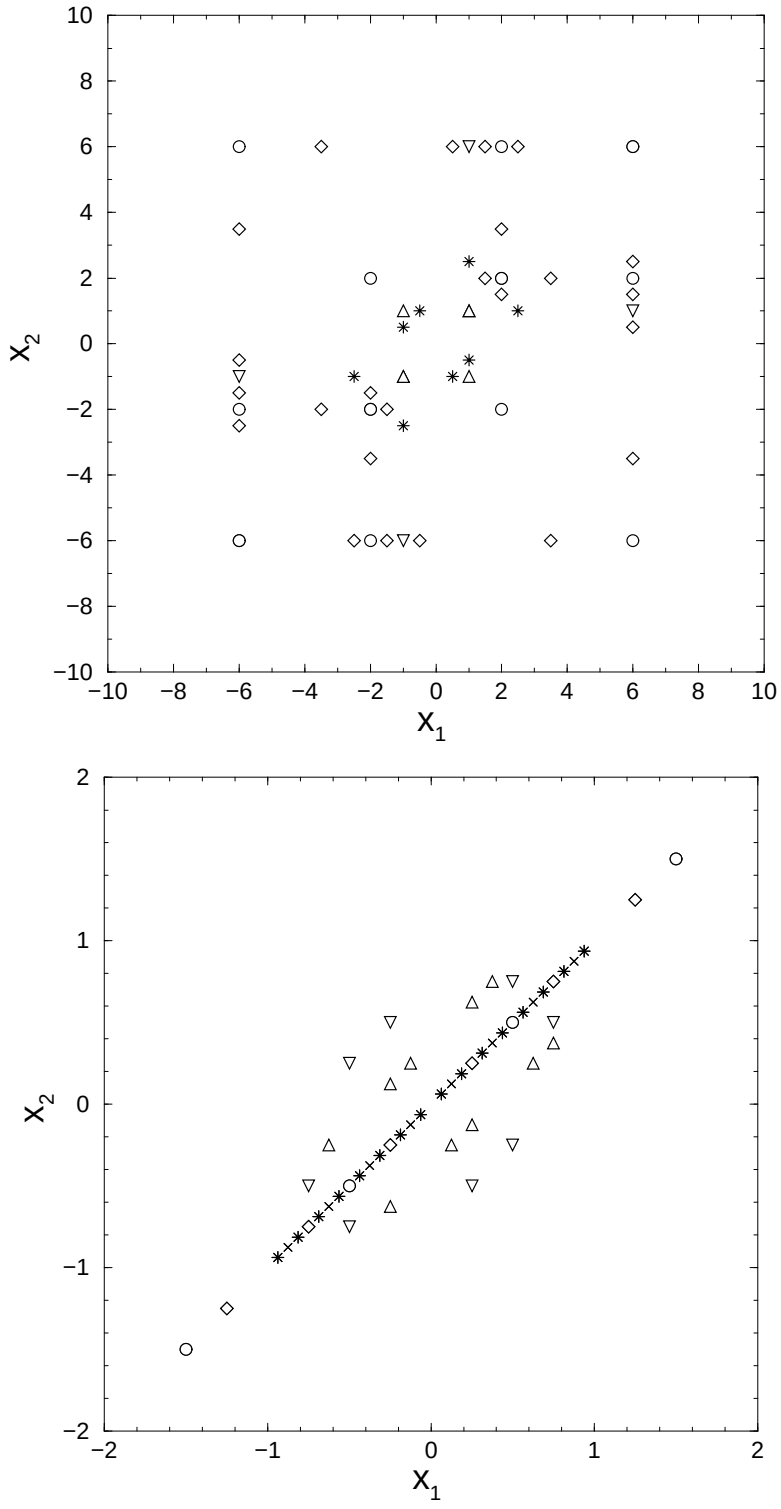

Figure 3: Fully adaptive wavelet scheme, based on the contribution of tensor products $\psi_{j_1,a_1}(x_1)\ \psi_{j_2,a_2}(x_2)$ to the energy, for the two-particle model. a) Tensor products on coarse levels (j_1, j_2): ◯ (-2,-2), ▽ (-2,-1), ♢ (-2,0), △ (-1,-1), ∗ (-1,0). b) Tensor products on fine levels (j_1, j_2): ◯ (0,0), ▽ (0,1), ♢ (1,1), △ (1,2), × (2,2), ∗ (3,3).

