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ORIGINAL PAPER

The kinetic energy operator in the subspaces of wavelet analysis

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Abstract 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 its 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.

Keywords Kinetic energy operator · Operator representation · Wavelet analysis

1 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,

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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. [5] a new approach for magnetic ordering was presented. Arias and his coworkers developed Kohn–Sham equations based wavelet method [6], and also tested for various systems (e.g., [7] and [8]).

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., [9,10]) 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 MRA. 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.

2 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

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

The algebraic representation of the Schrödinger equation

$$H\Psi_i = E_i\Psi_i \tag{2}$$

for the ith 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 $\mathcal{H}^{[M]} = \mathrm{span}\{s_{M\ell}(x)|\ell \in \mathbb{Z}\}$, where the orthonormal basis functions

$$s_{M\ell}(x) = 2^{M/2}s(2^M x - \ell) \tag{3}$$

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 [9] the complete Hilbert space $\mathcal{H}$ and the projectors

$$P_M = \sum_{\ell\in\mathbb{Z}} |s_{M\ell}\rangle\langle s_{M\ell}| \tag{4}$$

of $\mathcal{H}^{[M]}$ "approximate" the identity operator. By inserting P_M into (2) one arrives at

$$H P_M \Psi_i \cong E_i \Psi_i . \tag{5}$$

Multiplying (5) by the basis element s_{Mj} from the left results in

$$\sum_{\ell \in \mathbb{Z}} \langle s_{Mj} | H | s_{M\ell} \rangle \, \langle s_{M\ell} | \Psi_i \rangle \cong E_i \langle s_{Mj} | \Psi_i \rangle . \tag{6}$$

How well approximation (5) works is far from being understood. Nevertheless, the above method of algebraization is conventional, which in a general form was introduced in 1915 by B. G. Galerkin, for converting continuous operator problems to discrete problems [15]. Galerkin's method is widely known in engineering and applied mathematics, however, this terminology has not become an established custom in the quantum mechanics community, and later on, we will simply refer to this procedure as "canonical".

Of course, the canonical method includes the solution of the eigenvalue problem

$$\sum_{\ell \in \mathbb{Z}} H_{j\ell}^{[M]} c_{M\ell} = E_i^{[M]} c_{Mj} \tag{7}$$

of the Hamiltonian matrix $H_{j\ell}^{[M]} = \langle s_{Mj} | H | s_{M\ell} \rangle$. 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

$$\Phi_i^{[M]}(x) = \sum_{\ell \in \mathbb{Z}} c_{M\ell} \; s_{M\ell}(x) \tag{8}$$

of the wave function $\Psi_i(x)$. One cannot expect, of course, that (8) gives a better result than the best approximation

$$\Psi_i^{[M]} = P_M \Psi_i = \sum_{\ell \in \mathbb{Z}} \langle s_{M\ell} | \Psi_i \rangle \, s_{M\ell} \tag{9}$$

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. Figure 1 shows the exact excited state Ψ_5, its projection $\Psi_5^{[0]}$ to the subspace of resolution $M = 0$, and the solution $\Phi_5^{[0]}$ 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

$$\begin{aligned} T_{j\ell}^{[M]} &= \frac{1}{2} \, \langle s_{Mj} | - \Delta | s_{M\ell} \rangle = \frac{1}{2} \, \langle (-i\nabla) s_{Mj} | (-i\nabla) s_{M\ell} \rangle \\ &= \frac{1}{2} \int s'_{Mj}(x) s'_{M\ell}(x) dx . \end{aligned} \tag{10}$$

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

$$V(x) = \begin{cases} 0 & \text{if } |x| \leq L, \\ W & \text{if } |x| > L. \end{cases} \tag{11}$$

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

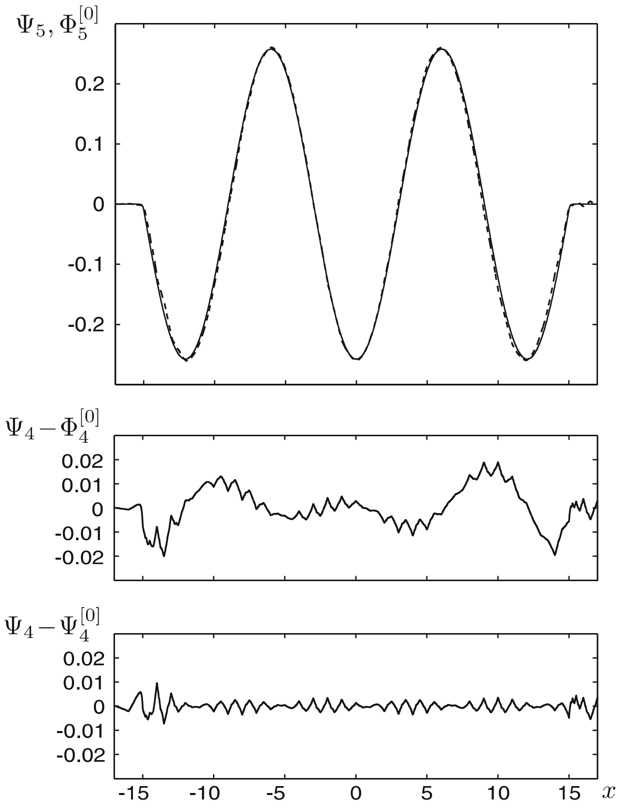

Fig. 1 Exact (solid line) and approximate (dashed line) wave functions Ψ_5 and $\Phi_5^{[0]}$ of the potential box (11), with $L = 15$ a.u., $W = 100$ a.u. The difference of the exact wave function and the solution of the canonical eigenvalue problem is also shown. For a reference the difference of the exact wave function and its projection to subspace $\mathcal{H}^{[0]}$ is plotted as well. Atomic units were used

cannot 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.

