The kinetic energy operator in the subspaces of wavelet analysis

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At any resolution level of wavelet expansions the physical observable of the kinetic energy is represented by an infinite matrix which is “canonically” chosen as the projection of the operator $-\Delta/2$ onto the subspace of the given resolution. It is shown, that this canonical choice is not optimal, as the regular grid of the basis set introduces an artificial consequence of periodicity, and it is only a particular member of possible operator representations. We present an explicit method of preparing a near optimal kinetic energy matrix which leads to more appropriate results in numerical wavelet based calculations. This construction works even in those cases, where the usual definition is unusable (i.e., the derivative of the basis functions does not exist). It is also shown, that building an effective kinetic energy matrix is equivalent to the renormalization of the kinetic energy by a momentum dependent effective mass compensating for artificial periodicity effects.

I. INTRODUCTION

Wavelets are commonly used for analyzing and for a compact storage of complex distributions like two dimensional images, temporal signals, and even for solving partial differential equations. Goedecker and Ivanov [1] solved the Poisson equation, Cho et al. employed wavelets in solving the Schrödinger equation for Hydrogen-like atoms [2]. Using this tool, all electron calculations were also performed within the framework of the local density approximation applying pseudopotentials and supercells [3]. Car–Parinello algorithm [4] and in Ref. [2] a new approach for magnetic ordering was presented. Arias and his coworkers developed Kohn–Sham equations based wavelet method [5], and also tested for various systems (e.g., [6] and [7]).

Wavelet analysis is a popular label applied for the concept of multiresolution analysis (MRA), which covers a systematically refined basis function set of Hilbert spaces. We refer to basic textbooks (see e.g., [9] and [10]) for the details.

In our previous works we have shown that the surroundings of a molecule can be described at a rather rough resolution level [11, 12]. We have also demonstrated [13] that electron-electron cusp singularity of the two-electron density operator can be easily reproduced by the method of multiresolution analysis. In [14] we have studied the detail structure of the wave function at various refinement levels using MRA. An adaptive method was also developed for identifying the fine structure localization regions, where further refinement of the wave function is necessary without solving the eigenvalue equation in the whole subspace expanded by the basis functions of the given resolution level.

II. SYSTEMATIC ERROR IN FINITE RESOLUTION EIGENFUNCTIONS

While having studied the question, which physical regions of the potential need a high resolution expansion of the wave function, we have solved numerically the matrix form of the one particle Schrödinger equation of exactly solvable models, with the Hamiltonian

$$H = -\frac{1}{2}\Delta + V(x).$$

The algebraic representation of the Schrödinger equation

$$H\Psi_i = E_i \Psi_i$$

for the $i$th excited state is derived by considering that according to the MRA construction, at the resolution level $M$, the Hilbert space $\mathcal{H}$ is approximated by one of its subspaces $\mathcal{H}^{[M]} = \text{span}\{s_M(x)\ell | \ell \in \mathbb{Z}\}$, where the orthonormal basis functions

$$s_M(x) = 2^{M/2}s(2^M x - \ell)$$

are the scaled and translated versions of the “mother” scaling function $s(x)$. The translated scaling functions are “sitting” on an equidistant grid of grid length $2^{-M}$. The series of subspaces $\mathcal{H}^{[M]} (M \to \infty)$ “approximates” in a given sense [8] the complete Hilbert space $\mathcal{H}$ and the
projectors
\[ P_M = \sum_{\ell \in \mathbb{Z}} |s_{M\ell}\rangle \langle s_{M\ell}| \]  

of \( \mathcal{H}^{[M]} \) “approximate” the identity operator (although, in the strict mathematical sense the limit of \( P_M \) does not exist).

By inserting the approximate identity \( P_M \) into \( \Phi \) one arrives at
\[ HP_M \Phi_i \approx E_i \Phi_i. \]  

Multiplying \( \Phi \) by the basis element \( s_{M\ell} \) from the left results in
\[ \sum_{\ell \in \mathbb{Z}} \langle s_{M\ell}|H|s_{M\ell}\rangle \langle s_{M\ell}|\Phi_i\rangle \approx E_i \langle s_{M\ell}|\Phi_i\rangle. \]  

How well approximation \( \Phi \) works is far from being understood. Nevertheless, the above method of algebraization is conventional, and later on, we will refer to this procedure as “canonical”.