Table 3: Errors in the energy $\Delta E(\ell)$ (Hartree) at level ℓ for the three-particle model. Results are presented for the hyperbolic wavelet approximation (*hyperbolic*) and its adaptively refined scheme by means of wavelet tensor products along the diagonal (*diagonal*) as well as for the corresponding scheme based on contracted tensor products (*contracted*). For comparison, a fully adaptive treatment with respect to the energy (*adaptive*) has been performed on the coarse levels. A wavelet with six vanishing moments has been taken from Sweldens [30]. Percentages refer to the relative error with respect to the total defect energy (23). The number of basis functions n is given for each scheme.

	adaptive				*hyperbolic*			*diagonal*			*contracted*		
ℓ	n	$\Delta E(\ell)$	%	$\tilde{Q}$	n	$\Delta E(\ell)$	%	n	$\Delta E(\ell)$	%	n	$\Delta E(\ell)$	%
-2	35	0.0625	93.8	1	5	0.4374	56.3	25	0.0678	93.2	10	0.1794	82.1
-1	69	0.0369	96.3	2	19	0.0841	91.6	87	0.0352	96.5	36	0.0604	94.0
0	177	0.0182	98.2	3	63	0.0449	95.5	315	0.0181	98.2	109	0.0244	97.6
1	274	0.0095	99.1	4	151	0.0331	96.7	617	0.0097	99.0	233	0.0147	98.5
2				5	335	0.0269	97.3	1177	0.0057	99.4	468	0.0091	99.1
3				6	651	0.0195	98.1	2677	0.0036	99.6	900	0.0057	99.4

Table 4: Same as in Table 3 for the four-particle model, except for missing results for the fully adaptive treatment with respect to the energy.

		hyperbolic			*diagonal*			*contracted*		
ℓ	$\tilde{Q}$	n	$\Delta E(\ell)$	%	n	$\Delta E(\ell)$	%	n	$\Delta E(\ell)$	%
-2	1	5	1.0695	57.2	35	0.2164	91.3	20	0.407	83.7
-1	2	19	0.2827	88.7	187	0.0882	96.5	82	0.134	94.6
0	3	63	0.1752	93.0	835	0.0370	98.5	297	0.065	97.4
1	4	186	0.0739	97.0	2271	0.0189	99.2	711	0.035	98.6
2	5	450	0.0512	98.0				1514	0.022	99.1
3	6	1026	0.0385	98.5						

three-particle terms are of the form $|x_i - x_j|\,|x_j - x_k|$. An optimal representation of these terms, however, requires products of the form $\chi_m(x_i, x_j)\,\chi_n(x_j, x_k)$ in the wavelet expansion, which were not included in our scheme. Due to the restricted flexibility of our contracted wavelet basis, we obtained a slightly deteriorated accuracy in the energy. As we have already mentioned above, this effect is enhanced by the bosonic character of our model. At least for the three-particle system, we were able to demonstrate that a fully adaptive treatment with respect to the energy yields results in close agreement with our diagonal refinement scheme.

4 Comparative studies for the helium atom

The three-dimensional analog of the two-particle model is the helium atom. It is fairly straightforward to transfer to it the adaptive approximation schemes, discussed above for the two-particle model. Due to the increase of computational complexity, we cannot afford the same range of numerical results. Instead we have to limit ourselves to a simplified approach. We took our best approximation for the helium wavefunction from paper I, which recovers 98

Table 5: Same as in Table 3 for the five-particle model, except for missing results for the fully adaptive treatment with respect to the energy.

		hyperbolic			*diagonal*			*contracted*		
ℓ	$\tilde{Q}$	n	$\Delta E(\ell)$	%	n	$\Delta E(\ell)$	%	n	$\Delta E(\ell)$	%
-2	1	5	2.4802	50.4	45	0.7138	85.7	30	1.0928	78.1
-1	2	19	0.9374	81.3	273	0.3113	93.8	168	0.4149	91.7
0	3	63	0.5928	88.1	1529	0.1529	96.9	755	0.2664	94.7
1	4	186	0.2553	94.9	4628	0.0785	98.4	2036	0.1310	97.4
2	5	506	0.1499	97.0						
3	6	1222	0.1059	97.9						

