An application of interpolating scaling functions to wave packet propagation

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Abstract

Wave packet propagation in the basis of interpolating scaling functions (ISF) is studied. The ISF are well known in the multiresolution analysis based on spline biorthogonal wavelets. The ISF form a cardinal basis set corresponding to an equidistantly spaced grid. They have compact support of the size determined by the order of the underlying interpolating polynomial that is used to generate ISF. In this basis the potential energy matrix is diagonal and the kinetic energy matrix is sparse and, in the 1D case, has a band-diagonal structure. An important feature of the basis is that matrix elements of a Hamiltonian are exactly computed by means of simple algebraic transformations efficiently implemented numerically. Therefore the number of grid points and the order of the underlying interpolating polynomial can easily be varied allowing one to approach the accuracy of pseudospectral methods in a regular manner, similar to high order finite difference methods. The results of numerical simulation of a H+H₂ collinear collision show that the ISF provide one with an accurate and efficient representation for use in the wave packet propagation method.

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1 Introduction

A direct on-the-grid solution of the time-dependent Schrödinger equation (TDSE) has become a common tool in quantum chemistry. In a dynamical context, it provides with quantitative predictions on the efficiency of different pathways of chemical reactions and deepens our understanding of their details [1, 2, 3]. Approaches based on the TDSE in connection with the filter diagonalization technique [4] are also used in the static context in order to compute states of complex molecules [5, 6]. To simulate the time evolution of a wave packet, repeated computations of the action of the system Hamiltonian $H$, or its exponential $\exp(-i\Delta t H)$, on the wave function $\Psi$ are required. Here $\Delta t$ is a time step. Therefore a lot of effort has been devoted to developing accurate and efficient methods to reduce computational costs of computing $H\Psi$. The numerical techniques used can be classified into several categories: (i) finite differences (FD), (ii) finite elements (FE), (iii) pseudospectral global grid representation approaches such as the discrete variable representation (DVR) and Fourier grid Hamiltonian method (FGH) [7, 8, 9, 10, 11]. Finite differences and finite elements lead to a sparse Hamiltonian matrix but exhibit a slow algebraic convergence with the number of grid points. The pseudospectral approaches result in dense Hamiltonian matrices, which, a priori, increases the number of operations needed to compute $H\Psi$. At the same time, the exponential convergence with the number of grid points counterbalances the aforementioned drawback. This is why pseudospectral methods are so widely used in time-dependent molecular dynamics [1, 2, 3, 12], as well as in stationary S-matrix [13, 14, 15] and eigenvalue [6] calculations. In particular, the FGH method based on the fast Fourier transform (FFT) algorithm is very advantageous since for a mesh of $N$ points the action of the kinetic energy operator is computed by $N \log_2 N$ elementary multiplications and is easily implemented numerically [16].

When discussing the slow algebraic convergence of finite differences and finite elements, one usually refers to the convergence with the number of grid points while the order of finite differences or the order of the polynomial for finite elements is kept fixed. In fact, an exponential (spectral) convergence can be achieved if not only the number of grid points, but also the order of the underlying polynomial is increased [7, 17]. Exploiting this property, as well as the sparsity of the Hamiltonian matrix and the possibility to distribute mesh points only along the reaction path, thus reducing the size of calculation, makes the high order FD and FE a competitive alternative to pseudospectral methods. Much work has recently been devoted to developing these techniques [18, 19, 20, 21, 22, 23, 24, 25].

In this paper we present a treatment of reactive scattering based on the wave function representation in the basis of interpolating scaling functions corresponding to interpolating (spline) wavelets [28]. Basis functions are generated from a single function, called the scaling function, by appropriate scalings and shifts of its argument. The scaling function is a solution of a functional equation which is found iteratively by using interpolating polynomials of a specific order. By construction, the basis functions have compact support with the width determined by the order of the interpolating polynomial and the resolution level (the mesh
The basis is biorthogonal and cardinal, which leads to a simple representation of the wave function. The resulting Hamiltonian matrix is sparse. The potential energy matrix appears to be diagonal, while, in the one-dimensional case, the kinetic energy matrix is band diagonal with the band width determined by the size of support of the scaling function. Matrix elements of the kinetic energy operator can be evaluated exactly via simple algebraic operations so that the order of the underlying interpolating polynomial and the step of the mesh can easily be varied allowing one to achieve a fast convergence. Thus our algorithm offers flexibility similar to that achieved in the case of finite differences of an arbitrary order with the Fornberg algorithm [7, 26]. In fact, the proposed approach can be seen as an alternative to high-order finite difference techniques. Applications of the method are illustrated with the example of a collinear H+H₂ collision.

