Numerical solution of eigenvalue problems by means of a wavelet-based Lanczos decomposition

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Abstract

The simple Lanczos process is very efficient for finding a few extreme eigenvalues of a large symmetric matrix. The main task in each iteration step consists in evaluating a matrix-vector product. It is shown in this paper how to apply a fast wavelet-based product in order to speed up computations. Some numerical results are given for three different monodimensional cases: the Harmonic Oscillator case, the hydrogenlike atoms and a problem with a pseudo-double well potential.

1 Introduction

For many applications in Quantum Chemistry, a few smallest eigenvalues of a large matrix are requested (e.g. first excited states above the ground state of a chemical system) [1, 2, 3]. In these cases, the direct methods, as Givens or Householder methods, which employ explicit similarity transformations on the matrix are useless and iterative methods, as the Conjugate Gradient or the Lanczos algorithm, are more efficient [4]. The only way the matrix enters these latter agorithms is through a matrix-vector product. It is then strongly recommended to exploit sparseness and compact storage in the coding of the program.
The method described in this paper is based on the wavelet transform which provides sparse representations of many operators. This transform consists in expanding a given function or an operator over a set of basis functions obtained by dilations and translations of an elementary function, called the mother wavelet, localized in both direct and Fourier spaces [5]. Wavelet decompositions, well known for providing several advantages in the representation of many operators, seem to be particularly suitable to iterative algorithms.
Few results concerning the Conjugate Gradient have already been published [6, 7], and we want to present in this paper an application of wavelets decomposition in a Lanczos computation. In the worst case, without any assumption on the data, the

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wavelet decomposition lead to an algorithm of $O(N)$ instead of $O(N^2)$ for usual methods (these orders correspond to the cost of the matrix-vector product required in the iterative algorithms). One of the main advantages of the wavelet methods is that the wavelets adapt themselves automatically in the sense that only few coefficients are needed to describe smooth data and more coefficients are needed for the singular points. So wavelet-based methods lead in general to computations whose cost is less than N.
Operators written as,

$$Hf(x) = Tf(x) + Vf(x) \tag{1}$$

where T denotes the kinetic term and V the potential term are considered in this paper. Three problems are particularly studied:

- the computation of the first ten eigenvalues of the simple Harmonic Oscillator,

$$Tf(x) + Vf(x) = -\frac{\Delta f(x)}{2} + \frac{x}{2} f(x), \tag{2}$$

- the computation of the ground state of the radial Schrödinger operator for the hydrogen atom,

$$Tf(x) + Vf(x) = -\frac{\Delta f(x)}{2} - \frac{f(x)}{\mid x \mid}, \tag{3}$$

- the computation of the fifth excited state of an operator with a pseudo-double well potential,

$$Tf(x) + Vf(x) = -\frac{\Delta f(x)}{2} - \frac{f(x)}{\sqrt{(x-1/2)^2 + a^2}} - \frac{f(x)}{\sqrt{(x+1/2)^2 + a^2}}, a = 0.01. \tag{4}$$

This last case has been initially chosen by J. Modisette [8] in order to show the capability of wavelets to separate close eigenvalues (the fifth eigenvalue of this operator is very close to the sixth one) for this problem.
We refer to T. Arias for a general review of the application of wavelet theory to the determination of electronic structure [9]. Theoretically, "multiresolution analysis provides the first practical possibility for a unified, systematic treatment of core and valence behavior in the electronic structure of molecular and condensed-matter systems" (quoting T.A. Arias [9]).

2 A review on wavelets

In Quantum Chemistry, equations and quantities are usually expressed with position coordinates, **r**, where electrons are referenced by the components of their position in the three-dimensional configuration space. Any classical physical quantity can be

defined from pairs of canonically conjugated variables from which the corresponding quantum mechanical hamiltonian can be constructed [10]. Since momentum, $\mathbf{p}$ is canonically conjugated to $\mathbf{r}$, an alternative representation can be obtained using momentum coordinates where electrons are referenced by the components of their momentum in the three-dimensional momentum space. The momentum representation is obtained by means of a Fourier Transform. It allows to obtain momentum densities and as such yields a direct interpretation of experimental results such as Compton profiles [11] and cross section from (e,2e) spectroscopy [12].
However in this representation, one cannot directly describe local properties, such as singularities, from spectral properties.
Therefore the possibility of a simultaneous visualization of position and momentum densities seems a necessary improvement to apprehend better chemical structures. Some investigations in signal or image analyses have led scientists to switch from Fourier analysis to some more specific algorithms better suited to analyse abrupt changes in signals whenever tricky interactions between events occuring at different scales appear. Among these new methods, the wavelet transform allows to keep advantages from position and momentum representations thanks to the visualization of wave functions in both spaces. The building block functions of the Fourier analysis, which depend only on a momentum parameter, are replaced by wavelets, the building block functions of the wavelet analysis, which depend on both position and momentum parameters.

2.1 Continuous wavelets

Since all the results presented in the sequel are one dimensional, only 1D wavelets theory is introduced in this part. The generalization to higher dimension is relatively easy and is based on tensor products of basis functions.
Functions depending on two variables a and b respectively linked to momentum and position are used to define the mathematical transformation:

$$d_b^a = \int dx\, f(x)\, \psi_{a,b}(x), \tag{5}$$

where $\psi_{a,b}(x)$ play the same part than the exponential functions in the Fourier transform. A possibility is to construct $\{\psi_{a,b}(x)\}_{a,b}$ from a function $g(x)$ by translating and modulating it:

$$\psi_{a,b}(x) = g(x-b)\, e^{iax}, a, b \in \mathbb{R} \tag{6}$$

where $g(x)$ is a window function. In spite of the improvement brought by this "pseudo-spectral" representation, this transformation is not perfect and in particular it is not adapted to describe accurately functions which exhibit high variations. This kind of phenomenon is generally very localized in space whereas low variations often spread over a large area. To overcome this disadvantage (a fixed size window function), analysing functions with position support widths adapted to their momentum need obviously to be defined.

