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Filter diagonalization with finite Fourier transform eigenfunctions

T. Levitina*

Institut Computational Mathematics, TU Braunschweig, Pockelsstrasse 14, D-38106, Braunschweig, Germany
E-mail: t.levitina@tu-bs.de

E. J. Brändas

Department of Quantum Chemistry, Uppsala University, PO Box 518, SE–75 120, Uppsala, Sweden

Below, we briefly report on the progress in the development of the Filter Diagonalization technique when filtering is carried out with the aid of Finite Fourier Transform (FFT) eigenfunctions. During recent years interest in these functions, also known as 'prolates', or 'slepians', has increased among scientists doing research in the field of signal processing. The main explanation to this follows from the set of very special extremal and orthogonality properties exibited by the FFT eigenfunctions. Recent results of Walter and Shen on sampling with prolate spheroidal functions will necessary produce a new wave of interest. In the presented, Filter diagonalization machinery, we show that the sampling formula of Walter and Shen simplifies essentially the computation of matrix elements as certain 2D–integrals involving FFT eigenfunctions.

KEY WORDS: filter diagonalization, spectral analysis, auto-correlation function, finite Fourier transform, prolates, sampling theorem

1. Introduction

It is well-known by now that signal and image processing mainly developed in applied sciences and engineering have much in common with the basic description of quantum mechanics and quantum chemistry. The recently developed procedure of Filter Diagonalization is such a typical example when the spectral information, extracted from the dynamics of a quantum system, directly mimics general procedures and implementations of high-resolution signal and image processing. In the present contribution, we report on the recent development of the filter diagonalization technique with implication for methods and computations in quantum chemistry.

*Corresponding author.

The Filter Diagonalization Technique was first introduced with particular reference to problems in quantum chemistry by Neuhauser and coworkers [1–3]. Significant developments by Mandelshtam and Taylor [4] and many others have now become among the most commonly used methods for solving spectral problems in quantum dynamics.

2. Filter diagonalization

Filter diagonalization is a method to investigate the detailed spectrum of an operator (Hamiltonian) $\hat{H}$ at a selected energy range. The spectral information is directly extracted from a short ($-T \leqslant t \leqslant T$) segment of the auto-correlation function $C(t) = \langle\varphi(\vec{x}, 0)|\varphi(\vec{x}, t)\rangle = \langle\varphi(\vec{x}, 0)|e^{-i\hat{H}t}|\varphi(\vec{x}, 0)\rangle$ associated with a given wave packet $\varphi(\vec{x}, t)$ subject to the time–dependent Schrödinger equation:

$$\frac{\partial\varphi}{\partial t}(\vec{x}, t) = -i\hat{H}\varphi(\vec{x}, t).$$

To filter the auto-correlation function $C(t)$, implies filtering the functional space on which $\hat{H}$ is acting. For a purely discrete spectrum, one extracts a subspace spanned by the eigenfunctions corresponding to the eigenvalues situated within the considered energy interval. Note that the filtering procedure is generally not exact, since contributions from eigenvectors associated with eigenvalues outside this interval are suppressed rather than eliminated completely.

3. Filtering with prolates

In Ref. [5], we have discussed the advantages of using the Finite Fourier Transform (FFT) eigenfunctions as tapering windows for the filtering procedure. The exclusive properties of FFT eigenfunctions have been widely discussed since the original paper [6] appeared, in particular, we refer to Ref. [7–9] for more details. The main advantage of using FFT eigenfunctions is that such filtering is exact, resulting in a system of non-linear equations reduced to treating only eigenvalues located within the prescribed interval $\left[\omega^* - \Omega, \omega^* + \Omega\right]$:

$$\sum_{\omega_k \in (\omega^*-\Omega, \omega^*+\Omega)} |d_k|^2 \theta_l(\omega^* - \omega_k) = (-1)^l \frac{\mu_l}{2\pi}\sqrt{\frac{\Omega}{T}} \int_{-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}\omega^* t}\, C(t)\, \Theta_l(t)\, \mathrm{d}t.$$

Above ω_k is an eigenvalue of the Hamiltonian $\hat{H}$; $\theta_l(t)$ and $\Theta_l(t)$ are FFT eigenfunctions, scaled and squeezed to become Ω-band-limited and T–concentrated, i.e.

$$F[\theta_l(\omega)] = (-1)^l \mu_l \sqrt{\frac{\Omega}{T}}\, \Theta_l(t),$$

$$F^{-1}[\theta_l(\omega)] = \frac{\mu_l}{2\pi} \sqrt{\frac{\Omega}{T}}\, \Theta_l(t),$$

further, $[-T, T]$ is the interval at which the wave packet propagation is known, and finally μ_l is the associated FFT eigenvalue.

Having filtered the Hilbert space of quantum states, we obtain the 'eigen subspace' of the hamiltonian $\hat{H}$ associated with the interval $\left[\omega^* - \Omega, \omega^* + \Omega\right]$. In this reduced 'eigen subspace' the eigenvalue problem for $\hat{H}$ takes the form

$$\mathbf{U}\vec{b}_k = \omega_k \mathbf{W}\vec{b}_k,$$

where **U** and **W** are finite matrices with entries being 2D integrals involving the the auto-correlation function and the tapering functions $\Theta_l(t)$:

$$\mathbf{U}_{sl} = (-1)^{s+l} \frac{\Omega \mu_s \mu_l}{4\pi^2 T} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{e}^{i\omega^*(t-\tau)} c(t-\tau) \Theta_s(t) \left\{ \omega^* \Theta_l(\tau) - i \frac{\mathrm{d}\Theta_l(\tau)}{\mathrm{d}\tau} \right\} \mathrm{d}\tau\, \mathrm{d}t \tag{1}$$

$$\mathbf{W}_{sl} = (-1)^{s+l} \frac{\Omega \mu_s \mu_l}{4\pi^2 T} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{e}^{i\omega^*(t-\tau)}\, c(t-\tau) \Theta_s(t)\, \Theta_l(\tau)\, \mathrm{d}\tau\, \mathrm{d}t.$$