2 Theory

2.1 Biorthogonal spline bases

Here we summarize some necessary facts about interpolating biorthogonal bases of scaling functions in the space of square integrable functions and describe the algorithm to construct such bases. Biorthonormal bases of scaling functions are used in the multiresolution analysis associated with interpolating wavelets. A more detailed description of such bases can be found in the mathematical literature, e.g., [27, 28, 29].

In general, a biorthogonal basis consists of two sets of elements \( \phi_a(x) \) and \( \tilde{\phi}_a(x) \) where the index \( a \) labels the basis elements. Any function \( \Psi(x) \) can be decomposed into a linear combination of the basis functions \( \phi_a(x) \),

\[
\Psi(x) = \sum_a s_a \phi_a(x),
\]

where the decomposition coefficients are determined by the dual basis functions

\[
s_a = \int dx \tilde{\phi}_a(x) \Psi(x).
\]

The basis is (bi)orthogonal in the sense that

\[
\int dx \tilde{\phi}_a(x) \phi_b(x) = \delta_{ab}.
\]

Consider a special class of biorthogonal bases that provide a multiresolution analysis. A biorthogonal basis with a multiresolution analysis is generated by a scaling function \( \phi(x) \) and its dual \( \tilde{\phi}(x) \) which satisfy accordingly the equations (the scaling relations)

\[
\phi(x) = 2 \sum_k h_k \phi(2x - k),
\]

\[
\tilde{\phi}(x) = 2 \sum_k \tilde{h}_k \tilde{\phi}(2x - k),
\]

\[
\int dx \tilde{\phi}_a(x) \phi_b(x) = \delta_{ab}.
\]
where the real coefficients $h_k (\tilde{h}_k)$ are called a (dual) filter. The scaling function and its dual are required to be orthogonal in the sense that
\[ \int dx \, \tilde{\phi}(x) \phi(x - j) = \delta_{0j} \] (6)
for all integers $j$. The orthogonality relation imposes a condition on the filters which is readily deduced from (6) by substituting the scaling relations (11) and (5) are rescaling the integration variable.

Consider two sets of functions, labeled by two integers $n$ and $j$,
\[ \phi_{n,j}(x) = 2^{n/2} \phi(2^n x - j), \quad \tilde{\phi}_{n,j}(x) = 2^{n/2} \tilde{\phi}(2^n x - j). \] (7)
Subspaces $V_n$ of the space of square integrable functions spanned by $\phi_{n,j}$ with a fixed value of $n$ form a ladder structure
\[ \cdots \subseteq V_n \subseteq V_{n+1} \subseteq \cdots . \] (8)
It is straightforward to convince oneself that $\phi_{n,j}$ form a biorthogonal basis in $V_n$:
\[ \int dx \, \tilde{\phi}_{n,j}(x) \phi_{n,j'}(x) = \delta_{jj'} . \] (9)
Any function $\Psi$ can be projected on a subspace $V_n$,
\[ P_n : \Psi(x) \rightarrow \Psi_n(x) = \sum_j s_{n,j} \phi_{n,j}(x) , \quad s_{n,j} = \int dx \, \tilde{\phi}_{n,j}(x) \Psi(x) . \] (10)
Taking successively larger values of $n$ allows one to reproduce a successively finer structure of $\Psi$. Thus, the index $n$ specifies a resolution level. If the filters are finite, then the scaling function $\phi$ has finite support and so do the basis functions $\phi_{n,j}$. The index $j$ is then naturally associated with the position of support of $\phi_{n,j}$.