Of course, the canonical method includes the solution of the eigenvalue problem
\[ \sum_{\ell \in \mathbb{Z}} H^{[M]}_{j\ell} c_{M\ell} = E_i^{[M]} c_{M\ell} \]  
of the Hamiltonian matrix \( H^{[M]}_{j\ell} = \langle s_{M\ell}|H|s_{M\ell}\rangle \). The eigenvalue \( E_i^{[M]} \) is only an approximation to the exact eigenvalue \( E_i \) (an upper bound for the ground state), and the eigenvectors \( c_{M\ell} \) define an approximation
\[ \Phi_i^{[M]}(x) = \sum_{\ell \in \mathbb{Z}} c_{M\ell} s_{M\ell}(x) \]  
of the wave function \( \Phi_i(x) \). One can not expect, of course, that \( \Phi_i^{[M]} \) gives a better result than the best approximation
\[ \Phi_i^{[M]} = P_M \Phi_i = \sum_{\ell \in \mathbb{Z}} \langle s_{M\ell}|\Phi_i\rangle s_{M\ell} \]  
in the subspace \( \mathcal{H}^{[M]} \).

For an illustration, we have chosen the simplest analytically solvable model of the potential box. The alternative of the free electron problem was singled out, as the wave functions should be square integrable in order to be able to successfully describe it with matrix methods.

Fig. 1 shows the exact excited state \( \Psi_s \), its projection \( \Psi_s^{[0]} \) to the subspace of resolution \( M = 0 \), and the solution \( \Phi_s^{[0]} \) related to the eigenvalue problem (7). The Hamiltonian matrix was calculated using the compactly supported 6 parameter Daubechies scaling functions [9]. As the first derivative of these basis functions exists, the kinetic energy matrix elements were determined by
\[ T^{[M]}_{j\ell} = \frac{1}{2} \langle s_{M\ell}| - \nabla |s_{M\ell}\rangle = \frac{1}{2} \langle s_{M\ell}|(-i\nabla) s_{M\ell}\rangle = \frac{1}{2} \int s^*_M(x)s'_M(x)dx. \]  

Here we have used the fact, that the momentum operator \(-i\nabla\) is self adjoint. The potential energy matrix elements were calculated numerically with the potential function
\[ V(x) = \begin{cases} 0 & \text{if } |x| \leq L, \\ W & \text{if } |x| > L. \end{cases} \]  

FIG. 1: Exact (solid line) and approximate (dashed line) wave functions \( \Psi_s \) and \( \Psi_s^{[0]} \) of the potential box \([11]\), with \( L = 15 \) a.u., \( W = 100 \) a.u. The difference of the exact wave function and the solution of the canonical eigenvalue problem is also shown. For a reference the difference of the exact wave function and its projection to subspace \( \mathcal{H}^{[0]} \) is plotted as well. Atomic units were used.

By a careless analysis of the results one can easily draw erroneous conclusions. One might think, that at the regions, where the difference of the exact and approximate solution is large, a further refinement of the basis set is necessary. Theoretically, this could be accomplished by adding wavelets sitting in the regions of large errors. Wavelets are localized basis functions of the orthogonal complement subspace \( \mathcal{W}^{[M]} \) of \( \mathcal{H}^{[M]} \) in the embedding subspace \( \mathcal{H}^{[M+1]} = \mathcal{H}^{[M]} \oplus \mathcal{W}^{[M]} \).

According to Fig. 1 the large error regions are located at the steepest parts of the oscillating wave function. At these places, however, the scaling function expansion can not be of bad quality, considering that any linear function of the form \( ax + b \) can be exactly expanded in \( \mathcal{H}^{[M]} \) at any resolution level \( M \). As the wave functions at the
steepest parts are almost linear, we do not expect large errors in the scaling function expansion. This prediction is justified in the third plot of Fig. 1, where the difference of the exact and projected wave function is shown. The large deviations in the approximate wave function $\Phi_i^M$ should have a different origin.

A careful study of the first part of Fig. 1 leads to the conclusion, that the solution of the eigenvalue problem has (apart from small irregularities) an oscillatory form similar to the exact solution. The essential difference between the two wave functions is that the approximate wave function $\Phi_i^M$ has a slightly smaller wavelength than the exact one, leading, of course, to a larger kinetic energy. In the case of the excited state $i = 5$, e.g., $\langle \psi_5 | T | \psi_5 \rangle = 0.1352$, while $\langle \Phi_5^0 | T | \Phi_5^0 \rangle = 0.1389$. The same general experience was gained by studying other excited states of the box model as well as those of the harmonic oscillator.

In the following sections we will analyze the reasons, why the above effects appear, and suggest a possible solution.