3 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 [16] the equivalence of both descriptions with the abstract Hilbert space equipped with linear operators for physical quantities. One can consider here that the subspace $\mathcal{H}^{[M]} \subset \mathcal{H}$ is itself 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 $K_{j\ell}^{[M]}$ corresponding to the physical quantity of the kinetic energy differs from the matrix elements $T_{j\ell}^{[M]} = \langle s_{Mj}|-\Delta/2\,|s_{M\ell}\rangle$, since $-\Delta/2$ is the operator representation of the kinetic energy in a different Hilbert space. We would like to emphasize, that by choosing an appropriate infinite matrix representation $K^{[M]}$ of the kinetic energy we do not aim to give an improved discretization of the Laplacian operator. Instead, our approach is not algorithmic, but specifically physical. We refer to one of the basic tasks of quantum mechanical descriptions, i.e., for a given physical quantity, we search for an operator in the Hilbert space $\mathcal{H}^{[M]}$ which is able to provide the expectation value as well as all possible measurable values of this quantity. As we will see later, this intention can be achieved even if the matrix elements of the Laplacian do not exist.

In order to avoid any weird representations, we would like to keep some properties of the "canonical" (Galerkin) approach, which are summarized below.

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

$$T_{j\ell}^{[M]} = \left(T_{\ell j}^{[M]}\right)^{*} = T_{\ell j}^{[M]}. \tag{12}$$

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

$$T_{j\ell}^{[M]} = T_{j-\ell}^{[M]}, \tag{13}$$

   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),

$$T_{\ell}^{[M]} = \frac{1}{2}\int s'_{M\ell}(x)s'_{M0}(x)dx = 0, \quad \text{if } |\ell| > N-2. \tag{14}$$

   Here N is the number of parameters which define the mother scaling function.
4. Using definition (3) in (10) leads to a scaling property

$$T_{j\ell}^{[M]} = 2^{2M}T_{j\ell}^{[0]}. \tag{15}$$

   This simple scaling behavior is a consequence of the MRA definition (3) of the basis set and holds generally for the canonical matrix elements in the framework of MRA.
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 applying the three (x_1, x_2, x_3) Cartesian coordinates. As the Laplacian is a simple sum of second derivatives according to the three spatial variables, orthonormality of the basis functions results in

$$\begin{aligned}\langle j_1 j_2 j_3| - \Delta/2|\ell_1\ell_2\ell_3\rangle = T_{j_1\ell_1}^{[M]}\delta_{j_2\ell_2}\delta_{j_3\ell_3} \\ +\delta_{j_1\ell_1}T_{j_2\ell_2}^{[M]}\delta_{j_3\ell_3} \\ +\delta_{j_1\ell_1}\delta_{j_2\ell_2}T_{j_3\ell_3}^{[M]}.\end{aligned} \tag{16}$$

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

Hermiticity (12) and translational invariance (13) 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

$$K_{j\ell}^{[M]} = \left(K_{\ell j}^{[M]}\right)^* = K_{\ell j}^{[M]}, \tag{17}$$

$$K_{j\ell}^{[M]} = K_{j-\ell}^{[M]} = K_{|j-\ell|}^{[M]}, \tag{18}$$

$$K_{\ell}^{[M]} = 0, \qquad \text{if } |\ell| > N-2. \tag{19}$$

In three dimensions we additionally apply

$$\begin{aligned} K_{j_1 j_2 j_3, \ell_1 \ell_2 \ell_3}^{[M]} &= K_{j_1 \ell_1}^{[M]} \delta_{j_2 \ell_2} \delta_{j_3 \ell_3} \\ &\quad + \delta_{j_1 \ell_1} K_{j_2 \ell_2}^{[M]} \delta_{j_3 \ell_3} \\ &\quad + \delta_{j_1 \ell_1} \delta_{j_2 \ell_2} K_{j_3 \ell_3}^{[M]}. \end{aligned} \tag{20}$$

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

$$\sum_{\ell \in \mathbb{Z}} K_{j\ell}^{[M]} \langle s_{M\ell} | e^{ikx} \rangle \stackrel{?}{=} \frac{k^2}{2} \langle s_{Mj} | e^{ikx} \rangle \tag{21}$$

is satisfied.

Defining the Fourier transform by $\hat{f}(\xi) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} f(x) e^{-i\xi x} dx$ and using definition (3) we have

$$\langle s_{M\ell} | e^{ikx} \rangle = 2^{-M/2} e^{ik_M \ell} (2\pi)^{1/2} \, \hat{s}(-k_M), \tag{22}$$

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

$$\sum_{\ell\in\mathbb{Z}} K^{[M]}_{j\ell}\langle s_{M\ell}|e^{ikx}\rangle$$
$$= \sum_{\ell\in\mathbb{Z}} K^{[M]}_{j\ell}\, e^{ik_M(\ell-j)}2^{-M/2}e^{ik_M j}(2\pi)^{1/2}\,\hat{s}(-k_M)$$
$$= \left(\sum_{\ell\in\mathbb{Z}} K^{[M]}_{j-\ell}\, e^{ik_M(\ell-j)}\right)\langle s_{Mj}|e^{ikx}\rangle. \tag{23}$$