The idea is to apply dilations on top of translations previously introduced. Starting with a function ψ well localized in position and momentum spaces, a family of analysing functions can be constructed:

$$\psi_{a,b}(x) = |a|^{1/2}\,\psi\left(\frac{x-b}{a}\right), a \in \mathbb{R}*, b \in \mathbb{R}. \tag{7}$$

The initial function is called the mother wavelet. Here b is a position parameter and $1/a$ is homogeneous to a momentum.
The continuous wavelet transform is an isometry from $L^2(\mathbb{R})$ into $L^2(\mathbb{R}\times\mathbb{R}, a^{-2}dadb)$. Similar to the definition of the inverse Fourier transform, it is possible to define a reconstruction formula that allows to rewrite $f(x)$ as an expansion. The following theorem specifies few characteristics of continuous wavelet theory:

Theorem 1 *Let ψ be a normalized function belonging to $L^1(\mathbb{R}) \cap L^2(\mathbb{R})$, of which the Fourier transform $\hat{\psi}$ verifies the following equality:*

$$\int d\xi \frac{|\hat{\psi}|^2}{|\xi|} = K < \infty. \tag{8}$$

Then, the conservation of the norm defined by,

$$\frac{1}{K}\int\int \frac{dadb}{a^2}\,|d_b^a|^2 = \int dx\,|f(x)|^2, \tag{9}$$

and the possibility to recover the function $f(x)$ using the reconstruction formula defined as follows:

$$f(x) = \frac{1}{K}\int\int \frac{dadb}{a^2} d_b^a \psi_{a,b}(x), \tag{10}$$

are ensured.

The condition (8) means that any oscillating function localized in both spaces and whose integral over the whole space $\mathbb{R}$ is null can be used as a mother wavelet. A typical choice for ψ is,

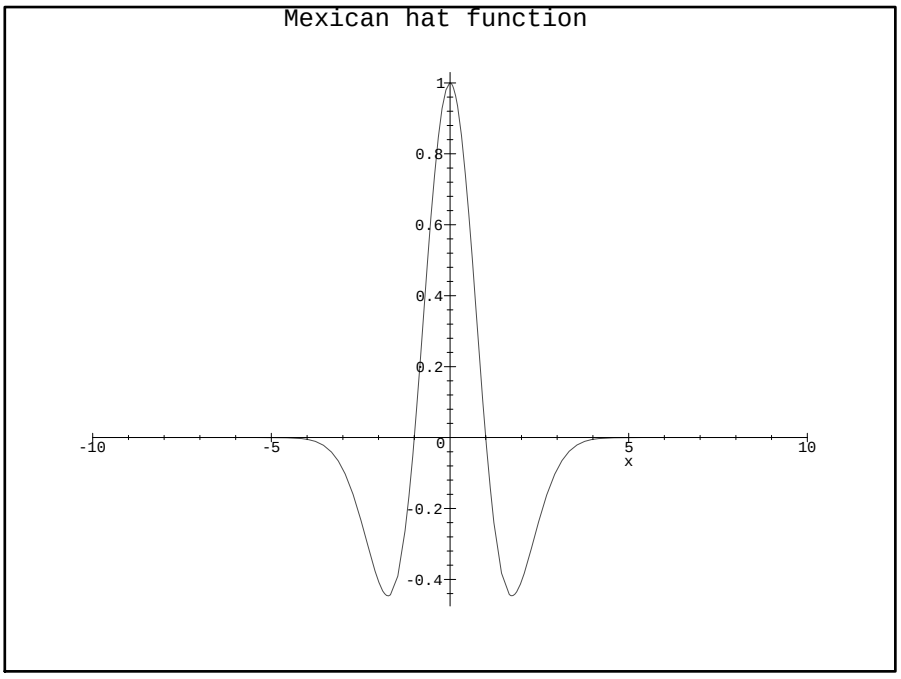
$$\psi(x) = (1-x^2)e^{-\frac{x^2}{2}} \tag{11}$$

the second derivative of the Gaussian function, sometimes called the mexican hat function.

2.2 Discrete and orthonormal wavelets

Discrete wavelets correspond to the choices $a = a_0^m, b = nb_0a_0^m$, indicating that the translation parameter b depends on the chosen dilation rate. The family of wavelets becomes, then, for $m, n \in \mathbb{Z}$,

$$\psi_{m,n} = a_0^{-m/2}\psi(a_0^{-m}x - nb_0). \tag{12}$$



The dilation step a_0 is generally taken greater than one and the translation step b_0 different from zero. It is also possible to define wavelets that constitute an orthonormal basis. They are defined as the collection,

$$\psi_{j,k} = 2^{-j/2}\psi(2^{-j}x - k), j, k \in \mathbb{Z}. \tag{13}$$

The simplest and most famous example of orthonormal wavelet basis is the Haar system already known at the beginning of the century [13]:

$$\psi(x) = \begin{cases} 1 & 0 \leq x < 1/2 \\ -1 & 1/2 \leq x < 1 \\ 0 & \text{otherwise} \end{cases}$$

The construction of orthonormal wavelet bases is presented in the next part describing the BCR algorithm.