III. THE KINETIC ENERGY OPERATOR IN THE SUBSPACES $\mathcal{H}^M$

As in the previous example the systematic error in the wave function occurred in regions without a potential energy contribution, we conclude, that the effect is due to the representation of the kinetic energy operator. Posing this question is not as heretical as one might think for the first sight. In the original formulation of matrix mechanics by Heisenberg, Born and Jordan, the physical quantities are represented by infinite matrices satisfying the appropriate commutation rules. There is no specific prescription for the determination of their matrix elements. On the other hand, Schrödinger works in the Hilbert space of the square integrable functions $\mathcal{H}$, with a specific prescription for the operator representation of physical quantities, in particular, $T = -\Delta/2$. Von Neumann has shown the equivalence of both descriptions with the abstract Hilbert space equipped with linear operators for physical quantities. One can consider here that the subspace $\mathcal{H}^M$ is an infinite dimensional separable Hilbert space, and as such, can serve for a complete description of any quantum mechanical system, on its own right. The significant difference of the multiresolution expansion from the usual atomic orbital expansions is that the latter span a finite dimensional subspace, which is in principle unable to describe a quantum system in all details.

As the subspace $\mathcal{H}^M$ essentially differs from the complete space of square integrable functions, it is natural that the elements of the infinite matrix $K_{ji}^M$ corresponding to the physical quantity of the kinetic energy differs from the matrix elements $s_{ij}^M = \langle s_{MJ_1} | -\Delta/2 | s_{MJ_2} \rangle$, since $-\Delta/2$ is the operator representation of the kinetic energy in a different Hilbert space. However, to avoid any weird representations, we would like to keep some properties of the “canonical” approach, which are summarized below.

1. Considering, that the scaling functions are usually (but not necessarily) real, according to (10)

$$T_{ji}^M = \left( T_{ji}^{[M]} \right)^* = T_{ji}^{[M]}.$$

2. Using the definition of $s_{MN}(x)$ and after a simple variable transformation in (10), one arrives at the shift invariance property

$$T_{ji}^M = T_{j-i}^M,$$

indicating that the kinetic energy is represented by a band matrix.

3. If the scaling functions are compactly supported on the interval $[0, N-1]$ (as in the case of Daubechies-N bases),

$$T_{ji}^M = \frac{1}{2} \int s_{Mj}^i(x) s_{Mo}^j(x) dx = 0,$$

if $|j| > N - 2.$

4. Using definition (3) in (10) leads to a scaling property

$$T_{ji}^M = 2^M T_{ji}^{[0]}.$$

5. In three spatial dimensions a direct product basis function set $| j_1, j_2, j_3 \rangle = s_{MJ_1}(x_1) s_{MJ_2}(x_2) s_{MJ_3}(x_3)$ is used. As the Laplacian is a simple sum of second derivatives according to the three spatial variables, orthonormality of the basis functions results in

$$\langle j_1, j_2, j_3 | -\Delta/2 | \ell_1, \ell_2, \ell_3 \rangle = T_{j_1 \ell_1}^{[M]} \delta_{j_2 \ell_2} \delta_{j_3 \ell_3} + \delta_{j_1 \ell_1} T_{j_2 \ell_2}^{[M]} \delta_{j_3 \ell_3} + \delta_{j_1 \ell_1} \delta_{j_2 \ell_2} T_{j_3 \ell_3}^{[M]},$$

Consequently, the case of the 3D kinetic energy operator is straightforwardly reduced to the one dimensional representation.

Hermiticity and translational invariance are natural requirements for any operator representations of the kinetic energy. Though we are not obliged to keep property (14), this is one of the most attractive features of using compactly supported basis sets, thus this prescription is applied as well. Transformation of the kinetic energy matrix elements with increasing resolution (like the scaling property (15)) will be discussed later.
For the matrix $K^{[M]}$ representing the kinetic energy we require the followings at any resolution level $M$

$$K^{[M]}_{j\ell} = (K^{[M]}_{\ell j})^* = K^{[M]}_{\ell j}, \quad (17)$$

$$K^{[M]}_{j\ell - \ell} = K^{[M]}_{j-\ell \ell}, \quad (18)$$

$$K^{[M]}_{\ell \ell} = 0, \quad \text{if } |\ell| > N - 2. \quad (19)$$

In three dimensions we additionally apply

$$K^{[M]}_{j_1j_2j_3,\ell_1\ell_2\ell_3} = K^{[M]}_{j_1\ell_1} \delta_{j_2\ell_2} \delta_{j_3\ell_3}$$

$$\quad + \delta_{j_1\ell_1} K^{[M]}_{j_2\ell_2} \delta_{j_3\ell_3}$$

$$\quad + \delta_{j_1\ell_1} \delta_{j_2\ell_2} K^{[M]}_{j_3\ell_3}, \quad (20)$$

The role of operators assigned to observables is to provide the possible and expectation values of the corresponding physical quantities. A proper representation of the kinetic energy should give the known $k^2/2$ eigenvalues with eigenvectors which give reasonable approximations of the free electron wave function $e^{ikx}$. In the following considerations we will prove that the best approximation $P_M e^{ikx}$ is really an eigenvector of any matrix satisfying the requirements (17)-(19). The question remains to clarify how well the equality

$$\sum_{\ell \in Z} K^{[M]}_{j\ell} \langle s_M|e^{ikx}\rangle = \frac{k^2}{2} \langle s_M|e^{ikx}\rangle$$

is satisfied.