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

$$\varepsilon^{[M]}(k) = \sum_{\ell\in\mathbb{Z}} K^{[M]}_{\ell} e^{-ik_M\ell}. \tag{24}$$

An analogous statement for finite difference differentiation operator approximations can be found in [17,18]. Further connections between wavelet and finite difference approaches can be found in [19]. As according to (17) $K^{[M]}_\ell$ is Hermitian, its eigenvalues $\varepsilon^{[M]}(k)$ are real and

$$\varepsilon^{[M]}(-k) = \sum_{\ell\in\mathbb{Z}} K^{[M]}_{\ell} e^{ik_M\ell} = \sum_{\ell\in\mathbb{Z}} K^{[M]}_{-\ell} e^{-ik_M\ell} = \varepsilon^{[M]}(k), \tag{25}$$

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

The fundamental question is how well $\varepsilon^{[M]}(k)$ approximates the free electron kinetic energy $k^2/2$. In order to understand this, some properties of $\varepsilon^{[M]}(k)$ 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 $\varepsilon^{[M]}(k)$. Due to the symmetry of $\varepsilon^{[M]}(k)$ all its odd order derivatives should be zero in $k = 0$. This condition is equivalent to $\sum_{\ell\in\mathbb{Z}} \ell^{2n+1} K^{[M]}_\ell = 0$ for any $n = 0, 1, \ldots$, which follows from (18). In the ideal case $\varepsilon^{[M]}(k)$ would be equal to $k^2/2$ requiring

$$\varepsilon^{[M]}(0) = \sum_{\ell\in\mathbb{Z}} K^{[M]}_{\ell} = 0, \tag{26}$$

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

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

for $n \geq 2$. In Appendix A, we have shown that for the canonical kinetic energy matrix sum rules (A1) and (A3) ensure that (26) and (27) are satisfied. It is easy to see, however, that regardless of the choice of $K^{[M]}_\ell$ the equivalence of $\varepsilon^{[M]}(k)$ and $k^2/2$ can never be perfect. According to (19) $\varepsilon^{[M]}(k)$ is a finite trigonometric polynomial,

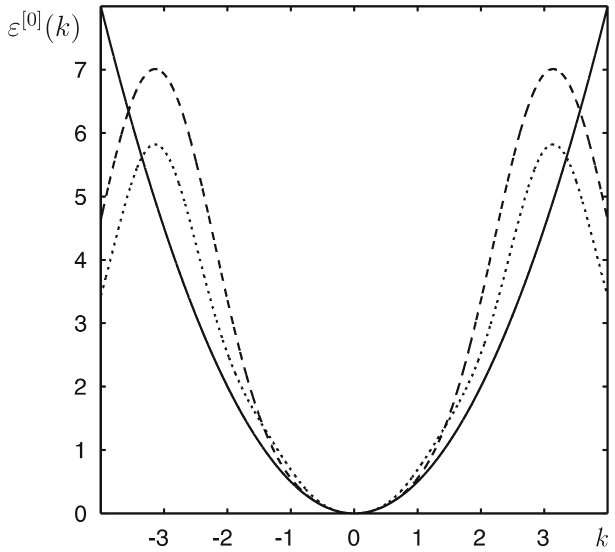

Fig. 2 The canonical kinetic energy function $\varepsilon^{[0]}_{\text{can}}(k)$ (dashed line) of the Daubechies-6 basis set compared to the free particle kinetic energy $k^2/2$ (solid line). The kinetic energy $\varepsilon^{[0]}_{\mathcal{F}}(k)$ of the Fourier type approximation with the same number of matrix elements is plotted by a dotted line. Atomic units were used

consequently it is 2π periodic, and cannot coincide with the free electron energy in the whole range $-\infty < k < \infty$.

Figure 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 2π periodic $\varepsilon^{[M]}(k)$ 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

$$\varepsilon^{[M]}_{\text{can}}(k) = 2^{2M} \sum_{\ell \in \mathbb{Z}} T^{[0]}_\ell e^{-ik_M \ell} = 2^{2M} \varepsilon^{[0]}_{\text{can}}(2^{-M} k). \tag{29}$$

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 a relatively low resolution M. At these resolutions the function $\varepsilon^{[M]}_{\text{can}}(k)$ performs rather poorly for larger k, and there is a reasonable hope to find matrix elements $K_\ell^{[M]}$ which provide significantly better approximation of the function $k^2/2$.

4 Assignment strategies for the optimal kinetic energy matrix

There are several possible decisions for choosing the matrix elements $K_\ell^{[M]}$ in order to approximate $k^2/2$ by a finite trigonometrical polynomial expansion of the form (24). As a first remark, we recall the scaling property (15) of the canonical kinetic energy matrix. Since the values of $K_\ell^{[M]}$ are not determined by a mathematical formula (similar to (10)), their scaling behavior cannot be derived. On the other hand, however, the necessary requirement (27) implies that in the leading order the kinetic energy matrix elements should scale as $K_\ell^{[M]} \sim 2^{2M}$. We would like to emphasize, that choosing the scaling formula

$$K_\ell^{[M]} = 2^{2M} K_\ell^{[0]} \tag{30}$$

is by no means a must, we have decided to apply it in order to decrease the many degrees of freedom of the problem. After this, we still have to determine the values of the zeroth level matrix elements, for which we consider two different philosophies.