Table 6: Errors in the energy ΔE (mHartree) for hyperbolic wavelet schemes with respect to a standard tensor product wavelet expansion of the helium atom ($E = -2.903004$ Hartree) published in paper I. In the first scheme (*hyperbolic*) only hyperbolic wavelets up to level $\tilde{Q}$ have been taken into account, whereas in the second scheme (*diagonal*) all diagonal tensor products were additionally included. For comparison, we present the corresponding error of the standard tensor product expansion at levels ℓ (*standard*). The number of basis functions n is given for each scheme.

	standard			*hyperbolic*		*diagonal*	
ℓ	n	ΔE	$\tilde{Q}$	n	ΔE	n	ΔE
-1	703	1.989	2	59	7.001	77	2.928
0	1540	0.266	3	401	3.958	437	0.585
1	2701	0.	4	914	1.790	950	0.151

% of the correlation energy, as a reference. The single-particle wavelet basis extends over four levels, ranging from level $j = -2$ up to $j = 1$. No restrictions have been imposed on the combinations of these wavelets in the standard tensor products. With respect to this wavefunction, we have studied the performance of hyperbolic wavelets and the corresponding adaptive approximation scheme.

It can be seen from Table 6 that taking hyperbolic wavelets alone leads to a considerable increase of the errors compared to the standard tensor product expansion. Concerning the convergence behavior, we can compare our results with the finite element calculations of Garcke and Griebel [36]. They performed calculations for the hydrogen and helium atom on sparse grids, using piecewise linear basis functions, and observed a convergence of $O(2^{-\tilde{Q}})$. This is in agreement with our results and demonstrates again that, with respect to the convergence rate, no improvement can be achieved by using higher order elements. In combination with an adaptive refinement along the diagonal, however, we have obtained a considerable improvement with only a very small number of additional basis functions. These preliminary results just indicate that the model system is a useful starting point to study approximation schemes for many-electron systems. Further work is required in order to get more insights concerning the convergence behavior of these schemes in the case of the helium atom.

5 Generalized contraction scheme in three dimensions

We have seen in Section 3 that a considerable reduction of the number of degrees of freedom has been achieved by contraction of wavelets on fine scales. However in the one-dimensional case, the situation is simplified due to the fact that the two-particle correlation factor $\mathcal{F}(x_1, x_2)$ is constant along the cusp $x_1 = x_2$. Obviously this is not the case for the helium atom where the correlation factor $\mathcal{F}(\mathbf{r}_1, \mathbf{r}_2)$ varies on the diagonal $\mathbf{r}_1 = \mathbf{r}_2$. However it has been observed that the variations are rather smooth and can be described by a relatively small number of degrees of freedom [37]. Similar conclusions can be drawn from the homogeneous electron gas [38], conjecturing the transferability of short-range correlations to inhomogeneous systems like atoms and molecules.

The two-particle cusp represents a three-dimensional sub-manifold of configuration space and requires $O(2^{3j})$ wavelets for its resolution up to level j. Contraction schemes for wavelets reduce the number of degrees of freedom in the ideal case to $O(j)$. However such schemes have no immediate effect on the computational complexity. At the outset it just corresponds to a re-summation of matrix elements, leading to the same computational costs for the $\mathbf{H}$ and $\mathbf{M}$ matrices as in the un-contracted case. Based on regularity arguments, we have pointed out in paper I, that one can expect an asymptotic convergence of the energy of $O(2^{-3j})$ with respect to the wavelet levels j. The cost to benefit ratio of $O(1)$, is therefore not very favorable in this case. Beyond a pure reduction of the number of degrees of freedom, we furthermore require from the contraction scheme to be beneficial with respect to the evaluation of the matrix elements. This can be achieved by choosing an ansatz of the form

$$\mathcal{F}^c_{j,\mathbf{w},\alpha}(\mathbf{r}_1, \mathbf{r}_2) = \mathcal{F}^c_{j,w_x,\alpha_x}(x_1, x_2)\ \mathcal{F}^c_{j,w_y,\alpha_y}(y_1, y_2)\ \mathcal{F}^c_{j,w_z,\alpha_z}(z_1, z_2), \tag{45}$$