Defining the Fourier transform by $\hat{f}(\xi) = (2\pi)^{-1/2} \int f(x)e^{-ikx}dx$ and using definition (2) we have

$$\langle s_M|e^{ikx}\rangle = 2^{-M/2}e^{ikM(2\pi)^{1/2}} \delta(-k_M), \quad (22)$$

where $k_M = 2^{-M}k$ is the scaled wave number. Using this expression in the left hand side of (21)

$$\sum_{\ell \in Z} K^{[M]}_{j\ell} \langle s_M|e^{ikx}\rangle =$$

$$\sum_{\ell \in Z} K^{[M]}_{j\ell} e^{ikM(\ell-j)} 2^{-M/2} e^{ikM(2\pi)^{1/2}} \delta(-k_M)$$

$$= \left( \sum_{\ell \in Z} K^{[M]}_{j-\ell} e^{ikM(\ell-j)} \right) \langle s_M|e^{ikx}\rangle. \quad (23)$$

It is clear that just the shift invariance (18) ensures that the projection of the free electron wave function to $\mathcal{H}^{[M]}$ is an eigenfunction of $K^{[M]}$, with the eigenvalue

$$e^{[M]}(k) = \sum_{\ell \in Z} K^{[M]}_{\ell} e^{-ikM\ell}. \quad (24)$$

As according to (17) $K^{[M]}_{\ell}$ is Hermitian, its eigenvalues $e^{[M]}(k)$ are real and

$$e^{[M]}(-k) = \sum_{\ell \in Z} K^{[M]}_{\ell} e^{ikM\ell} = \sum_{\ell \in Z} K^{[M]}_{-\ell} e^{-ikM\ell} = e^{[M]}(k), \quad (25)$$

i.e., $e^{[M]}(k)$ is symmetric in $k$. The above natural physical requirements are satisfied for all reasonably chosen $K^{[M]}$.

The fundamental question is how well $e^{[M]}(k)$ approximates the free electron kinetic energy $k^2/2$. In order to understand this, some properties of $e^{[M]}(k)$ will be studied below. As the argument $k_M$ in definition (24) exponentially decreases with increasing resolution $M$, it is natural to consider the Taylor expansion of $e^{[M]}(k)$. Due to the symmetry of $e^{[M]}(k)$ all its odd order derivatives should be zero in $k = 0$. This condition is equivalent to

$$\sum_{\ell \in Z} 2^{2n+1} K^{[M]}_{\ell} = 0 \quad \text{for any } n = 0, 1, \ldots, \quad (26)$$

$$d^2 \varepsilon^{[M]}(0) = -2^{-2M} \sum_{\ell \in Z} \ell^2 K^{[M]}_{\ell} = 1, \quad (27)$$

$$d^{2n} \varepsilon^{[M]}(0) = (-1)^n 2^{-2nM} \sum_{\ell \in Z} \ell^{2n} K^{[M]}_{\ell} = 0, \quad (28)$$

for $n \geq 2$. In Appendix A we have shown that for the canonical kinetic energy matrix sum rules $(20)$ and $(21)$ ensure that $(20)$ and $(21)$ are satisfied. It is easy to see, however, that regardless of the choice of $K^{[M]}$ the equivalence of $e^{[M]}(k)$ and $k^2/2$ can never be perfect. According to $(19)$ $e^{[M]}(k)$ is a finite trigonometric polynomial, consequently it is $2\pi$ periodic, and can not coincide with the free electron energy in the whole range $-\infty < k < \infty$.

Fig. 2 shows that the canonical kinetic energy function approaches the “Brillouin zone” boundaries at $k = -\pi$ and $k = \pi$ with a horizontal tangent. This difficulty can never be resolved by choosing any set of $K^{[M]}_{\ell}$ values for $2\pi$ periodic $e^{[M]}(k)$ functions, which leads to the conclusion, that any multiresolution quantum mechanics loses its applicability for the energies with $|k| = 2\pi/\lambda \approx \pi$. In other words, for the wavelength of the particle we get the condition $\lambda/2 \ll 1$. It is not surprising from the physical point of view, since 1 is the grid length of the scaling function basis set at resolution level $M = 0$ and no wave functions with a wavelength comparable to the grid length are expected to be described in a satisfactory manner. If the resolution increases, however, the scaling property (15) results in

$$\varepsilon^{[M]}(k) = 2^{2M} \sum_{\ell \in Z} T^{[0]}_{\ell} e^{-ikM\ell} = 2^{2M} \varepsilon^{[0]}(2^{-M}k). \quad (29)$$