4.1 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

$$\frac{k^2}{2} = \frac{\pi^2}{6} + 2\sum_{\ell=1}^{\infty} \frac{(-1)^\ell}{\ell^2} \cos(\ell k). \tag{31}$$

Applying (19) leads to a truncation of (31) at $\ell = N - 2$. It is clear that identifying $K_\ell^{[0]}$ 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 (criterion (26)). On the other hand, in the large resolution limit we should recover the exact kinetic energy, and as we have discussed above, this is equivalent to (27). Considering these arguments, we suggest the following truncation process

$$\alpha \mathcal{F}_\ell^N = \begin{cases} \frac{\pi^2}{6} & \text{for } \ell = 0, \\ \frac{(-1)^\ell}{\ell^2} & \text{for } 1 \le |\ell| \le N-3, \\ -\frac{1}{2}\left(\frac{\pi^2}{6} + 2\sum_{\ell=1}^{N-3} \frac{(-1)^\ell}{\ell^2}\right) & \text{for } |\ell| = N-2. \end{cases} \tag{32}$$

The definition $K_\ell^{[M]} = 2^{2M} \mathcal{F}_\ell^N$ automatically satisfies sum rule (26), whereas with an appropriate choice of the normalization factor α, (27) can also be fulfilled. The kinetic

Table 1 The error of the total energy $E_i^{[0]\mathcal{F}}$ and the wave function $\Phi_i^{[0]\mathcal{F}}$ 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

i	$\lvert E_i - E_i^{[0]}\rvert$	$\lvert E_i - E_i^{[0]\mathcal{F}}\rvert$	$\lVert \Psi_i - \Phi_i^{[0]}\rVert$	$\lVert \Psi_i - \Phi_i^{[0]\mathcal{F}}\rVert$
1	1.0802×10^{-4}	2.7721×10^{-4}	1.0392×10^{-2}	1.4545×10^{-2}
2	4.4247×10^{-4}	1.6186×10^{-3}	1.8878×10^{-2}	2.1309×10^{-2}
3	1.0681×10^{-3}	5.4125×10^{-3}	2.7654×10^{-2}	2.6331×10^{-2}
4	2.1982×10^{-3}	1.3550×10^{-2}	3.6618×10^{-2}	2.8380×10^{-2}
5	4.3310×10^{-3}	2.7925×10^{-2}	4.5968×10^{-2}	2.7997×10^{-2}

E_i and Ψ_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.

energy function $\varepsilon_{\mathcal{F}}^{[0]}(k)$ calculated according to (24) 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 Table 1; 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.

4.2 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 $K_\ell^{[M]}$. We suggest the following scheme for determining the optimal kinetic energy matrix. According to (18) 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

$$K_\ell^{[M]} = 2^{2M} \mathcal{T}_\ell^N(t) \tag{33}$$

with

$$\alpha \mathcal{T}_\ell^N(t) = \begin{cases} 1 & \text{for} \quad \ell = 0, \\ t & \text{for} \quad |\ell| = 1, \\ t_\ell(t) & \text{for} \quad 2 \le |\ell| \le N - 2. \end{cases} \tag{34}$$

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

$$\begin{pmatrix} 1 & 1 & \dots & 1 \\ 2^4 & 3^4 & \dots & (N-2)^4 \\ 2^6 & 3^6 & \dots & (N-2)^6 \\ \vdots & \vdots & \ddots & \vdots \\ 2^{2(N-3)} & 3^{2(N-3)} & \dots & (N-2)^{2(N-3)} \end{pmatrix} \begin{pmatrix} t_2 \\ t_3 \\ \vdots \\ t_{N-2} \end{pmatrix} = \begin{pmatrix} -1/2 - t \\ -t \\ \vdots \\ -t \end{pmatrix}. \quad (35)$$

The normalization factor

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

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 Eq. 35 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

$$V(x) = \begin{cases} 0 & \text{if } -L \le x < 0, \\ V_0 & \text{if } 0 \le x \le L, \\ W & \text{if } |x| > L, \end{cases} \quad (37)$$

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. Figure 3 shows the exact and the $M = 0$ level approximated wave function of the

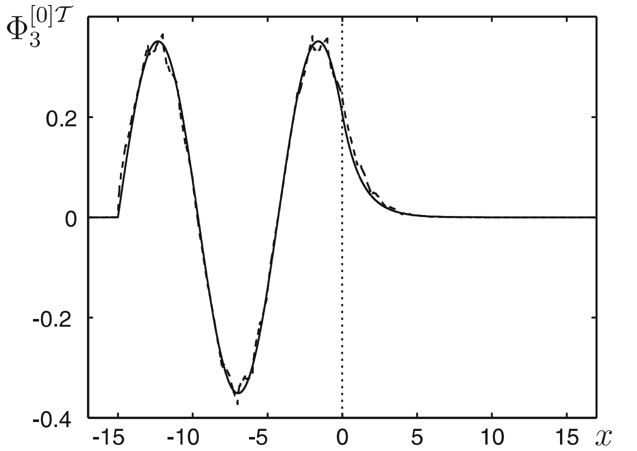

Fig. 3 Exact (solid line) and approximate (dashed line) wave functions Ψ_1 and $\Phi_1^{[0]\mathcal{T}}$ of the potential model (37), with $L = 15$ a.u., $W = 100$ a.u. and $V_0 = 0.5$ a.u., using the Daubechies-4 scaling function in the Taylor series method. Atomic units were applied