where the contraction is done for each dimension separately

$$\mathcal{F}^c_{j,w,\alpha}(x_1, x_2) = \begin{cases} \sum_b f_\alpha(b)\, \varphi_{j,b}(x_1)\, \varphi_{j,b}(x_2) & w = 0 \\ \sum_b f_\alpha(b)\, [\varphi_{j,b}(x_1)\, \psi_{j,b}(x_2) + \psi_{j,b}(x_1)\, \varphi_{j,b}(x_2)] & w = 1 \\ \sum_b f_\alpha(b)\, \psi_{j,b}(x_1)\, \psi_{j,b}(x_2) & w = 2 \end{cases}. \tag{46}$$

The index $\mathbf{w}$ characterizes possible combinations for three-dimensional wavelets, which can be described by the ansatz (45). With this ansatz, we have introduced a set of functions $f_\alpha(x)$, which constitute the new degrees of freedom. In principle we can choose for f_α any convenient set of functions, like Chebyshev polynomials, for which we can easily evaluate their values at the grid points. However it is tempting to stay within multi-resolution analysis and use again wavelets for this purpose. Especially wavelets based on interpolating scaling functions, like those used in the present work, seem to be appropriate. Choosing $f_\alpha = \varphi_{j,\alpha}$ yields a complete decoupling of the contracted wavelet basis, whereas coarser scales with $k < j$ generate an increasingly stringent coupling scheme.

We want to exemplify our discussion of integral evaluation by considering two-electron Coulomb integrals for a combination of contracted and un-contracted tensor product wavelets

$$\int\int d^3r_1 d^3r_2\ \mathcal{F}^c_{j,\mathbf{w},\alpha}(\mathbf{r}_1, \mathbf{r}_2)\phi_s(\mathbf{r}_1)\phi_t(\mathbf{r}_2)\ \frac{1}{\mid \mathbf{r}_1 - \mathbf{r}_2 \mid}\ \gamma^{(p_1)}_{m_1,\mathbf{a}_1}(\mathbf{r}_1)\gamma^{(p_2)}_{m_2,\mathbf{a}_2}(\mathbf{r}_2)\phi_u(\mathbf{r}_1)\phi_v(\mathbf{r}_2), \tag{47}$$

where the ϕ_s represent arbitrary orbitals from the mean-field part Φ. Typically, contracted wavelets belong to finer levels than un-contracted ones, therefore we assume $j \geq m_1, m_2$ in the following. Applying the Gaussian transform method to the Coulomb interaction, it can be expressed via an integral over a Gaussian function

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \frac{2}{\sqrt{\pi}} \int_0^\infty dt\ \exp(-|\mathbf{r}_1 - \mathbf{r}_2|^2 t^2). \tag{48}$$

According to our discussion in paper I, we assume that the orbitals are represented in terms of linear combinations of GTOs. Therefore we can trace back our expansion of the wavefunction to products of univariate functions

$$\chi^{(w)}_{k,j,b}(x) = \begin{cases} (x-A_k)^{\ell_k} \exp\left[-\alpha_k (x-A_k)^2\right] & w=0 \\ \varphi_{j,b}(x)\,(x-A_k)^{\ell_k} \exp\left[-\alpha_k (x-A_k)^2\right] & w=1 \\ \psi_{j,b}(x)\,(x-A_k)^{\ell_k} \exp\left[-\alpha_k (x-A_k)^2\right] & w=2 \end{cases}, \tag{49}$$

where the indices j, b can be dropped in the case $w = 0$. Inserting Eqs. (46), (48) and (49) into the integral (47) and changing the order of integration, the integral over the spatial variables factorizes into products of one-dimensional integrals of the form

$$L_{\alpha,j}(t) = \sum_b f_\alpha(b) \int\int dx_1 dx_2 \, \exp\left[-(x_1-x_2)^2 t^2\right] \, \eta^{(1)}_{j,b}(x_1)\, \eta^{(2)}_{j,b}(x_2), \tag{50}$$

where we have introduced the products

$$\eta^{(i)}_{j,b}(x_i) := \chi^{(w_i)}_{k_i,j,b}(x_i)\, \chi^{(v_i)}_{\ell_i,m_i,a_i}(x_i). \tag{51}$$