A special class of biorthogonal bases is obtained when filters are finite and of a special form
\[ h_k = \frac{1}{2} \phi(k/2) , \quad k = 0, \pm 1, \pm 2, \ldots, \pm m , \] (11)
\[ \tilde{h}_k = \delta_{k0} , \quad \tilde{\phi}(x) = \delta(x) . \] (12)
The expansion coefficients are simply values of the function at dyadic lattice sites
\[ s_{n,j} = 2^{-n/2} \Psi(2^{-n} j) . \] (13)
Larger values of the resolution level $n$ correspond to finer grids. In what follows $m$ is chosen to be odd for convenience.

To find the filter $h_k$ and an explicit form of the scaling function $\phi(x)$, Eq. (11) is solved iteratively for $\phi(x)$. First, one observes that the equation is satisfied at the integer valued
argument by \( \phi(l) = \delta_{0l} \) with \( h_0 = \frac{1}{2} \). Thus, the scaling function vanishes at integral \( x \) except for \( x = 0 \) where \( \phi(0) = 1 \) as is required by the orthogonality condition (10) with our choice of the filters (11) and (12). To compute \( \phi(x) \) at half-integer values of the argument, \( \phi(j + 1/2) \) \( (j \) is a fixed integer), one uses the polynomial (spline) interpolation with polynomials \( P_m^{(j)} \) of order \( m \) passing through \( M = (m + 1)/2 \) integer points neighboring to \( x = j + 1/2 \) to the left and \( M \) integer points to the right: \( x = j - M + 1, j - M + 2, \ldots, j + M \). Having found such a polynomial, we set \( \phi(j + 1/2) = P_m^{(j)}(j + 1/2) \). Note that for different points \( x = j + 1/2 \), polynomials \( P_m^{(j)} \) are different. To find \( \phi(j \pm 1/4) \), the same procedure is applied, but now the values of \( \phi \) at \( M \) half-integer points neighboring to \( x = j \pm 1/4 \) to the left and \( M \) half-integer points to the right are used to construct the corresponding interpolating polynomial. For example, for \( x = j + 1/4 \) the sequence will be: \( x = j - (M - 1)/2, j - (M - 2)/2, \ldots, j + M/2 \). In other words, any \( x \) can be squeezed into successively smaller intervals of length \( 1/2, 1/4, \ldots, 1/2^N, N \to \infty \). The limiting procedure allows one to compute \( \phi(x) \) at any \( x \), in principle.

An important property of \( \phi(x) \) is that it has compact support, an interval of width \( D = 2m \), that is, \( \phi(x) = 0 \) for all \( |x| \geq m \) as can be inferred from the construction procedure described above.

In Fig. 1 we show an example of the scaling function \( \phi(x) \equiv \phi_{0,0}(x) \) where \( \phi_{0,0}(x) \) is the basis function centered at position \( x = 0 \) and corresponding to the zero resolution level (the mesh mesh equals 1). The length of the filter is \( m = 15 \) so that support of the scaling function is the interval \(-15 \leq x \leq 15\).

### 2.2 Hamiltonian matrix

Consider first a simple 1D example. Let \( H \) be a Hamiltonian of a system in the coordinate representation. A solution of the Schrödinger equation \( i \partial / \partial t \ \Psi(x, t) = H \Psi(x, t) \) for a given initial wave packet \( \Psi(x, t = 0) \) is approximated by its projection into a finite dimensional subspace spanned by \( \phi_{n,j} \) where \( j \) enumerates basis functions whose support lies in a box, \( x \in [0, L] \), that is, \( \Psi(x, t) = \sum_j s_{n,j}(t) \phi_{n,j}(x) \). Each basis function \( \phi_{n,j} \) has support of the length \( D_n = 2m/2^n \). Therefore the number of the basis functions \( N \) is given by: \( N = 2^n L/2m \). Our choice of the basis implies also zero boundary conditions for the wave function. The initial wave packet \( \Psi(x, t = 0) \) is projected into the corresponding subspace of \( V_n \) according to (10) to determine \( s_{n,j}(0) \). The Hamiltonian is projected by the rule \( H \to P_n H P_n \) and becomes a finite matrix with elements

\[
H_{k,j}^{(n)} = \int dx \phi_{n,k}(x) H \phi_{n,j}(x). \tag{14}
\]