Since the argument of $\varepsilon^{[0]}_{\text{can}}$ decreases exponentially with increasing resolution, the quality of the Taylor expansion becomes increasingly better, as it can be traced in Fig. 2 in the close neighborhood of $k = 0$. Although it is very satisfying that the canonical kinetic energy can reproduce the exact values in the infinite resolution limit, in a practical calculation, however, one should stay at
of (24). As a first remark, we recall the scaling property (15) of finite trigonometrical polynomial expansion of the form (27) implies that in the leading order the kinetic energy matrix elements should scale as $K^2/2$. On the other hand, however, the necessary requirement (similar to (10)), their scaling behavior can not be derived. Consequently, we have decided to keep only one independent parameter $t$ and to define the kinetic energy matrix elements by

$$K^M_k = 2^{2M} T^N_k (t)$$

A. The Fourier series approach

The best possibility we can expect using an expression of the form (24) is that the function $k^2/2$ is correctly described in the interval $(-\pi, \pi)$. This, however, requires the infinite Fourier series expansion

$$\frac{k^2}{2} = \frac{\pi^2}{6} + 2 \sum_{\ell=1}^{\infty} \frac{(-1)^{\ell}}{\ell^2} \cos(\ell k).$$

Applying (19) leads to a truncation of (31) at $\ell = N - 2$. It is clear that identifying $K^{[0]}_k$ with the expansion coefficients of the truncated series would not satisfy any of the criteria (26)–(28). It is an elementary requirement that a particle with zero momentum should have zero kinetic energy, and as we have discussed above, this is equivalent to (27). Considering these arguments, we suggest the following truncation process

$$\alpha F^N_k = \begin{cases} \frac{\pi^2}{6} & \text{for } \ell = 0, \\ \frac{(-1)^{\ell}}{\ell^2} & \text{for } 1 \leq |\ell| \leq N - 3, \\ -\frac{1}{3} \left( \frac{\pi^2}{6} + 2 \sum_{\ell=1}^{N-3} \frac{(-1)^{\ell}}{\ell^2} \right) & \text{for } |\ell| = N - 2. \end{cases}$$

The definition $K^{[M]}_k = 2^{2M} F^N_k$ automatically satisfies sum rule (26), whereas with an appropriate choice of the normalization factor $\alpha$, (27) can also be fulfilled. The kinetic energy function $\varepsilon^{[0]}(k)$ calculated according to (29) using the matrix elements determined by (32) is plotted in Fig. 2. According to the figure, the Fourier type approach results in a weaker quality approximation than the canonical calculation, especially in the low energy region. This effect can be traced in Tab. I; both the total energy and the wave function deviate more from the exact quantities than those of the canonical calculation, except for the wave function of higher excited states.

B. The Taylor series approach

As we have seen, the quality of the $\varepsilon^{[0]}(k)$ for smaller $k$ values is essential both in rough resolutions and also in the limit $M \to \infty$. This leads to the conclusion that the Taylor expansion of the kinetic energy function should satisfy as much conditions of (26)–(28) as possible with the given number of non-zero matrix elements $K^{[M]}_k$. We suggest the following scheme for determining the optimal kinetic energy matrix. According to (13) and (19) the number of non-zero, essentially different matrix elements is $N - 1$, offering too much freedom in the optimization process. Consequently, we have decided to keep only one independent parameter $t$ and to define the kinetic energy matrix elements by

$$K^{[M]}_k = 2^{2M} T^N_k (t)$$

FIG. 2: The canonical kinetic energy function $\varepsilon^{[0]}_\text{can}(k)$ (dashed line) of the Daubechies-6 basis set compared to the free particle kinetic energy $k^2/2$ (solid line). The kinetic energy $\varepsilon^{[0]}(k)$ of the Fourier type approximation with the same number of matrix elements is plotted by a dotted line. Atomic units were used.
TABLE I: The error of the total energy $E_{i}^{[0,F]}$ and the wave function $\Phi_{i}^{[0,F]}$ of the Fourier method compared to the ones of the canonical quantities $E_{i}^{[0]}$ and $\Phi_{i}^{[0]}$ for the Daubechies-6 basis set. $E_{i}$ and $\Psi_{i}$ are the exact total energy and wave function, respectively. Label $i = 1$ indicates the ground state, whereas $i = 2, 3, 4, 5$ are the successive excited states of the potential box $[11]$, with $L = 15$ a.u., $W = 100$ a.u.