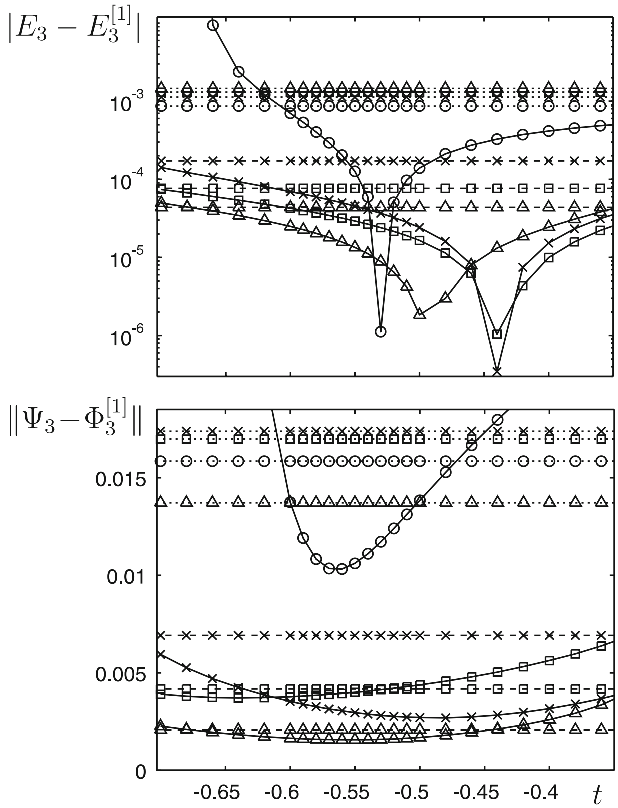

Fig. 4 The deviation of the approximate total energy $E_3^{[1]\mathcal{T}}$ and wave function $\Phi_3^{[1]\mathcal{T}}$ from their exact counterparts E_3 and Ψ_3 (solid lines) of the potential model (37), with $L = 17$ a.u., $W = 10$ a.u. and $V_0 = 0.01$ a.u., using the Taylor series method. As references, 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, $\times$, $\square$ and $\triangle$ mean Daubechies-6, Daubechies-8 and Daubechies-10 calculations, respectively. Atomic units were applied

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 (34)–(36) we have plotted the deviation of the approximate total energy from the exact one as a function of the parameter t in Fig. 4. Similarly, the norm of the difference of the exact and approximated wave function of 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.

Table 2 The recommended kinetic energy matrix parameter t for the Taylor series based construction (33)–(36) in case of Daubechies-N scaling function sets ($N = 4, 6, 8, 10$)

N	4	6	8	10
t	−0.54	−0.47	−0.57	−0.58

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 ± 0.06. Also, by playing around the 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

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

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 ω^{-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 Table 2 we summarize our recommendations for 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 ± 10 percent without a considerable change in the quality of the total energy and wave function approximations.

5 Optimal kinetic energy matrix in systematically refined wavelet subspaces

The main advantage of wavelet based calculations is that besides the scaling function basis set $\{s_{M\ell}\}$ of

$$\begin{aligned} \mathcal{H}^{[M]} &= \mathcal{H}^{[M-1]} \oplus \mathcal{W}^{[M-1]} && (39)\\ &= \mathcal{H}^{[M-2]} \oplus \mathcal{W}^{[M-2]} \oplus \mathcal{W}^{[M-1]} && (40)\\ &= \mathcal{H}^{[0]} \oplus \mathcal{W}^{[0]} \oplus \mathcal{W}^{[1]} \oplus \cdots \oplus \mathcal{W}^{[M-1]} && (41) \end{aligned}$$

equivalent sets like $\{s_{M-1\,\ell}, w_{M-1\,\ell}\}$ or $\{s_{M-2\,\ell}, w_{M-2\,\ell}, w_{M-1\,\ell}\}, \ldots,$ $\{s_{0\ell}, w_{0\ell}, \ldots, w_{M-1\,\ell}\}$ exist, where the wavelets of level m are defined by the mother wavelet $w(x)$ as

$$w_{m\ell}(x) = 2^{m/2} w(2^m x - \ell) \tag{42}$$

for any $m = 0, \ldots, M-1$. The wavelets are added only at those positions where the description of the wave function is not sufficiently precise [14]. The question arises, how an optimum kinetic energy matrix can be built for these systematic refinements of the basis set.

In the previous sections we have concentrated on the methods for replacing $\langle s_{Mj}|\hat{T}|s_{M\ell}\rangle$ type matrix elements. In the wavelet function basis sets there appear canonical matrix elements of type $\langle s_{m_0 j}|\hat{T}|w_{m_1\ell}\rangle$, $\langle w_{m_1 j}|\hat{T}|w_{m_2\ell}\rangle$, as well. In this section we will show that there exists a method for a systematic choice of optimal kinetic matrix elements in the wavelet basis, too.