3 BCR Algorithm

The method of decomposition, first proposed by Beylkin, Coifman and Rokhlin (BCR) [14, 15], is based on the notion of multiresolution analysis [16, 17]. Orthonormal

wavelets, constructed by Daubechies [18, 19] are used as basis functions to represent some operators. These wavelets are compactly supported and lead to sparse matrix representations. The study of the derivative and of the multiplicative (by a function) operators allows to analyze operators like (1) whose wavelet transform is performed by sorting out the operator in two parts which are treated individually. The matrix coefficients corresponding to the kinetic term are given by an iterative process defined from relations existing between different scales and those related to the potential term are given by a quadrature formula constructed from a Taylor expansion of the integral kernel corresponding to the potential.

3.1 Multiresolution analysis

The theoretical construction of orthogonal wavelet families is intimately related to the notion of multiresolution analysis:
Definition:
A MultiResolution Analysis is a decomposition of the Hilbert space $L^2(\mathbb{R})$ of physically admissible functions (i.e square integrable functions) into a chain of closed subspaces,

$$\ldots \subset V_2 \subset V_1 \subset V_0 \subset V_{-1} \subset V_{-2} \ldots$$

such that

- $\bigcap_{j\in\mathbb{Z}} V_j = \{0\}$ and $\bigcup_{j\in\mathbb{Z}} V_j$ is dense in $L^2(\mathbb{R})$
- $f(x) \in V_j \Leftrightarrow f(2x) \in V_{j-1}$
- $f(x) \in V_0 \Leftrightarrow f(x-k) \in V_0$
- There is a function $\varphi \in V_0$ such that $\{\varphi(x-k)\}_{k\in\mathbb{Z}}$ is an orthonormal basis of V_0

Let W_j be the orthogonal complementary subspace of V_j in V_{j-1}:

$$V_j \oplus W_j = V_{j-1} \tag{14}$$

This space contains the difference in information between V_j and V_{j-1}, and allows the decomposition of $L^2(\mathbb{R})$ as a direct form:

$$L^2(\mathbb{R}) = \oplus_{j\in\mathbb{Z}} W_j \tag{15}$$

Then, there exists a function $\psi \in W_0$, called the mother wavelet, such that $\{\psi(x-k)\}_{k\in\mathbb{Z}}$ is an orthonormal basis of W_0. The corresponding wavelet bases are then characterized by:

$$\varphi_{j,k}(x) = 2^{-j/2}\varphi(2^{-j}x - k), \quad k, j \in \mathbb{Z}, \tag{16}$$
$$\psi_{j,k}(x) = 2^{-j/2}\psi(2^{-j}x - k), \quad k, j \in \mathbb{Z}. \tag{17}$$

The mother wavelet corresponding to the chosen wavelet basis verifies:

$$\int_{\mathbb{R}} dx\, \psi(x)\, x^m = 0, \quad m = 0, \ldots, M-1 \ , \tag{18}$$

which means that it has M vanishing moments.

Since the scaling function $\varphi(x)$, and the mother wavelet $\psi(x)$ belong to V_{-1}, they admit the following expansions:

$$\varphi(x) = \sqrt{2} \sum_{k=0}^{L-1} h_k\, \varphi(2x-k), \quad h_k = \langle \varphi, \varphi_{-1,k} \rangle \ , \tag{19}$$

$$\psi(x) = \sqrt{2} \sum_{k=0}^{L-1} g_k\, \varphi(2x-k), \quad g_k = (-1)^k h_{L-k-1} \ , \tag{20}$$

where the number L of coefficients is connected to the number M of vanishing moments and is also connected to other properties that can be imposed to $\varphi(x)$. Functions verifying (19) or (20) have their support included in $[0, \ldots, L-1]$. Furthermore, if there exists a coarsest scale, $j = n$, and a finest one, $j = 0$, the bases can be rewritten as:

$$\varphi_{j,k}(x) = \sum_{l=0}^{L-1} h_l\, \varphi_{j-1,2k+l}(x), \quad j = 1, \ldots, n \ , \tag{21}$$

and

$$\psi_{j,k}(x) = \sum_{l=0}^{L-1} g_l\, \varphi_{j-1,2k+l}(x), \quad j = 1, \ldots, n \ . \tag{22}$$

The wavelet transform of a function $f(x)$ is then given by two sets of coefficients defined as

$$d_k^j = \int_{\mathbb{R}} dx\, f(x)\, \psi_{j,k}(x) \ , \tag{23}$$

and

$$s_k^j = \int_{\mathbb{R}} dx\, f(x)\, \varphi_{j,k}(x) \ . \tag{24}$$

Starting with an initial set of coefficients s_k^0, and using (21) and (22), coefficients d_k^j and s_k^j can be computed by means of the following recursive relations:

$$d_k^j = \sum_{l=0}^{L-1} g_l\, s_{2k+l}^{j-1} \ , \tag{25}$$

and

$$s_k^j = \sum_{l=0}^{L-1} h_l \, s_{2k+l}^{j-1} \ . \tag{26}$$

Coefficients d_k^j, and s_k^j are considered in (25) and (26) as periodic sequences with the period 2^{n-j}. The set d_k^j, is composed by coefficients corresponding to the decomposition of $f(x)$ on the basis $\psi_{j,k}$ and s_k^j may be interpreted as the set of averages at various scales.