The Hamiltonian matrix acts in a vector space of the expansion coefficient \( s_{n,j}(t) \). Solving the time dependent Schrödinger equation thus implies computing \( s_n(t) = \exp(-i t H^{(n)}) s_n(0) \), where \( s_n \) is regarded as a vector with components \( s_{n,j} \) and \( H^{(n)} \) as a matrix with elements given in (14).
A typical Hamiltonian is a sum of kinetic and potential energies. For matrix elements of the potential energy $V$ we have

$$V_{k,j}^{(n)} = \int dx \tilde{\phi}_{n,j}(x)V(x)\phi_{n,j}(x) = V(2^{-n}j)\delta_{kj}.$$  

(15)

This is a great advantage of the basis under consideration: The potential energy matrix is diagonal. To compute the kinetic energy matrix we apply a general procedure to compute derivative operators $d^l/dx^l$ in a basis of compactly supported (spline) wavelets [30]. By rescaling the integration variable, and using Eqs. (7) and (12) one can find

$$D_{k,j}^{(n,l)} = \int dx \tilde{\phi}_{n,k}(x)(d/dx)^l\phi_{n,j}(x) = 2^{nl}\int dx \tilde{\phi}(x)(d/dx)^l\phi(x-k+j) = 2^{nl}(d/dx)^l\phi(x-k+j)|_{x=0} \equiv 2^{nl}D_{j-k}^{(l)}.$$  

(16)

Using the scaling relation for the scaling function (4) we infer

$$D_{i}^{(l)} = 2^{l+1}\sum_{k}D_{2^{l-k}}^{(l)}h_{k} \equiv \sum_{j}A_{i,j}^{(l)}D_{j}^{(l)},$$  

(17)

$$A_{i,j}^{(l)} = 2^{l+1}h_{2^{l-j}} = 2^{l}\phi(i-j/2).$$  

(18)

Thus, $D^{(l)}$ is an eigenvector of the matrix $A^{(l)}$ corresponding to the eigenvalue 1.

Finally, we need a normalization of the vector $D^{(l)}$. Note that, since the value of $\phi$ at any $x$ is given by a polynomial of order $m$, the monomial $x^l$, $l \leq m$, should be a linear combination of $\phi_{0,j}(x) = \phi(x-j)$, that is, $x^l = \sum_{j} s_{0,j} \phi_{0,j}(x)$ with $s_{0,j} = j^l$. Differentiating this relation $l$ times, multiplying by $\tilde{\phi}(x)$ and integrating over $x$ we obtain the normalization relation

$$l! = \sum_{j} j!D_{j}^{(l)}.$$  

(19)

The matrix $D^{(n,l)}$ satisfies the symmetry relation $D_{k,j}^{(n,l)} = (-1)^lD_{j,k}^{(n,l)}$, which follows from (16) after changing the integration variable $x \rightarrow -x$ and making use of $\phi(x) = \phi(-x)$ (the same for the dual). In particular, $D^{(n,2)}$ is a symmetric matrix. Since support of $\phi(x)$ lies within $|x| \leq m$, the $D^{(n,l)}$ matrix is band diagonal: $D_{k,j}^{(n,l)} = 0$, if $|k-j| > m$ as follows from Eq. (16). Therefore the action of the Hamiltonian of the system $H^{(n)} = -\frac{1}{2}D^{(n,2)} + V^{(n)}$ on the wave function $s_n$ requires $N \times 2m$ elementary multiplications. The above approach allows easy and fast evaluation of the Hamiltonian matrix for any desirable resolution level $n$ (any number of the basis functions) and any length of the filter $m$ (any interpolating polynomial order).