The basis sets $\{s_{M\ell}\}$ and $\{s_{M-1\,\ell}, w_{M-1\,\ell}\}$ are connected by the unitary transformation

$$s_{M-1\,\ell}(x) = \sum_{j\in\mathbb{Z}} h_{j-2\ell}\, s_{Mj}(x), \tag{43}$$

$$w_{M-1\,\ell}(x) = \sum_{j\in\mathbb{Z}} g_{j-2\ell}\, s_{Mj}(x) \tag{44}$$

according to [9]. Here the constants h_k define the mother scaling function $s(x)$ by the refinement Eq. 43. The wavelets are generated from these values by applying $g_k = (-1)^k h^*_{-k+1}$. The expansion coefficients satisfy the orthonormality conditions

$$\sum_{k\in\mathbb{Z}} h^*_{k-2i}\, h_{k-2j} = \delta_{ij}, \tag{45}$$

$$\sum_{k\in\mathbb{Z}} g^*_{k-2i}\, g_{k-2j} = \delta_{ij}, \tag{46}$$

$$\sum_{k\in\mathbb{Z}} h^*_{k-2i}\, g_{k-2j} = 0. \tag{47}$$

We have already criteria (17)–(18) and (26)–(28) for building the matrix elements $K^{ss[M-1]}_{j\ell}$ among the scaling functions $s_{M-1\,j}$ and $s_{M-1\,\ell}$ which give better results than the canonical ones. The question arises, how to complete this matrix with the blocks $K^{sw[M-1]}_{j\ell}$, $K^{ws[M-1]}_{j\ell}$ and $K^{ww[M-1]}_{j\ell}$ in order to have an optimum description at resolution level M. The basic idea is that we will require the kinetic energy matrix $K^{ss[M]}_{j\ell}$ among scaling functions at level M to satisfy the criteria (17)–(18) and (26)–(28). As we have mentioned it previously, the application of the scaling property (30) is not obligatory, and we will not assume (30) in the following considerations. The matrices

$$\begin{pmatrix} K^{ss[M-1]} & K^{sw[M-1]} \\ K^{ws[M-1]} & K^{ww[M-1]} \end{pmatrix} \longleftrightarrow K^{ss[M]} \tag{48}$$

are connected by the unitary transformations (43), (44) as

$$K_{ij}^{ss[M-1]} = \sum_{k,\ell} h_{k-2i}^{*} h_{\ell-2j} K_{k\ell}^{ss[M]}, \tag{49}$$

$$K_{ij}^{sw[M-1]} = \sum_{k,\ell} h_{k-2i}^{*} g_{\ell-2j} K_{k\ell}^{ss[M]}, \tag{50}$$

$$K_{ij}^{ws[M-1]} = \sum_{k,\ell} g_{k-2i}^{*} h_{\ell-2j} K_{k\ell}^{ss[M]}, \tag{51}$$

$$K_{ij}^{ww[M-1]} = \sum_{k,\ell} g_{k-2i}^{*} g_{\ell-2j} K_{k\ell}^{ss[M]}, \tag{52}$$

and by its inverse transformation. Requiring shift invariance all matrix elements depend only on the difference of their indices (18). With simple index transformations one arrives at

$$K_{\ell}^{ss[M-1]} = \sum_{k,n} h_{k}^{*} h_{k-n+2\ell} K_{n}^{ss[M]}, \tag{53}$$

$$K_{\ell}^{sw[M-1]} = \sum_{k,n} h_{k}^{*} g_{k-n+2\ell} K_{n}^{ss[M]}, \tag{54}$$

$$K_{\ell}^{ws[M-1]} = \sum_{k,n} g_{k}^{*} h_{k-n+2\ell} K_{n}^{ss[M]}, \tag{55}$$

$$K_{\ell}^{ww[M-1]} = \sum_{k,n} g_{k}^{*} g_{k-n+2\ell} K_{n}^{ss[M]}. \tag{56}$$

At any level M the matrix $K^{[M]}$ can be decomposed as

$$K^{[M]} = 2^{2M} T^{[0]} + \Delta^{[M]}, \tag{57}$$

where $T^{[0]}$ is the canonical kinetic energy matrix and $\Delta^{[M]}$ is a correction, provided that the canonical representation exists. For $\Delta^{[M]} = 0$ Eqs. 53–56 lead to a system of eigenvalue equations for the variables $T_n^{[0]}$. These equations are satisfied by the canonical matrix elements according to [20]. All that remains is to find a set of correction matrix elements by replacing the $K^{[M]}$ submatrices in (53)–(56) with the corresponding elements of $\Delta^{[M]}$. We will not further assume any scaling property for $\Delta^{[M]}$ similar to (30) and we also drop limitation (19). We now apply a specific choice,

$$\Delta_n^{[M]} = \begin{cases} \Delta_{2j}^{[M]} & \text{if } n = 2j, \\ 0 & \text{if } n \text{ is odd.} \end{cases} \tag{58}$$

Substituting (58) in (53)–(56), in place of the $K_n^{[M]}$ matrix elements, and applying (45)–(47) we have

$$\Delta_\ell^{ss[M-1]} = \Delta_{2\ell}^{ss[M]}, \tag{59}$$
$$\Delta_\ell^{sw[M-1]} = 0, \tag{60}$$
$$\Delta_\ell^{ws[M-1]} = 0, \tag{61}$$
$$\Delta_\ell^{ww[M-1]} = \Delta_{2\ell}^{ss[M]}. \tag{62}$$

Considering this result, the following strategy for harmonizing the determination of the optimum kinetic energy matrix with an iterative refinement of resolution can be developed. As we have proved in Sect. 4.2 the requirement that the expansion of the function $\varepsilon(k)$ approximates the exact $k^2/2$ leads to a considerable advance of the results. This is equivalent with satisfying (26), (27) and as many (28) equations as possible.