3.2 Non Standard form of integral operators

Let us consider operators that can be written in an integral form,

$$Tf(x) = \int_{\mathbb{R}} dy \, K(x,y) \, f(y) \tag{27}$$

where $K(x,y)$ is the integral kernel associated to the operator T. In order to carry out computations, the representation of an operator consists in writing the corresponding kernel as a matrix. The Non Standard (NS) form related to a wavelet basis decomposition leads to sparse matrices and, as a result, speeds up calculations. It is obtained by developing the kernel on the following two dimensional family:

$$\Big\{ \psi_{j,k}(x) \, \psi_{j,k'}(y), \ \psi_{j,k}(x) \, \varphi_{j,k'}(y), \ \varphi_{j,k}(x) \, \psi_{j,k'}(y) \Big\}_{j,k,k' \in \mathbb{Z}} \ . \tag{28}$$

(the Standard Form is obtained by tensor products of the 1D basis functions [14, 15]). Hence, the three sets of coefficients,

$$\alpha_{k,k'}^j = \iint_{\mathbb{R}^2} dx \, dy \, K(x,y) \, \psi_{j,k}(x) \, \psi_{j,k'}(y) \ , \tag{29}$$

$$\beta_{k,k'}^j = \iint_{\mathbb{R}^2} dx \, dy \, K(x,y) \, \psi_{j,k}(x) \, \varphi_{j,k'}(y) \ , \tag{30}$$

$$\gamma_{k,k'}^j = \iint_{\mathbb{R}^2} dx \, dy \, K(x,y) \, \varphi_{j,k}(x) \, \psi_{j,k'}(y) \ , \tag{31}$$

have to be computed. By applying formulae (21) and (22), equations (29), (30), and (31) may be rewritten as:

$$\alpha_{k,k'}^j = \sum_{l,l'=0}^{L-1} g_l \, g_{l'} \, r_{2k+l,2k'+l'}^{j-1} \ , \tag{32}$$

$$\beta_{k,k'}^j = \sum_{l,l'=0}^{L-1} g_l \, h_{l'} \, r_{2k+l,2k'+l'}^{j-1} \ , \tag{33}$$

$$\gamma_{k,k'}^j = \sum_{l,l'=0}^{L-1} h_l \, g_{l'} \, r_{2k+l,2k'+l'}^{j-1} \ , \tag{34}$$

where $r^j_{k,k'}$ is a fourth set of coefficients defined as,

$$r^j_{k,k'} = \iint_{\mathbb{R}^2} dx\, dy\, K(x,y)\, \varphi_{j,k}(x)\, \varphi_{j,k'}(y)\ , \tag{35}$$

which verifies the recursive rule:

$$r^j_{k,k'} = \sum_{l,k'=0}^{L-1} h_l\, h_{l'}\, r^{j-1}_{2k+l,2k'+l'}\ , \tag{36}$$

where $k, k' = 0, \ldots, 2^{n-j} - 1$, $j = 1, \ldots, n$.

If one denotes by P_j the projection operator from $L^2(\mathbb{R})$ on the subspace spanned by the basis $\{\phi_{j,k}\}_{k\in\mathbb{Z}}$, and by R_j the projection operator on the subspace spanned by the basis $\{\psi_{j,k}\}_{k\in\mathbb{Z}}$, then $\{\alpha^j_{k,k'}\}_{k,k'\in\mathbb{Z}}$, $\{\beta^j_{k,k'}\}_{k,k'\in\mathbb{Z}}$, $\{\gamma^j_{k,k'}\}_{k,k'\in\mathbb{Z}}$, $\{r^j_{k,k'}\}_{k,k'\in\mathbb{Z}}$ represent the operators $A_j = R_j T R_j$, $B_j = R_j T P_j$, $G_j = P_j T R_j$, and $T_j = P_j T P_j$, respectively. The discretization T_0 of the operator T on the finest scale $j = 0$ may be written as:

$$T_0 = \sum_{j=1}^{n} (A_j + B_j + G_j) + T_n\ . \tag{37}$$

The matrix representation of an operator applied to a function is then depicted by:

$$\begin{pmatrix} A_1 & B_1 & & & & \\ G_1 & & & & & \\ & & A_2 & B_2 & & \\ & & G_2 & & & \\ & & & & A_3 & B_3 \\ & & & & G_3 & T_3 \end{pmatrix} * \begin{pmatrix} d^1 \\ s^1 \\ d^2 \\ s^2 \\ d^3 \\ s^3 \end{pmatrix} = \begin{pmatrix} d'^1 \\ s'^1 \\ d'^2 \\ s'^2 \\ d'^3 \\ s'^3 \end{pmatrix}\ . \tag{38}$$

After applying the NS form to a vector, the result is obtained with the following reconstruction formula:

$$T_0 f(x) = \sum_{j=1}^{n} \sum_{k=0}^{2^{n-j}} d'^j_k \psi_{j,k}(x) + s'^j_k \varphi_{j,k}(x). \tag{39}$$