| $i$ | $|E_{i} - E_{i}^{[0]}|$ | $|E_{i} - E_{i}^{[0,F]}|$ | $||\Psi_{i} - \Phi_{i}^{[0]}||$ | $||\Psi_{i} - \Phi_{i}^{[0,F]}||$ |
|-----|-----------------|-----------------|-----------------|-----------------|
| 1   | $1.0802 \times 10^{-4}$ | $2.7721 \times 10^{-4}$ | $1.0392 \times 10^{-2}$ | $1.4545 \times 10^{-2}$ |
| 2   | $4.4247 \times 10^{-4}$ | $1.6186 \times 10^{-3}$ | $1.8878 \times 10^{-2}$ | $2.1309 \times 10^{-2}$ |
| 3   | $1.0681 \times 10^{-3}$ | $5.4125 \times 10^{-3}$ | $2.7654 \times 10^{-2}$ | $2.6331 \times 10^{-2}$ |
| 4   | $2.1982 \times 10^{-3}$ | $1.3550 \times 10^{-2}$ | $3.6618 \times 10^{-2}$ | $2.8380 \times 10^{-2}$ |
| 5   | $4.3310 \times 10^{-3}$ | $2.7925 \times 10^{-2}$ | $4.5968 \times 10^{-2}$ | $2.7997 \times 10^{-2}$ |

with

$$\alpha T_{\ell}^{N}(t) = \begin{cases} 1 & \text{for } \ell = 0, \\ t & \text{for } |\ell| = 1, \\ t_{\ell}(t) & \text{for } 2 \leq |\ell| \leq N - 2. \end{cases}$$

Quantities $t_{\ell}(t)$ are determined by the solution of the linear system of equations

$$\begin{pmatrix} 1 & 1 & \ldots & 1 \\
2 & 3 & \ldots & (N - 2)^{4} \\
2^{6} & 3^{6} & \ldots & (N - 2)^{6} \\
\vdots & \vdots & \ddots & \vdots \\
2^{2(N-3)} & 3^{2(N-3)} & \ldots & (N - 2)^{2(N-3)} \\
\end{pmatrix} \begin{pmatrix} t_{2} \\
t_{3} \\
\vdots \\
t_{N-2} \end{pmatrix} = \begin{pmatrix} -1/2 - t \\
t \\
\vdots \\
-t \end{pmatrix}.$$ (35)

The normalization factor

$$\alpha = -2t - 2 \sum_{\ell=2}^{N-2} \ell^{2}t_{\ell}(t).$$ (36)

It is easy to verify that the conditions (26) and (27) are always satisfied by these values and (28) fulfills until $n = N - 3$.

Notice, that equations (34)–(36) have a solution even in the case of $N = 4$, i.e., for the Daubechies-4 scaling functions, where the canonical kinetic energy matrix elements are not defined at all, as the application of formula (10) requires the derivative of the scaling function, which does not exist in this case. For an illustration we have carried out a calculation for the potential

$$V(x) = \begin{cases} 0 & \text{if } -L \leq x < 0, \\
V_{0} & \text{if } 0 \leq x \leq L, \\
W & \text{if } |x| > L, \end{cases}$$ (37)

with Daubechies-4 scaling functions and with the Taylor series based method outlined above. The optimal value of the parameter $t$ was determined as described later. Fig. 3 shows the exact and the $M = 0$ level approximated wave function of the 2nd excited state of the model (37). This state was selected in order to demonstrate the capabilities of the method, not only in the free electron case but in the classically unavailable regions (right hand side of the box, $E_{i} < V_{0}$), as well. It is seen that the construction of the kinetic energy matrix by the Taylor expansion method leads to a rather satisfactory result even at this low resolution approximation.

For finding the optimal values of $t$ in the construction of the wave function, we have plotted the deviation of the approximate total energy from the exact one as a function of the parameter $t$ in Fig. 3. Similarly, the norm of the difference of the exact and approximated wave function of

Fig. 3: Exact (solid line) and approximate (dashed line) wave functions $\Psi_{1}$ and $\Phi_{3}^{[0,F]}$ of the potential model (37), with $L = 15$ a.u., $W = 100$ a.u. and $V_{0} = 0.5$ a.u., using the Daubechies-4 scaling function in the Taylor series method. Atomic units were applied.
The deviation of the approximate total energy $E_1^{[T]}$ from their exact counterparts $E_1$ and $\Psi_1$ (solid lines) of the potential model (37), with $L = 17$ a.u., $W = 10$ a.u. and $V_0 = 0.01$ a.u., using the Taylor series method. As references, horizontal lines indicate the values of the canonical (dashed line) and the Fourier series method (dotted line) results. Sign $\bigcirc$ stands for the results of the Daubechies-4 scaling function, $\times$, $\Box$ and $\triangle$ mean Daubechies-6, Daubechies-8 and Daubechies-10 calculations, respectively. Atomic units were applied.