At resolution level $M = 0$ we can either determine the independent kinetic energy matrix elements $K_\ell^{ss[0]}$, $(\ell = 0, \ldots, N-2)$ using the Taylor series method described above, or by separating $K_\ell^{ss[0]} = T_\ell^{ss[0]} + \Delta_\ell^{[0]}$ and substituting it into (26), (27) and the next $N-3$ pieces of Eq. 28, we can determine the set of corrections $\Delta_\ell^{[0]}$. (In fact, the number of $\Delta_\ell^{[0]}$ parameters is not restricted, however, it seems to be rather obvious to limit their number to $N-1$.) If a refinement step is necessary, we extend our basis set by introducing the $M = 0$ level wavelets $\{w_{0\ell}\}$. As this basis is equivalent to the set of the $M = 1$ level scaling functions $\{s_{1\ell}\}$, the correction to the canonical kinetic energy matrix is determined at this level by choosing $K_\ell^{ss[1]} = 2^2 T_\ell^{ss[0]} + \Delta_\ell^{[1]}$, where the correction set $\Delta_\ell^{[1]}$ is subject to the constraint $\Delta_{2\ell_0}^{[1]}$, $(\ell_0 = 0, \ldots, N-2)$. We allow corrections only at even indices ℓ in order to be able to apply (59)–(62). Solving the system of Eqs. 26–28, the resulting values $\Delta_{2\ell_0}^{[1]}$ are added as corrections to each off-diagonals in the scaling function-wavelet representation as $K_{\ell_0}^{ss[0]} = T_{\ell_0}^{ss[0]} + \Delta_{\ell_0}^{[0]}$ and $K_{\ell_0}^{ww[0]} = T_{\ell_0}^{ww[0]} + \Delta_{\ell_0}^{[0]}$. The mixed components remain uncorrected, $K_{\ell_0}^{sw[0]} = T_{\ell_0}^{sw[0]}$ and $K_{\ell_0}^{ws[0]} = T_{\ell_0}^{ws[0]}$.

By further refinements, adding additional levels of wavelets, the corrections are determined at the Mth scaling function level by choosing $K_\ell^{ss[M]} = 2^{2M} T_\ell^{ss[0]} + \Delta_\ell^{[M]}$ with the non-zero corrections $\Delta_{2^M\ell_0}^{[M]}$, $(\ell_0 = 0, \ldots, N-2)$. The solution of Eqs. 26–28 determines the correction values. The block structure of the kinetic energy matrix similar to (48) contains blocks belonging to the several wavelet levels, e.g., $K^{s_0s_0}$, $K^{w_0w_0}$, $K^{w_1w_1}$, …, $K^{w_{M-1}w_{M-1}}$, and $K^{s_0w_0}$, $K^{w_0w_1}$, etc. None of the mixed blocks, like $K^{s_0w_0}$, $K^{w_0w_1}$, need any correction. The diagonal block $K^{w_{M-1}w_{M-1}}$ is adjusted in every 2^{M-1}th off-diagonal by the values $\Delta^{[M]}$, the block $K^{w_1w_1}$ is corrected in every second off-diagonal by the same series of $\Delta^{[M]}$, while both $K^{s_0s_0}$ and $K^{w_0w_0}$

Table 3 Suggested $T^{[0]}$ matrix elements for the Daubechies-4 basis set

ℓ	-3	-2	-1	0	1	2	3
$\beta^{-1}T_\ell^{sw[0]}$	$-\frac{2-\sqrt{3}}{6}$	$\frac{2}{3}$	$-\frac{\sqrt{3}}{3}$	$-\frac{2}{3}$	$\frac{2+\sqrt{3}}{6}$		
$\beta^{-1}T_\ell^{ws[0]}$			$\frac{2+\sqrt{3}}{6}$	$-\frac{2}{3}$	$-\frac{\sqrt{3}}{3}$	$\frac{2}{3}$	$-\frac{2-\sqrt{3}}{6}$
$\beta^{-1}T_\ell^{ww[0]}$		$-\frac{1}{6}$	2	7	2	$-\frac{1}{6}$	

needs an addition of $\Delta^{[M]}$ to each off-diagonals. (Naturally, the diagonals have to be also modified by $\Delta_0^{[M]}$).

This procedure seems to extend the spatial range of the kinetic energy operator with increasing resolution. This argumentation is, however, misleading in two sense. In the algorithmic sense, the number of essential off-diagonals does not increase to infinity (a maximum factor of 2 is possible only). In the physical sense, on the other hand, the spatial range of the kinetic energy operator remains constant, considering, that the grid-length of the $w_{M\ell}(x)$ wavelets decreases as $\sim 2^{-M}$. Numerical calculations show, that the extension of resolution leads to an exponential decrease of the average magnitude of $\Delta_\ell^{[M]}$, indicating that the corrected kinetic energy matrix tends to the canonical one at the infinitely fine resolution limit.

In the above considerations we have supposed, that the canonical kinetic energy matrix elements do exist, which is, however, not satisfied for the Daubechies-4 basis set. This problem can be resolved by noticing that for the expansion coefficients $h_0 = (1+\sqrt{3})/(4\sqrt{2})$, $h_1 = (3+\sqrt{3})/(4\sqrt{2})$, $h_2 = (3-\sqrt{3})/(4\sqrt{2})$ and $h_3 = (1-\sqrt{3})/(4\sqrt{2})$ the set of "canonical" matrix elements

$$\begin{aligned} T_0^{ss[M]} &= \beta\, 2^{2M}, \\ T_{-1}^{ss[M]} &= T_1^{ss[M]} = -\beta\, 2^{2M}\frac{2}{3}, \\ T_{-2}^{ss[M]} &= T_2^{ss[M]} = \beta\, 2^{2M}\frac{1}{6} \end{aligned} \tag{63}$$

fulfills the transformation rule (53), and the wavelet blocks of the kinetic energy matrix are defined by (54)–(56) leading to the values listed in Table 3. Choosing the normalization parameter $\beta \approx 1.3$ reproduces the results from Sect. 4.2 acceptable. Of course, a correction $\Delta_\ell^{[M]}$ is necessary even in the $M = 0$ case, as the values (63) alone do not satisfy Eq. 27. The calculation of the correction values is similar to the procedure described above.