4 The Lanczos algorithm

Simple processes, like the Power Method, require, in principle, an infinite number of matrix-vector products to converge to an eigenvector. On the other hand, the Lanczos iterations expands each eigenvector in a convergent series with a finite number of terms [4]. The Lanczos method can be viewed as a process of computing a tridiagonal matrix T orthogonally congruent to A (i.e. $T = Q^*AQ, Q = (q_1, q_2, \ldots, q_n), Q^* = Q^{-1}$). The algorithm need not to go the whole way; it builds up $Q_j = (q_1, q_2, \ldots, q_j)$ and $T_j = Q_j^* A Q_j$ by step j and can often be stopped at values of j as small as $2\sqrt{n}$. To compete in accuracy the Lanczos has to be supplemented with the explicit orthogonalization of the Lanczos vectors which, in exact arithmetic, would be orthogonal automatically. Roundoff errors at each iteration step lead to the loss of orthogonality and make the Lanczos algorithm very unstable. The version used in this paper includes a reorthogonalization routine whose detailed features can be found in [20]. Our purpose here being not to discuss or to compare the various orthogonalization strategies, we refer to the original papers for more details [21, 22, 23, 24].
The computation of the eigenvalues from the tridiagonal matrix obtained from the Lanczos process is then performed using a basic Givens bisection [4] which gives, in some cases, better results than the usual QR algorithm. Indeed, for problems whose eigenvalues are very close to each other, the convergence factor of the QR algorithm is close to 1 whereas it remains bounded by 1/2 for the bisection method.

4.1 The theoretical Lanczos iteration

The simple Lanczos process for a symmetric $n \times n$ matrix A (if A is not hermitian then a variant exists and is called the Arnoldi process) computes a sequence of Lanczos vectors q_j and scalars α_j, β_j as follows:

1. choose a starting vector $r_1 \neq 0$, set $q_0 \equiv 0, \beta_1 = \|r_1\|$
2. for $j = 1, 2, \ldots, do$
   $q_j = r_j / \beta_j$
   $u_j = A q_j - \beta_j q_{j-1}$
   $\alpha_j = u_j^* q_j$
   $r_{j+1} = u_j - \alpha_j q_j$
   $\beta_{j+1} = \|r_{j+1}\|$

One pass through step 2 is a Lanczos step. The equation for one Lanczos step can be written as:

$$\beta_{j+1} q_{j+1} = A q_j - \alpha_j q_j - \beta_j q_{j-1} \tag{40}$$

In exact arithmetic, the Lanczos vectors q_j are orthogonal:

$$|q_i^* q_k| = 0, \tag{41}$$

for $i = 1, \ldots, j, k = 1, \ldots, j, k \neq j$.

4.2 Orthogonalization methods

Whereas in general, the loss of orthogonality is simply credited to an accumulation of roundoff and cancellation errors, it has been shown that this phenomena is just an amplification of the local errors which can be explained through recurrence formulas. A theorem quantifies how the local error is propagated in the algorithm [20]. Let the $j \times j$ matrix $N_j = (\omega_{ik})$ be defined by,

$$N_j = Q_j^* Q_j. \tag{42}$$

If the Lanczos vectors are orthogonal then $N_j = I_j$ (the $j \times j$ identity matrix).

Theorem 2 *The elements of the matrix N_j satisfy the following recurrence:*

$\omega_{kk} = 1$ *for* $k = 1, \ldots, j$,

$\omega_{kk-1} = \epsilon_k$ *for* $k = 2, \ldots, j$,

$\beta_{j+1}\omega_{j+1k} = \beta_{k+1}\omega_{jk+1} + (\alpha_k - \alpha_j)\omega_{jk} + \beta_k\omega_{jk-1} - \beta_j\omega_{j-1k} + q_j^* f_k - q^* f_j$,

$\omega_{jk+1} = \omega_{k+1j}$,

where $\omega_{k0} = 0, \epsilon_k = q_k^* q_{k-1}$, *and* f_k *denotes the local roundoff errors at step* k.

If the first j *Lanczos vectors satisfy,*

$$|q_i^* q_k| \leq \omega_j, \tag{43}$$

for $i = 1, \ldots, j, k = 1, \ldots, j, k \neq j$, *then the smallest* ω_j *will be called the level of orthogonality. If* $\omega_j = \sqrt{\epsilon}$, *where* ϵ *can be the machine roundoff unit or any threshold given by the user, then the Lanczos vectors are called semiorthogonal.*

Simon then showed that the Lanczos algorithm leads to accurate results as far as semiorthogonality is maintained among the Lanczos vectors. He also showed that both partial reorthogonalization and selective orthogonalization introduced by Parlett and Scott [21] or himself [24] are semiorthogonalization strategies. According to the result established by Simon, an adapted Gram-Schmidt orthogonalization routine has been included in the Lanczos step in order to keep the semiorthogonality among the Lanczos vectors during the process.

5 Effective implementation of the Non Standard Form

The two parts of the operators under study are separately treated with two differents techniques. The NS form of the Laplacian term is worked out in an iterative process and the potential term by a quadrature formula.

5.1 Representation of the Laplacian term

The analysis of the operator,

$$Lf = -\frac{\Delta f}{2}, \tag{44}$$

is, in fact, a particular case of the representation of the derivative operator d^p/dx^p. The method for finding the NS form of this operator is entirely described by Beylkin [15]. Only the most important points of this process are recalled. For the p^{th} derivative, the computations of the coefficients defined in (29), (30), (31) and (35) lead to the following scaling relations:

$$\alpha_{k,k'}^j = 2^{-pj}\,\alpha_{k-k'}, \tag{45}$$

$$\beta_{k,k'}^j = 2^{-pj}\,\beta_{k-k'}, \tag{46}$$

$$\gamma_{k,k'}^j = 2^{-pj}\,\gamma_{k-k'}, \tag{47}$$

$$r_{k,k'}^j = 2^{-pj}\,r_{k-k'}, \tag{48}$$

where

$$\alpha_l = \int_{\mathbb{R}} dx\,\psi(x-l)\,\psi^{(p)}(x) \tag{49}$$

$$\beta_l = \int_{\mathbb{R}} dx\,\psi(x-l)\,\varphi^{(p)}(x) \tag{50}$$

$$\gamma_l = \int_{\mathbb{R}} dx\,\varphi(x-l)\,\psi^{(p)}(x) \tag{51}$$

$$r_l = \int_{\mathbb{R}} dx\,\varphi(x-l)\,\varphi^{(p)}(x) \tag{52}$$

Using Equations (21) and (22), coefficients $\{\alpha_l\}_{l\in\mathbb{Z}}$, $\{\beta_l\}_{l\in\mathbb{Z}}$, $\{\gamma_l\}_{l\in\mathbb{Z}}$ can be written as expressions involving the set $\{r_l\}_{l\in\mathbb{Z}}$ which verifies itself an iterative rule:

$$\alpha_l = 2^p \sum_{m,m'=0}^{L-1} g_m\,g'_m\,r_{2l+m-m'}, \tag{53}$$

$$\beta_l = 2^p \sum_{m,m'=0}^{L-1} g_m\,h'_m\,r_{2l+m-m'}, \tag{54}$$

$$\gamma_l = 2^p \sum_{m,m'=0}^{L-1} h_m\,g'_m\,r_{2l+m-m'}, \tag{55}$$

$$r_l = 2^p \sum_{m,m'=0}^{L-1} h_m\,h'_m\,r_{2l+m-m'}. \tag{56}$$

Starting with an initial guessed set of coefficients, Equation (56) can be used in an iterative way in order to compute $\{r_l\}_{l\in\mathbb{Z}}$. The convergence of this process is reached in less than ten iterations with a sufficient accuracy.

5.2 Representation of the potential term

A quadrature formula proposed by Beylkin et al. [14] to compute wavelet coefficients of a smooth functions is described in this subsection. If the scaling function $\varphi(x)$ verifies the following condition,

$$\int_{\mathbb{R}} dx\, \varphi(x+\tau)x^m = 0, \quad m = 1, \ldots, M-1, \tau \in \mathbb{Z}, \tag{57}$$

$$\int_{\mathbb{R}} dx\, \varphi(x) = 1 \tag{58}$$

and if the function $f(x)$ that need to be analyzed is smooth enough, then coefficients s_k^j can be computed from an expansion of $f(x)$ into a Taylor series around $2^j(k+\tau)$. The result is,

$$s_k^j = 2^{j/2} f(2^j(k+\tau)) + O(2^{j(M+1/2)}). \tag{59}$$

This formula is only used for the finest scale where the discretization step size is about 2^{-n}, and then the relations (25), (26) are used to computes the coarser scales coefficients.

By applying the quadrature formula to each variable of the kernel $K(x,y)$ corresponding to the potential term, the wavelet decomposition can be easily obtained.

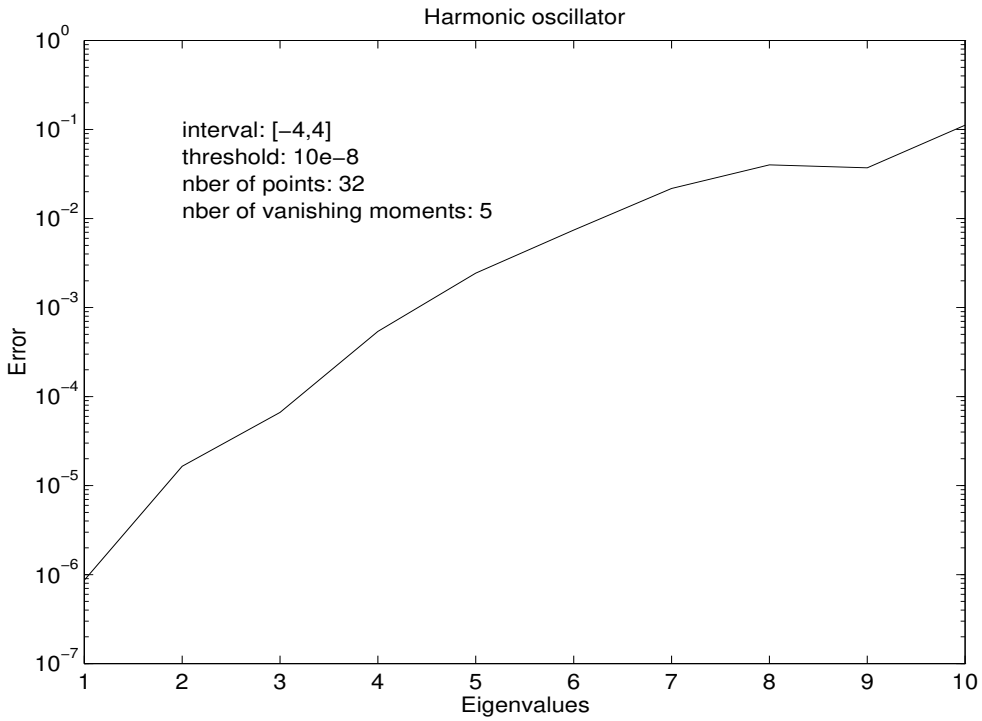
6 Numerical results

The Harmonic Oscillator case is studied in details in order to point out the importance of some parameters as the number of vanishing moments of the mother wavelet or the discretization step size. The numerical results given for the pseudo-double well problem and for the hydrogen atom have been obtained with parameters values leading to acceptable accuracies.