A multidimensional generalization is obtained by taking the direct product of $\phi_{n,j}$ for every independent variable $x_i$. The resolution level $n_i$ may be chosen independently for every variable $x_i$. For example, in the two dimensional case, the basis consists of functions $\phi_{n_1,j_1}(x_1)\phi_{n_2,j_2}(x_2)$. The spline order $m$ may also be chosen independently for every coordinate. In other words, the scaling functions for each $x_i$ may be different.
3 Numerical results

3.1 Harmonic oscillator example

In Fig. 2 we show the results of a test calculation of 30 first eigenvalues of a 1D harmonic oscillator, $H = -\frac{1}{2} \frac{d^2}{dx^2} + \frac{x^2}{2}$. We use a mesh in the interval $-L \leq x \leq L$ with $L = 10 \ a_0$ where $a_0$ is the Bohr radius. The Hamiltonian matrix in the basis of interpolating scaling functions $\phi_{n,j}(x)$ has been calculated according to the procedure described in the previous section and diagonalized yielding the eigenstate energies. The results of the present approach are compared with those obtained by the Fourier Grid Hamiltonian (FGH) approach. In the FGH method, the convergence is reached with 80 points of the grid and the error of the eigenvalue calculation is basically determined by the precision of the diagonalization procedure. In the ISF basis and low order $m$, convergence with the number of basis functions $N (N = 2^n \times 2L$, where $n$ is the resolution level) is slow. At the same time the convergence can dramatically be improved by increasing the order $m$ of the interpolating polynomial, i.e. by increasing the band width of the band-diagonal kinetic energy matrix. This observation is in line with the results reported by several authors for finite differences and finite elements where it has been shown that the pseudospectral convergence can be reached by increasing the order of finite differences or the order of an underlying polynomial in finite elements [1] [7] [8] [9] [25]. Thanks to the biorthogonality of the basis in our case, increasing the order $m$ and the resolution level $n$ is a quite simple procedure given by Eqs. (15)–(19) which is easy to implement numerically.

In the case of the harmonic oscillator the FGH method outperforms the ISF method. The latter, as well as finite difference methods, might compete with pseudospectral approaches for calculations involving complex reaction paths. Indeed, the FGH method, for example, generally uses hypercubic grid domains. In the present approach the calculation volume can sufficiently be reduced by the choice of the basis functions $\phi_{n,j}$ whose support lies in the vicinity of the reaction path, which is again a simple procedure because of the biorthogonality of the basis. We now turn to one such example.

3.2 $\text{H}+\text{H}_2(v = 0)$ collinear collision

Here we present a wave packet propagation treatment of an H+H$_2$ collision in collinear geometry with the energy of the collisional Hydrogen atom between 0.2 $eV$ and 1.1 $eV$. The system is described by Jacobi coordinates $r_{1,2}$ with $r_1$ being the distance between the two Hydrogen atoms in the molecule and $r_2$ being the distance of the collisional Hydrogen atom from the molecular center of mass. We use the Lanczos method [31] [32] to solve the time dependent Schrödinger equation (atomic units are used)

$$i \frac{\partial}{\partial t} \Psi(r_1, r_2; t) = \left( -\frac{1}{2m_H} \left[ 2 \frac{\partial^2}{\partial r_1^2} + 3 \frac{\partial^2}{\partial r_2^2} \right] + V(r_1, r_2) \right) \Psi(r_1, r_2; t) , \quad (20)$$
where $m_H$ is the mass of the Hydrogen atom. The interaction potential $V(r_1, r_2)$ is taken from [33]. A typical size of the mesh is $32 \times 32 \ a_0$. An absorbing potential [34, 35] is introduced at the grid boundaries for large $r_1$ and $r_2$ to avoid interference of the simulated wave packet with its reflection from the grid boundary. The initial state corresponds to the $\text{H}_2$ molecule in the $v = 0$ vibrational state and an impinging Gaussian wave packet in the reaction channel ($r_2$).