To simplify our notation, all indices which are not explicitly required have been omitted in the sequel. According to our assumption $j \geq m_1, m_2$, the spatial extend of a function $\eta^{(i)}_{j,b}$ is characterized by the support of the wavelet $\psi_{j,b}$ or scaling function $\varphi_{j,b}$ belonging to it, i.e. $\mathrm{supp}\{\eta^{(i)}_{j,b}\} \subset \mathrm{supp}\{\psi_{j,b}\}$. Based on our discussion of products involving wavelets in paper I, we therefore expect that the wavelet expansion of $\eta^{(i)}_{j,b}$ strongly peaks around $\psi_{j,b}$.

The integrals (50) can be efficiently calculated using a nonstandard representation [39] of their Gaussian kernels. This means that the matrix representation of the kernels contains no couplings between wavelets on different levels. Instead one has to introduce matrix elements for the coupling between wavelets and scaling functions on the same level. Due to the smoothness of the Gaussian kernels, we profit within this representation from the vanishing moment property of our wavelets. All the required integrals can be obtained from the basic integrals

$$G^{(w)}(a,t) = \int\int dx_1 dx_2 \, \exp\left[-(x_1-x_2)^2 t^2\right] \begin{cases} \varphi(x_1-a)\varphi(x_2) & w=0 \\ \psi(x_1-a)\varphi(x_2) & w=1 \\ \psi(x_1-a)\psi(x_2) & w=2 \end{cases} \tag{52}$$

via simple scaling relations, e.g.

$$\int\int dx_1 dx_2 \, \exp\left[-(x_1-x_2)^2 t^2\right] \, \psi_{\ell,a}(x_1)\psi_{\ell,b}(x_2) = 2^{-\ell} G^{(2)}(a-b, 2^{-\ell}t). \tag{53}$$

Furthermore we have the relations

$$G^{(1)}(a,t) = \sum_{b,c} g_{b+c-2a} h_c \, G^{(0)}(b, t/2), \tag{54}$$

$$G^{(2)}(a,t) = \sum_{b,c} g_{b+c-2a} g_c \, G^{(0)}(b, t/2), \tag{55}$$

by applying the refinement relations for wavelets and scaling functions, respectively. The numerical evaluation of the functions $G^{(0)}(a,t)$ has been discussed in detail in paper I [4].

[4] The function $G(a,t)$ of paper I differs by a pre-factor, i.e. $G(a,t) = 2\pi^{1/2} G^{(0)}(a,t)$

Applying the same type of telescopic expansion, which has been discussed for the Coulomb integrals in paper I, we obtain a nonstandard expression for the integrals (50)

$$\begin{aligned} L_{\alpha,j}(t) \quad = \sum_b f_\alpha(b) \quad & \Bigg[2^{-\ell} \sum_{c,d} \langle \eta^{(1)}_{j,b} | \tilde{\psi}_{\ell,c+d} \rangle \, \langle \tilde{\psi}_{\ell,d} | \eta^{(2)}_{j,b} \rangle \; G^{(2)}(c, 2^{-\ell} t) && (56) \\ & + 2^{-\ell} \sum_{c,d} \langle \eta^{(1)}_{j,b} | \tilde{\psi}_{\ell,c+d} \rangle \, \langle \tilde{\varphi}_{\ell,d} | \eta^{(2)}_{j,b} \rangle \; G^{(1)}(c, 2^{-\ell} t) && (57) \\ & + 2^{-\ell} \sum_{c,d} \langle \eta^{(1)}_{j,b} | \tilde{\varphi}_{\ell,c+d} \rangle \, \langle \tilde{\psi}_{\ell,d} | \eta^{(2)}_{j,b} \rangle \; G^{(1)}(-c, 2^{-\ell} t) && (58) \\ & \qquad \vdots \\ & + \; 2^{-\ell_0} \sum_{c,d} \langle \eta^{(1)}_{j,b} | \tilde{\varphi}_{\ell_0,c+d} \rangle \, \langle \tilde{\varphi}_{\ell_0,d} | \eta^{(2)}_{j,b} \rangle \; G^{(0)}(c, 2^{-\ell_0} t) \Bigg] && (59) \end{aligned}$$