According to Fig. 4 a minimum in the error functions can be identified which defines the optimum value of parameter $t$. We would like to emphasize, that around the minima the curves are flat, even for the energy deviations (consider, the logarithmic scale on the vertical axis). The error curves are similar to all of the lower energy excited states, and even the positions of the minima are almost the same. As the worst example, we adduce the case of Daubechies-8 scaling function where the average value of the optimal $t$ calculated for the energy and wave function error curves of several excited states is 0.57, with a standard deviation of $\pm 0.06$. Also, by playing around the

the model potential (37) is also shown. It can be realized, that in quite a broad range of the parameter $t$, the kinetic energy matrix of the Taylor’s expansion method leads to a considerably better quality result than the canonical choice, regarding both the total energy and the wave function. The Fourier series method, however, leads to unacceptable solutions.

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parameters $L, W$ and $V_0$ of model (37) we could realize, that the optimum $t$ values are essentially potential independent. Extending the scope of the investigations to finer resolution levels $M = 0, 1, 2, 3, 4$ we have found that the position of the minima of the error curves stabilizes at $M = 1$, there is no significant change at fine resolutions. Further, we have studied the exactly solvable model of the harmonic oscillator with the potential

$$V(x) = \frac{\omega^2}{2} x^2. \quad (38)$$

We have experienced the same behavior as in the case of the previous physical system (37). The positions of the optimum $t$ values are independent of the excitation level $i$, of the resolution $M$ and also of the value of the potential width $\omega^{-1}$. Finally, we conclude, that to a good approximation, the optimum values of parameter $t$ in the kinetic energy matrix definition (33)–(36) can be chosen model independently, which works also for many low lying excited states. In Tab. 11 we summarize our recommendations for the the best values of $t$ for various Daubechies basis function sets. As the error curves are rather flat around the minima, the values in the table can be changed by $\pm 10$ percent without a considerable change in the quality of the total energy and wave function approximations.

### V. SUMMARY

Studying exactly solvable models in the framework of multiresolution analysis we have found that the representation of the kinetic energy operator plays an essential role in the quality of the results achieved by approximate solutions at a given resolution level $M$. The regular grid of the scaling function basis set introduces an artificial consequence of periodicity. Instead of a free particle, the MRA expansion describes rather an electron with a momentum dependent effective mass $m^*(k) = k^2/(2\varepsilon^{[M]}(k))$, where the function $\varepsilon^{[M]}(k)$ is determined by the matrix elements of the kinetic energy matrix. We have shown that in the case of resolution level $M = 0$ the MRA expansion loses its applicability if the kinetic energy approaches or exceeds the value $E_{\text{kin}} = \pi^2/2$ a.u. (corresponding to the limit value $k = \pi$). By increasing the resolution, the applicability range extends exponentially as $k < 2^M \pi$, $E_{\text{kin}} < 2^{2M}\pi^2/2$ a.u., and artificial periodicity effects disappear in this limit.

| $N$ | 4  | 6  | 8  | 10 |
|-----|----|----|----|----|
| $t$ | 0.54 | 0.47 | 0.57 | 0.58 |

TABLE II: The recommended kinetic energy matrix parameter $t$ for the Taylor series based construction (33)–(36) in case of Daubechies-$N$ scaling function sets ($N = 4, 6, 8, 10$).
However, in the numerical practice the level of resolution should be kept as low as possible, in order to avoid the need for extensive computational resources. We have demonstrated that for low resolutions the kinetic energy of the numerical calculations is overestimated compared to the exact values. The effect is due to the fact that the free particle energy $k^2/2$ is improperly reproduced by its $2\pi$-periodic approximation $\varepsilon_{\text{can}}(k)$. This reproduction can considerably be improved by introducing alternative matrix elements of the kinetic energy matrix instead of the canonical ones. Both the total energy and wave function improvements are well pronounced at low resolutions as it can be traced from Fig. II. A close optimal, system and eigenstate independent choice of the kinetic energy matrix elements is derived from the formulas of the Taylor series approach \([33]–[36]\) and from our suggestion for its parameter value $t$ in Tab. II. At an arbitrary resolution level $M$ the kinetic energy matrix elements are calculated as

$$K_{j\ell}^{[M]} = K_{|j-\ell|}^{[M]} = 2^{2M}T_{|j-\ell|}^N,$$

where $N$ determines the number of essential matrix elements, as $T_{|j-\ell|}^N = 0$ if $|j-\ell| > N - 2$. Tab. III lists the values of $T_{|j-\ell|}^N$ for various Daubechies-$N$ scaling function sets. In three spatial dimensions expression \([20]\) should be applied. With the suggested method it is possible to define a kinetic energy matrix even in the case of the Daubechies-4 basis set, where the scaling function is not differentiable, thus the canonical approach is not applicable.