In the FGH method, convergent results are obtained with 192 points in the $r_1$ coordinate and 256 points in the $r_2$ coordinate. Two types of calculation have been performed by the ISF method. The first one corresponds to a rectangular grid where the basis functions are chosen as $\Phi_{n,j_1,j_2} = \phi_{n,j_1}(r_1) \phi_{n,j_2}(r_2)$. The resolution level $n = 4$ has been used, which corresponds to the mesh step $1/2^4 = 0.0625 \ a_0$ so that in total there are $360 \times 512$ basis functions. The order of the underlying interpolating polynomial (size of the filter) has been set to $m = 21$. In the second simulation the ISF basis has been chosen in such a way that the basis functions have support in the potential energy valley inside the 4.6 eV potential energy level curve as shown in Fig. 3. In this case only 48600 basis functions are needed. As a result, the computational time has been reduced by 3.8 times, which brings it to the level comparable to the FGH treatment. Results are presented in Fig. 4. We find that with our choice of the basis both simulations based on the interpolating scaling functions yield the total reaction probability $R$ which nicely agrees with the FGH method. The absolute difference $\left| \frac{R_{\text{ISF}} - R_{\text{FGH}}}{R_{\text{FGH}}} \right|$ is better than 0.1%.

4 Conclusions

We have shown that the wave function representation in bases of interpolating scaling functions can efficiently be used in wave packet propagation studies of molecular dynamics. The ISF originate from a multiresolution analysis associated with interpolating (spline) wavelets [27, 28, 29]. The ISF have a finite support whose width is determined by the order of the underlying interpolating polynomial and the resolution level (the mesh step). The basis is cardinal, which leads to a simple representation of the wave function. The resulting Hamiltonian matrix is sparse. In particular, the potential energy matrix is diagonal, while for the kinetic energy matrix there is an efficient and simple algebraic procedure for its exact computation so that the order of the underlying interpolating polynomial and the mesh step can easily be varied to achieve fast convergence. Thus, our algorithm provides one with flexibility similar to that achieved in the case of finite differences of an arbitrary order by, e.g., the Fornberg algorithm [7, 26]. In the 1D case the kinetic energy matrix has a band diagonal structure with the width of the band of off-diagonal elements given by the size of support of the scaling function. In our example of a collinear $\text{H} + \text{H}_2$ collision, a considerable reduction of computational costs has been reached when the basis functions are chosen in such a way that their support is localized only in the vicinity of the reaction path. The very possibility of the latter procedure and the simplicity of its numerical implementation, thanks
to the biorthogonality of the basis, is a general feature of the method proposed which can be used in simulations of systems with more complex reaction paths to reduce computational costs.

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**Figure captions**

Fig. 1. Scaling function $\phi(x)$ for the filter length $m = 15$.

Fig. 2 A 1D harmonic oscillator problem. A relative error in the eigenvalue calculation as a function of the oscillator quantum number. Lines: The FGH method with different numbers $N$ of mesh points; the gray line is for $N = 40$, the dashed line for $N = 80$, and the black line for $N = 160$. Symbols and lines with symbols: The ISF method. Circles show the results obtained with $n = 2$ resolution level corresponding to the $N = 80$ scaling functions basis ($N = 80$ points of the mesh). Triangles show the results obtained with $n = 3$ resolution level corresponding to the $N = 160$ scaling functions basis ($N = 160$ points of the mesh). Gray solid symbols: Results obtained with the filter length $m = 7$ (the interpolating polynomial order); open symbols: Results obtained with the filter length $m = 15$; black solid symbols: Results obtained with the filter length $m = 21$. The line with black solid symbols: results obtained with the filter length $m = 41$.

Fig. 3 A schematic representation of the arrangement of of the mesh (positions of the basis functions) in the wave packet propagation treatment of a collinear H-H$_2$ collision.

Fig. 4. Reaction probability calculated by different methods for the H+H$_2(v = 0)$ collinear collision as a function of energy. Solid line: Fourier Grid Hamiltonian method; Open circles: Results obtained by ISF method in the rectangular mesh; Triangles: Results obtained by the ISF method in the mesh arranged along the reaction coordinate (path) as depicted in Fig. 3.

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