starting at a sufficiently fine level ℓ down to a conveniently chosen coarse level ℓ_0. After a reordering of the sums, we can define the coefficients

$$g^{(w)}_{\alpha,k,c} = 2^{-k} \sum_b f_\alpha(b) \begin{cases} \sum_d \langle \eta^{(1)}_{j,b} | \tilde{\varphi}_{k,c+d} \rangle \langle \tilde{\varphi}_{k,d} | \eta^{(2)}_{j,b} \rangle & w = 0 \\ \sum_d \langle \eta^{(1)}_{j,b} | \tilde{\psi}_{k,c+d} \rangle \langle \tilde{\varphi}_{k,d} | \eta^{(2)}_{j,b} \rangle & w = 1 \\ \sum_d \langle \eta^{(1)}_{j,b} | \tilde{\varphi}_{k,c+d} \rangle \langle \tilde{\psi}_{k,d} | \eta^{(2)}_{j,b} \rangle & w = 2 \\ \sum_d \langle \eta^{(1)}_{j,b} | \tilde{\psi}_{k,c+d} \rangle \langle \tilde{\psi}_{k,d} | \eta^{(2)}_{j,b} \rangle & w = 3 \end{cases} . \qquad (60)$$

Due to the local character of the functions $\eta^{(i)}_{j,b}$, there are only a finite number of grid points c with non-vanishing coefficients $g^{(0)}_{\alpha,k,c}$. The coefficients (60) can therefore be calculated with $O(\Omega^{1/3} 2^j)$ effort, where Ω corresponds to the volume of the system under consideration. Consequently, all the sums (56) to (59), including the sum (59) with respect to scaling functions on the coarsest level, can be performed in a local manner, thereby avoiding a persistent sum as in the case of the Coulomb interaction. It therefore does not seem to make much sense to go to very coarse levels, instead it appears to be reasonable to choose $\ell_0 = j$.

From these considerations, we obtain an expression of the form

$$\begin{aligned} L_{\alpha,j}(t) \quad = \quad & \sum_{k=\ell_0}^{\ell} \sum_c \left[g^{(1)}_{\alpha,k,c} G^{(1)}(c, 2^{-k} t) + g^{(2)}_{\alpha,k,c} G^{(1)}(-c, 2^{-k} t) + g^{(3)}_{\alpha,k,c} G^{(2)}(c, 2^{-k} t) \right] && (61) \\ + \quad & \sum_c g^{(0)}_{\alpha,\ell_0,c} G^{(0)}(c, 2^{-\ell_0} t) \end{aligned}$$

for the one-dimensional integrals (50). It remains to perform the integral

$$\frac{2}{\sqrt{\pi}} \int_0^\infty dt \; L_{\alpha_x,j}(t) \, L_{\alpha_y,j}(t) \, L_{\alpha_z,j}(t) \qquad (62)$$

with respect to the auxiliary variable t. According to Eq. (62), this just requires integrals of the form

$$\int_0^\infty dt \; G^{(w_x)}(c_x, 2^{-k_x} t) \, G^{(w_y)}(c_y, 2^{-k_y} t) \, G^{(w_z)}(c_z, 2^{-k_z} t) \qquad (63)$$

within the range of the coefficients $g^{(w)}_{\alpha,k,c}$. These integrals do not depend on the system under consideration and can be precomputed and stored in a library.

The computation of Coulomb integrals envolving contracted wavelet tensor products can therefore be performed with $O(\Omega^{1/3} 2^j)$ effort, resulting in a favorable cost to benefit ratio of $O(\Omega^{1/3} 2^{-2j})$.