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**APPENDIX A: SOME ELEMENTARY PROPERTIES OF THE CANONICAL KINETIC ENERGY MATRIX**

We will prove here, that the canonical kinetic energy matrix elements defined by \([10]\) satisfy simple sum rules as

$$\sum_{\ell \in \mathbb{Z}} T_{\ell}^{[M]} = 0, \quad (A1)$$

$$\sum_{\ell \in \mathbb{Z}} \ell T_{\ell}^{[M]} = 0, \quad (A2)$$

$$\sum_{\ell \in \mathbb{Z}} \ell^2 T_{\ell}^{[M]} = -2^{2M}, \quad (A3)$$

with the notation introduced in \([13]\). Of course, these relations hold only if the canonical kinetic energy matrix exists, i.e., if the scaling function is differentiable. This condition is satisfied for the Daubechies basis sets with 6 or more parameters.

**Proof of \((A1)\).** At any resolution level $M$ the scaling function basis set is capable to exactly expand any constant function \([3,10]\), consequently, for any $x$

$$\sum_{\ell \in \mathbb{Z}} c_{\ell}^{[M]} s_{M\ell}(x) = 1$$

with the expansion coefficients $c_{\ell}^{[M]} = 2^{-M/2}$. Differentiating, multiplying by $s_r^{M\ell}(x)/2$ and integrating one gets

$$\sum_{\ell \in \mathbb{Z}} \frac{1}{2} \int s_r^{M\ell}(x)s_s^{M\ell}(x)dx = \sum_{\ell \in \mathbb{Z}} T_{\ell}^{[M]} = 0. \quad (A5)$$

**Proof of \((A2)\).** The basis set \($s_{M\ell}|\ell \in \mathbb{Z}\$) exactly expands the identity function, i.e., for all $x$

$$\sum_{\ell \in \mathbb{Z}} c_{\ell}^{[M]} s_{M\ell}(x) = x$$

with the appropriate expansion coefficients

$$c_{\ell}^{[M]} = \int xs_{M\ell}(x)dx = 2^{-3M/2}\mu_1 + \ell,$$ \(A7\)

where we have applied definition \([9]\), a proper integral variable transformation, and the fact that $\int s(y)dy = 1$ \([3]\). The quantity $\mu_1 = \int ys(y)dy$ is the first momentum of the mother scaling function. Differentiating \(A6\), multiplying by $s_r^{M\ell}(x)/2$ and integrating we arrive at

$$\sum_{\ell \in \mathbb{Z}} c_{\ell}^{[M]} \frac{1}{2} \int s_r^{M\ell}(x)s_s^{M\ell}(x)dx = \sum_{\ell \in \mathbb{Z}} c_{\ell}^{[M]} T_{\ell}^{[M]} =$$

$$\frac{1}{2} \int s_r^{M\ell}(x)dx = \frac{1}{2}(s_{M\ell}(x))_{-\infty}^\infty. \quad (A8)$$

As the scaling functions are square integrable, $s_{M\ell}(\pm\infty) = 0$, and

$$0 = \sum_{\ell \in \mathbb{Z}} c_{\ell}^{[M]} T_{\ell}^{[M]} = 2^{-3M/2}\mu_1 \sum_{\ell \in \mathbb{Z}} T_{\ell}^{[M]} + 2^{-3M/2} \sum_{\ell \in \mathbb{Z}} \ell T_{\ell}^{[M]}. \quad (A9)$$

Considering \(A1\) immediately follows \(A2\).

**Proof of \((A3)\).** For the compactly supported scaling functions of Daubechies with 6 or more parameters the function $x^2$ is still among the exactly expandable functions.

$$\sum_{\ell \in \mathbb{Z}} c_{\ell}^{[M]} s_{M\ell}(x) = x^2$$

where the expansion coefficients are

$$c_{\ell}^{[M]} = \int x^2 s_{M\ell}(x)dx = 2^{-5M/2}(2\ell\mu_1 + \ell^2), \quad (A10)$$
after similar steps applied in the previous proof. The notation \( \int y^2 s(y) dy = \mu_2 \) was introduced. Differentiating (A10) leads to

\[
\sum_{\ell \in \mathbb{Z}} [c_{\ell}^{M}] T_{\ell}^{[M]} = \int x s_{M0}(x) dx =
\]

\[-\int s_{M0}(x) dx = -2^{-M/2}. \quad (A12)
\]

The second equality follows from partial integration, and from the fact that the integrated part disappears due to \( s_{M0}(\pm \infty) = 0 \). Substituting (A11) into (A12) and using (A1) and (A2) gives (A3).

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