The idea to reformulate the original spectral problem to that of linear algebra, has been proposed earlier, (see e.g, [10]). The procedure looks very attractive, particularly since a preliminary computation employs only the auto-correlation function and does not require values of the original propagating wave packet. The approach discussed in Ref. [10] leads, however, to an almost degenerate matrix, and if the grid in the spectral interval is made finer, the degeneracy effect becomes stronger. This drawback follows from the fact that the Fourier basis, in which the matrix elements are computed, consists of almost linearly dependent functions. They are subsequently computed as the Fourier transform of the wave–packet propagation by shifting the spectral parameter to a neighbouring grid point and enumerating basis functions with this shifts.

Employing instead different filtering windows, we can remedy the above mentioned degeneracy problem. Thus we obtain a sufficient number of basis functions from the wave–packet Fourier transform, computed with various tapering functions at the same value of spectral parameter.

4. Sampling with prolates

In spite of the drawback mentioned above, the Mandelstam's procedure in Ref. [10] is clear and easily coded, while the necessity to integrate the auto-correlation function, weighted with a convolution of two FFT eigenfunctions in Ref. [5], made our present approach less promising.

The sampling formulas obtained in Ref. [7,8] have resolved this problem. The key to such a kind of formulas lies in the generalization of the famous Whittaker–Nyquist–Kotelnikov-Shannon sampling theorem. The theorem states that any band–limited function $f(x) \in \mathcal{L}_2(-\infty, +\infty)$ (i.e., function whose Fourier transform is of finite support) may be completely recovered from its equally spaced samples. Originally, for interpolation of these function, sinc–function translates have been used. However, although formally converging, expansions in terms of the sinc–function converge in practice very slowly. On the contrary the relevant expansions in terms of eigenfunctions of FFT converge considerably faster then the classical series of Shannon and others. A relatively high accuracy can now be achieved with only a few equally spaced samples and few eigenfunctions. Thus, if f is π–bandlimited and τ is the 'interval of concentration'

$$f(t) \approx \sum_{n=0}^{2[\tau]} \left(f(m) \sum_{m=-[\tau]}^{[\tau]} \Theta_n(\pi\tau, m) \right) \Theta_n(\pi\tau, t),$$

where $\Theta_n(\pi\tau, t)$ is the π–band limited, τ–concentrated FFT eigenfunction.

One can use these expressions to interpolate the internal integrals in the right-hand sides of (1):

$$\zeta_{sl}(t) = \int_{-\infty}^{\infty} \Theta_s(t+\tau) \left\{ \omega^* \Theta_l(\tau) - i \frac{\mathrm{d}\Theta_l(\tau)}{\mathrm{d}\tau} \right\} \mathrm{d}\tau,$$

$$\Upsilon_{sl}(t) = \int_{-\infty}^{\infty} \Theta_s(t+\tau)\, \Theta_l(\tau) \mathrm{d}\tau;$$

These convolutions are also Ω-band-limited, since $\Theta_s(t)$ and $\Omega_l(t)$ have this property.

5. Computational recipe

Thus the final recipe of our calculation of the matrix elements U_{sl}, W_{sl} is: (i) first to compute a few (namely, $\frac{2\Omega T}{\pi}$) equally spaced values $\zeta_{sl}(t_k)$, and $\Upsilon_{sl}(t_k)$, then (ii) using these samples to interpolate the functions $\zeta_{sl}(t)$, $\Upsilon_{sl}l(t)$ everywhere on $[-T, T]$ and (iii) to compute the remaining integrals

$$\mathbf{U}_{sl} = \frac{(-1)^{l+s}}{4\pi^2} \mu_l\, \mu_s \frac{\Omega}{T} \int_{-\infty}^{\infty} e^{i\omega^* t} c(t) \zeta_{sl}(t)\, \mathrm{d}t,$$

$$\mathbf{W}_{sl} = \frac{(-1)^{l+s}}{4\pi^2} \mu_l\, \mu_s \frac{\Omega}{T} \int_{-\infty}^{\infty} e^{i\omega^* t} c(t) \Upsilon_{sl}(t)\, \mathrm{d}t.$$

Before, the necessity to compute the integrals over an infinite interval has not been discussed. Obviously, we have to truncate the infinite integration interval to a finite one in the computations. Here the magic property of the FFT

eigenfunctions namely of being mostly concentrated at the interval [-T,T] (see [5]) should be used. On can prove, in particular, that

$$\int_{-\infty}^{\infty} |f(t)\Theta_s(\Omega T, t)|^2 \, \mathrm{d}t - \int_{-T}^{T} |f(t)\Theta_s(\Omega T, t)|^2 \, \mathrm{d}t \leqslant A \frac{1 - |\mu_s|^2}{|\mu_s|^2},$$

with the constant A depending on the function $f(t)$. For $s < \dfrac{2\Omega T}{\pi}$ the value $|\mu_s|^2 \approx 1$ up to a very high accuracy.

An accurate and efficient numerical technique for the evaluation of the FFT eigenfunction, as well as for computating various functionals of them (e.g., the matrix elements $\mathbf{U}_{sl}, \mathbf{W}_{sl}$) is considered in Ref. [11] and references therein.

A more detailed consideration will be presented elsewhere [12].

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