6 Conclusions

Data compression is a common theme of image processing and many-particle theory. Physically speaking it means to find a local representation of the essential degrees of freedom of a system. Thereby avoiding artificial couplings between almost independent degrees of freedom corresponding to physical processes on separate energy and length scales. The concepts of multi-scale analysis offer the framework for the development of methods going into this direction. Wavelets provide a hierarchical single-particle basis with basis functions simultaneously localized in position and momentum space according to Heisenberg's uncertainty principle. We proposed wavelets here as an alternative to atomic centered GTOs, still the most popular basis in *ab initio* quantum chemistry. Hyperbolic wavelets, based on the sparse grids approximation scheme of finite element methods, provide a starting point for the representation of many-particle wavefunctions. However their efficiency is mainly limited to the approximation of the smooth parts of the wavefunction. Additional adaptive refinement is required near the inter-electronic cusps.

In the present work, we have studied local representations of short-range correlations for a one-dimensional many-particle model, which provides considerable technical simplifications compared to real many-electron systems. Nevertheless our results provide some insight for the construction of adaptive approximation schemes in the many-electron case. Short-range correlations are of fundamental importance from the point of view of approximation theory because the inter-electronic cusps determine the regularity of the wavefunction. We devised a contraction scheme for wavelet tensor products, which serves to extract the physically relevant degrees of freedom and reduces the number of additional variables for the refinement considerably. Furthermore, we proposed a method for the efficient evaluation of matrix elements including contracted tensor products.

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Appendix

A Regularity considerations for correlated wavefunctions

In order to make a reference to error estimates of finite element methods, we require a detailed knowledge of the Sobolev regularity of the exact solution Ψ_0 of the two-particle model (3). To be more specific we have to determine the maximal real index s of the Sobolev spaces $H^s(\mathbf{R}^2)$ to which Ψ_0 belongs. By definition $\Psi_0 \in H^s(\mathbf{R}^2)$ requires the existence of the integral

$$\int\int d\omega_1 d\omega_2 \left(1+\omega_1^2+\omega_2^2\right)^s \left|\hat{\Psi}_0(\omega_1,\omega_2)\right|^2 \tag{64}$$

in Fourier space. We define the Fourier transform

$$\hat{\Psi}_0(\omega_1,\omega_2) = \int\int dx_1 dx_2 \exp(-i\omega_1 x_1)\exp(-i\omega_2 x_2)\Psi_0(x_1,x_2), \tag{65}$$

which can be explicitly calculated by introducing the new variables $y_1 = x_1 - x_2$, $y_2 = x_1 + x_2$ and $\tilde{\omega} = \frac{1}{2}(\omega_1 - \omega_2)$, $\omega = \frac{1}{2}(\omega_1 + \omega_2)$ for which we can factorize the integral and obtain and an explicit representation in terms of the error function with complex arguments [40]

$$\begin{aligned}
\hat{\Psi}_0'(\tilde{\omega},\omega) &= \frac{1}{2}\int dy_1 \exp\left(\frac{1}{2}|y_1| - \frac{1}{4}y_1^2\right)\exp\left(-i\tilde{\omega}y_1\right)\int dy_2 \exp\left(-\frac{1}{4}y_2^2\right)\exp\left(-i\omega y_2\right) \\
&= 2\sqrt{\pi}\exp\left(-\omega^2\right)\int_0^\infty dy_1 \exp\left(\frac{1}{2}y_1 - \frac{1}{4}y_1^2\right)\cos\left(\tilde{\omega}y_1\right) \qquad (66) \\
&= \pi\exp\left(-\omega^2\right)\left\{\exp\left[\left(\frac{1}{2}+i\tilde{\omega}\right)^2\right]\mathrm{erfc}\left(-\frac{1}{2}-i\tilde{\omega}\right)\right. \\
&+ \left.\exp\left[\left(\frac{1}{2}-i\tilde{\omega}\right)^2\right]\mathrm{erfc}\left(-\frac{1}{2}+i\tilde{\omega}\right)\right\}.
\end{aligned}$$

The prime indicates the change of variables in Fourier space. Furthermore we have ignored the normalization constant of the wavefunction. Using the asymptotic expansion of the complementary error function in the complex plane [41]

$$\mathrm{erfc}(z) = \frac{\exp(-z^2)}{\sqrt{\pi}z}\left(1 - \frac{1}{2z^2}\cdots\right) \quad \text{for} \quad |z| \to \infty, \quad |\mathrm{arg}(z)| < \frac{3\pi}{4}, \qquad (67)$$

we obtain an asymptotic expansion of the exact solution

$$\hat{\Psi}_0'(\omega,\tilde{\omega}) = \sqrt{\pi}\exp\left(-\omega^2\right)\left[-\frac{1}{\tilde{\omega}^2} + O\left(\frac{1}{\tilde{\omega}^4}\right)\right] \quad \text{for} \quad |\tilde{\omega}| \to \infty. \qquad (68)$$