6.1 The Harmonic Oscillator case

In order to test the method, the first ten eigenvalues of the Harmonic Oscillator have been computed. The initial discretization contains only 32 points since no more points were necessary to get accurate results. However, it is obvious that more points would lead to better results.

Different parameters connected to the wavelet decomposition have to be specified, the most important being the number of vanishing moments, M, of the mother wavelet. Numerical tests with various values for M have been performed, and only those corresponding to $M = 5$ and $M = 11$ are reported in this paper. The comparison of the results corresponding to these two values emphasizes the importance of this parameter: greater is the number of vanishing moments, better are the wavelets representations of the different mathematical object. Once the number of vanishing moments is fixed, another important parameter is the discretization step size. For a

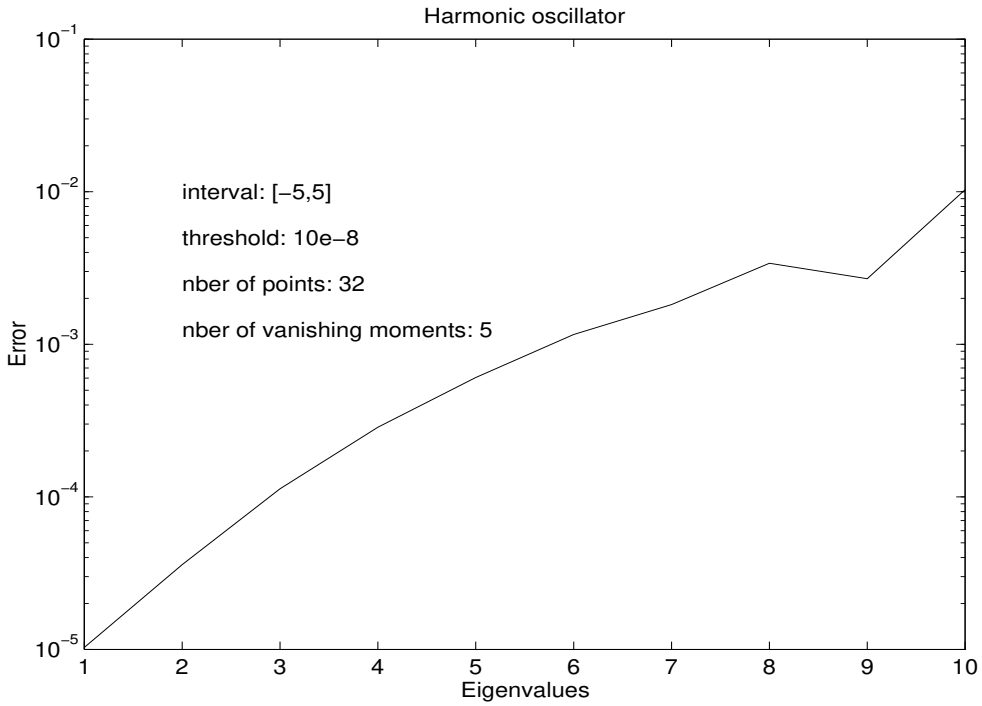


given number of points, this parameter can be modified by just changing the interval size. Results corresponding to three different sizes are given.

A treshold is necessary in two places in the algorithm. The first one concerns the thresholding of the wavelet decomposition: any wavelet coefficient below a given threshold ϵ is discarded in order to sparsify the datas; and the second one occurs in the semiorthogonalization keeping: the level of orthogonality is chosen to be equal to $\epsilon^{3/4}$ as suggested by Simon in [24]. The value of ϵ has been fixed equal to 10^{-8}. The numerical results for the first ten eigenvalues are given in the figures.

6.2 The Hydrogen atom and the pseudo-double well cases

The results and the different parameters used for these problems are given in table 1. It can be noticed that more points (than for the Harmonic Oscillator case) are required to reach reasonable accuracies. This is due to the fact that we are trying to described singular potentials with non sigular functions.
The result obtained for the pseudo-double well problem is a little bit worst than those obtained by Modisette in [8] for the same problem. Modisette had used a much