6 Summary

Studying exactly solvable models in the framework of MRA 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

Table 4 The recommended kinetic energy matrix elements for the Taylor series based construction in case of Daubechies-N scaling function sets

	$N = 4$	$N = 6$	$N = 8$	$N = 10$
$\mathcal{T}_0^N$	1.3157894737	1.0269360269	1.4668325041	1.5177613012
$\mathcal{T}_1^N$	−0.7105263158	−0.4826599327	−0.8360945274	−0.8803015547
$\mathcal{T}_2^N$	0.0526315789	−0.0586700337	0.1207733653	0.1495444216
$\mathcal{T}_3^N$		0.0326358826	−0.0206082682	−0.0344316374
$\mathcal{T}_4^N$		0.0047739298	0.0027102582	0.0074722170
$\mathcal{T}_5^N$			−0.0002005664	−0.0013201227
$\mathcal{T}_6^N$			0.0000034864	0.0001689233
$\mathcal{T}_7^N$				−0.0000133612
$\mathcal{T}_8^N$				0.0000004634

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.

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 2π-periodic approximation $\varepsilon_{\text{can}}^{[M]}(k)$. 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. 4. 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 Table 2. At an arbitrary resolution level M the kinetic energy matrix elements are calculated as

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

where N determines the number of essential matrix elements, as $\mathcal{T}_{|j-\ell|}^N = 0$ if $|j-\ell| > N-2$. Table 4 lists the values of $\mathcal{T}_\ell^N$ for various Daubechies-N scaling function sets.

The Taylor series approach can be extended to the cases where the basis set starts with scaling functions given on a relatively coarse grid, and consecutive refinements are added by wavelets of finer resolutions. We have given an explicit method for calculating corrected kinetic matrix elements. At the infinite resolution limit, the corrected matrix elements converge to the canonical ones.

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. In the general form, this procedure is well suited to adaptive refinement algorithms.

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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

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

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

$$\sum_{\ell\in\mathbb{Z}} \ell^2 T_\ell^{[M]} = -2^{2M} \tag{A3}$$

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 [9,10], consequently, for any x

$$\sum_{\ell\in\mathbb{Z}} c_\ell^{[M]} s_{M\ell}(x) = 1 \tag{A4}$$

with the expansion coefficients $c_\ell^{[M]} = 2^{-M/2}$. Differentiating, multiplying by $s'_{M0}(x)/2$ and integrating one gets

$$\sum_{\ell\in\mathbb{Z}} \frac{1}{2}\int s'_{M0}(x)s'_{M\ell}(x)dx = \sum_{\ell\in\mathbb{Z}} T_\ell^{[M]} = 0. \tag{A5}$$

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

$$\sum_{\ell\in\mathbb{Z}} c_\ell^{[M]} s_{M\ell}(x) = x \tag{A6}$$

with the appropriate expansion coefficients

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

where we have applied definition (3), a proper integral variable transformation, and the fact that $\int s(y)dy = 1$ [9]. The quantity $\mu_1 = \int ys(y)dy$ is the first momentum of the mother scaling function. Differentiating (A6), multiplying by $s'_{M0}(x)/2$ and integrating we arrive at

$$\begin{aligned}\sum_{\ell\in\mathbb{Z}} c_\ell^{[M]} \frac{1}{2} \int s'_{M0}(x)s'_{M\ell}(x)dx &= \sum_{\ell\in\mathbb{Z}} c_\ell^{[M]} T_\ell^{[M]} \\ = \frac{1}{2}\int s'_{M0}(x)dx &= \frac{1}{2}\left[s_{M0}(x)\right]_{-\infty}^{\infty}.\end{aligned} \tag{A8}$$

As the scaling functions are square integrable, $s_{M0}(\pm\infty) = 0$, and

$$\begin{aligned}0 &= \sum_{\ell\in\mathbb{Z}} c_\ell^{[M]} T_\ell^{[M]} \\ &= 2^{-3M/2}\mu_1 \sum_{\ell\in\mathbb{Z}} T_\ell^{[M]} + 2^{-3M/2} \sum_{\ell\in\mathbb{Z}} \ell\, T_\ell^{[M]}.\end{aligned} \tag{A9}$$

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.

$$\sum_{\ell\in\mathbb{Z}} c_\ell^{[M]} s_{M\ell}(x) = x^2 \tag{A10}$$

where the expansion coefficients are

$$c_\ell^{[M]} = \int x^2 s_{M\ell}(x)dx = 2^{-5M/2}(\mu_2 + 2\ell\mu_1 + \ell^2), \tag{A11}$$

after similar steps applied in the previous proof. The notation $\int y^2 s(y)dy = \mu_2$ was introduced. Differentiating (A10) leads to

$$\begin{aligned}\sum_{\ell\in\mathbb{Z}} c_\ell^{[M]} T_\ell^{[M]} &= \int x\, s'_{M0}(x)dx \\ &= -\int s_{M0}(x)dx = -2^{-M/2}.\end{aligned} \tag{A12}$$

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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