Taking into account the boundedness of the Fourier transform (65) and the inequality

$$|\omega_1^2 + \omega_2^2|^s \leq 2^{2s}\left(|\tilde{\omega}|^{2s} + |\omega|^{2s}\right) \quad \text{for} \quad s > 0 \qquad (69)$$

we can see that the integral (64) exists provided $s < 3/2$. We conclude that $\Psi_0 \in H^{3/2-\varepsilon}(\mathbf{R}^2)$ for $\varepsilon > 0$.

To our knowledge there exists no rigorous statement concerning the Sobolev regularity of the exact ground state solution of the helium atom. According to the classical work of Kato [23], Ψ_0 belongs to $H^2(\mathbf{R}^6)$, providing at least a lower bound on the Sobolev regularity. There exists a large number of very accurate approximate wavefunctions, which have in common a leading order linear dependence on $|\mathbf{r}_1 - \mathbf{r}_2|$ [12]. This property actually determines the regularity of these wavefunctions, where the electron-nuclear and tree-particle cusps have been neglected. It is therefore instructive to consider the three-dimensional analogue of the wavefunction Ψ_0

$$\Psi_{3d}(\mathbf{r}_1,\mathbf{r}_2) = \exp\left[\frac{1}{2}|\mathbf{r}_1 - \mathbf{r}_2|\right]\exp\left[-\frac{1}{2}(\mathbf{r}_1^2 + \mathbf{r}_2^2)\right]. \qquad (70)$$

as a representative for the whole class of these approximate wavefunctions. The Fourier transform

$$\hat{\Psi}_{3d}(\mathbf{k}_1,\mathbf{k}_2) = \int\int d^3r_1 d^3r_2 \exp(-i\mathbf{k}_1\mathbf{r}_1)\exp(-i\mathbf{k}_2\mathbf{r}_2)\Psi_{3d}(\mathbf{r}_1,\mathbf{r}_2) \qquad (71)$$

can be treated analogously to the one-dimensional case by introducing new variables $\mathbf{t} = \mathbf{r}_1 - \mathbf{r}_2$, $\mathbf{s} = \mathbf{r}_1 + \mathbf{r}_2$ and $\tilde{\mathbf{k}} = \frac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2)$, $\mathbf{k} = \frac{1}{2}(\mathbf{k}_1 + \mathbf{k}_2)$. After transformation of the new variables into polar coordinates we can easily perform the integrations analytically

$$\begin{aligned}
\hat{\Psi}_{3d}'(\tilde{k},k) &= 4\pi^{5/2}\exp\left(-k^2\right)\frac{1}{\tilde{k}}\int_0^\infty dt\, t\exp\left(\frac{1}{2}t - \frac{1}{4}t^2\right)\sin\left(\tilde{k}t\right) \qquad (72) \\
&= -4\pi^{5/2}\exp\left(-k^2\right)\frac{1}{\tilde{k}}\frac{d}{d\tilde{k}}\int_0^\infty dt \exp\left(\frac{1}{2}t - \frac{1}{4}t^2\right)\cos\left(\tilde{k}t\right)
\end{aligned}$$

except for the variable t, where we end up with an integral similar to the one appearing in Eq. (66). Performing the same kind of asymptotic analysis we obtain

$$\hat{\Psi}'_{3d}(k,\tilde{k}) = 4\pi^{5/2}\exp\left(-k^2\right)\left[-\frac{1}{\tilde{k}^4}+O\left(\frac{1}{\tilde{k}^6}\right)\right] \quad \text{for} \quad |\tilde{k}|\to\infty \tag{73}$$

Inserting the asymptotic expansion into the corresponding six-dimensional integral (64), we conclude that $\Psi_{3d}\in H^{5/2-\varepsilon}(\mathbf{R}^6)$ for $\varepsilon>0$.

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