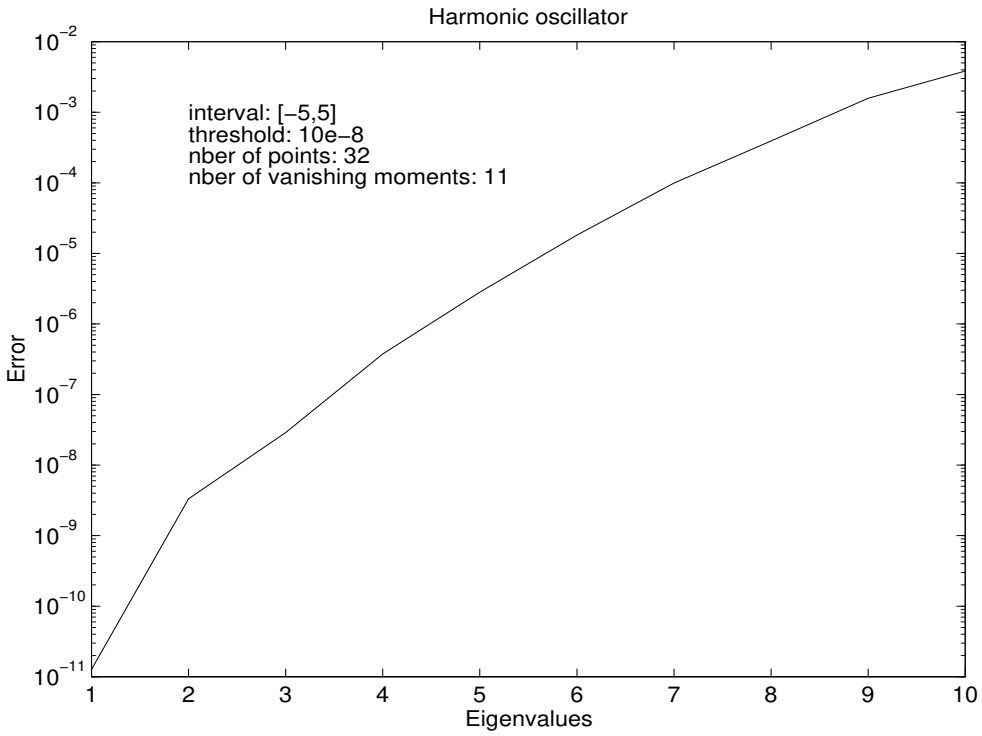
more complicated quadrature than the one point quadrature used in our computation. On the contrary, the accuracy achieved for the hydrogen atom is better than the one obtained by the author with another iterative scheme in [25]. These two experiments show the capability of wavelets to give a good representation of a real singular potential, and to separate close eigenvalues in a spectrum.

7 Comments

A first comment concerning the number of vanishing moments can be done. As already emphasized, this parameter acts directly onto the accuracy. A large number of vanishing moments leads to a better accuracy for the quadrature formula (in the Taylor expansion, more terms will be exactly equal to zero). This parameter also influences the quality of the Laplacian representation.

The importance of the discretization step size has already been pointed out in [25], and we refer to this paper for more details about this point.

With a threshold of 10^{-8}, the level of orthogonality is maintained around 10^{-6},



and as stated by Simon [24, 20], it is largely sufficient to get accurate results with the Lanczos algorithm.

It should be also emphasized that the Lanczos method is a very sensitive process, and a good accuracy in the description of the different parts of the operator is required to get good final results. The simple quadrature formula used for the potential term can be replaced by a more sophisticated one in order to improve the final accuracies. Many detailed studies have already been carried out, and we refer to these publications for more details [26].

No CPU times are given since the tests have been performed with a rudimentary code, and some technical improvements should be brought to make it competitive with codes which are running for many years. The aim of this paper was just to show that a $O(N)$ wavelet-based matrix-vector product can be used in any iterative method instead of a regular product in $O(N^2)$. The generalization of the method to three-dimensional problems is in progress and the results will be published in another issue.

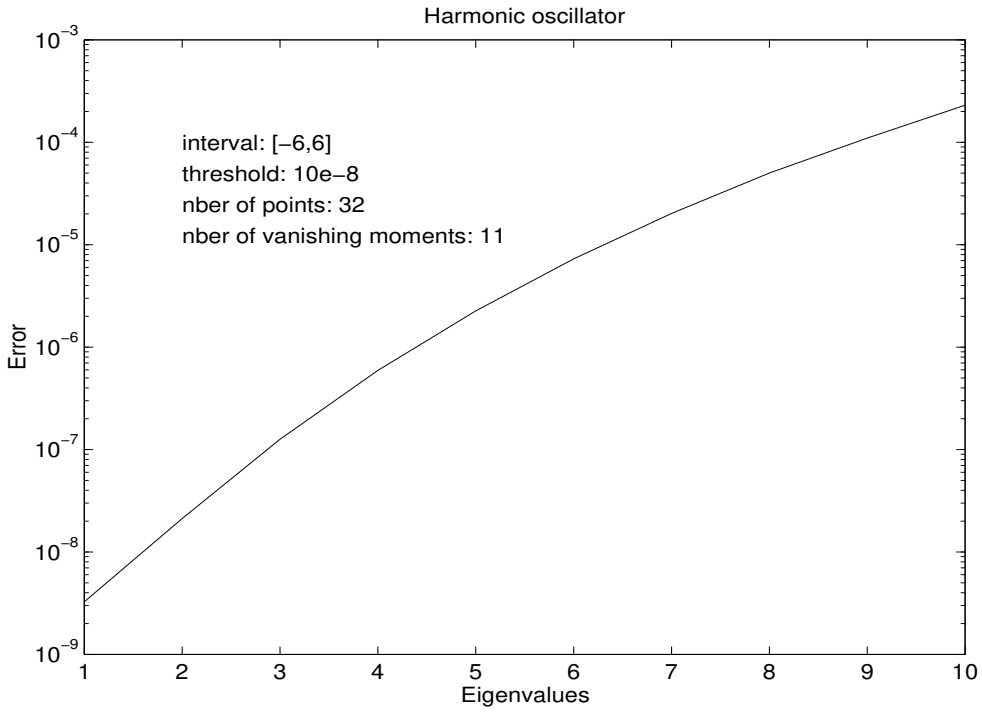


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Table 1: Numerical results for operators with a (pseudo) singular potential term

	Pseudo-double well 5^{th} excited state	Hydrogen Atom ground state
Interval	[-18,18]	[-7,7]
Threshold	10^{-8}	10^{-8}
Nber of points	512	512
Vanishing moments	5	5
Exact value	-0.24825962	-0.5
Result	-0.24825517	-0.499659345
Error	2.2×10^{-5}	6.8×10^{-4}