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Multitaper Techniques and Filter Diagonalization Methods—A Comparison

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In the present contribution we compare the new Multitaper Filtering technique with the very popular Filter Diagonalization Method. The substitution of a time-independent problem, like the standard Schrödinger equation, by a time-dependent one from the Filter Diagonalization Method allows the employment of and comparison with standard signal processing filtration machinery. The use of zero-order prolate spheroidal tapers as filtering functions is here extended and exactly formulated using techniques originating from general investigations of prolate spheroidal wave functions. We investigate the modifications presented with respect to accuracy and general effectiveness. The approach may be useful in various branches of physics and engineering sciences including signal processing applications as well as possibly also in general time-dependent processes.

KEY WORDS: multitaper techniques; filter diagonalization methods.

1. INTRODUCTION

The filter diagonalization method was introduced in Neuhauser (1990) for extracting highly excited rovibrational states from an arbitrary Hamiltonian, in any prespecified energy range. In this approach the values of the associated autocorrelation function were first filtered at various energies followed by an explicit diagonalization of the filtered functions. Hence a time-dependent propagation was combined with a time-independent procedure including a small matrix diagonalization. The filter technique of Neuhauser and coworkers thus overcomes the disadvantage of the long propagation time, avoiding the limitations of the time-dependent approach, caused by the uncertainty relations. At the same time it also avoided the needs for the diagonalization of large matrices necessary in a purely time-independent approach. It is also worth emphasizing that in the Neuhauser filtering method one does not need to store the filter states themselves. Their approach has been followed and extended by several other groups (see, e.g., Belkic *et al.*,

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2001; Chen and Guo, 1996; Mandelshtam and Taylor, 1997; Yu and Smith, 1997). In Pang *et al.* (1998) e.g., one extends the Filter Diagonalization Method to consider arbitrary functions as filters rather than box filters or Gaussian exponentials as it was done before.

Below we restrict our consideration to the filters of a special kind namely prolate spheroidal wave functions of zero-order known in signal processing literature as "prolates," or "Slepians." Such a choice is motivated by the very special and important properties possessed by these functions. We briefly review these in section 3 (for more details, see Komarov *et al.*, 1976; Landau and Pollak, 1961; Slepian, 1964; Slepian and Pollak, 1961, 1962).

To employ the prolate spheroidal wave functions for windowing an accurate numerical technique has been proposed in Abramov *et al.* (1984, 1991) and further developed in Levitina and Brandas (2001). The new technique serves to compute both the *prolates* themselves and various functionals of them, keeping at the same time a desired accuracy. This is an important advantage since it will allow us to exactly estimate the accuracy of the appropriate auxiliary computations and, therefore, also of the ultimate spectral definition.

Formally any of the above functions may be used to investigate the spectrum. However below we will show that the most accurate approach requires a set of such functions constituting a basis on the interval of interest. The method is to some extent resembling the multitaper method for spectral estimations.

The multitaper method was invented by Thomson (1982) and it is now known as a very powerful method for doing power spectrum analysis. In particular it is useful for cases where the spectral density is detailed or varies rapidly. It is presently of use in many branches of science, e.g., in astronomy, climatology, geophysics, etc. Using multitaper spectral estimations, zero-order prolate spheroidal tapers are applied to the time series followed by averaging the resulting spectral estimators ("eigenspectra") thereby reducing the variance (McCoy *et al.*, 1998; Percival and Walden, 1993).

In our approach, to be presented below, we will not average the windowed data (the autocorrelation function associated with a given solution to the Schrödinger equation), but rather combine them to constitute a simple exponential function, which explicitly depends on the desired eigenvalues. An attractive feature of our proposed technique is that it first allows us to localize the eigenvalues situated within the given interval under study and second to easily extract them from the auxiliary computations offered by the method. Thereby at each stage we can guarantee that the desired accuracy is always preserved.

We begin by making the idealistic assumption that the Hamiltonian spectrum is purely discrete and simple and that the eigenvalues are well-resolved or separated. In the last section we will discuss the possibilities to extend our approach to more general cases. In passing we note that the above assumptions are meaningful only in a local sense, i.e., within the interval of interest. In future applications

we expect to be able to give up such an assumption completely allowing us to investigate mixed spectra of a highly sophisticated behaviors.

2. FILTER DIAGONALIZATION METHOD FOR EXTRACTING DISCRETE SPECTRUM EIGENVALUES

Before the work of Feit *et al.* (1982) appeared conventional methods for computing the eigenvalues and eigenfunctions of the Schrödinger equation consisted mainly in the diagonalization of a Hamiltonian matrix or in finding iterative numerical solutions of a time-independent wave equation. The method proposed in Feit *et al.* (1982), in contrast, is based directly on the spectral properties of solutions to the time-dependent Schrödinger equation. The method requires the computation of an autocorrelation function defined from a numerical solution related to a given wave packet propagation. Resonant peaks of the Fourier transform of this autocorrelation function correspond to the stationary states of the system. The latter allows the localization of the actual eigenvalues with high accuracy. Because of its low storage requirements and high numerical efficiency, this method is particularly attractive for calculating high-energy eigenstates of many-dimensional problems.

Consider the evolution of an arbitrary initial wave packet[3] $\Psi(\vec{x}, t)|_{t=0}$ governed by the time-independent Hamiltonian $\hat{H}$ through the Schrödinger equation

$$\frac{\partial \Psi}{\partial t}(\vec{x}, t) = -i\hat{H}\Psi(\vec{x}, t). \tag{1}$$

Here $\hat{H}$ is a self-adjoint operator acting in a Hilbert space $\mathcal{H}$; its spectrum is assumed to be purely discrete and simple. In addition, since $\hat{H}$ is self-adjoint, its eigenvalues are real and its eigenfunctions $\Psi_k(\vec{x})$ constitute an orthonormal basis in $\mathcal{H}$ (see, e.g., Akhiezer and Glazman, 1993). In particular, this implies that the solution of (1) may be expanded in terms of $\Psi_k(\vec{x})$:

$$\Psi(\vec{x}, t) = \sum_{k=0}^{\infty} d_k \, e^{-i\epsilon_k t} \Psi_k(\vec{x}), \tag{2}$$

where d_k, $k = 0, 1 \ldots$, stand for the expansion coefficients of the initial wave packet:

$$d_k = \langle \Psi(\vec{x}, 0) | \Psi_k(\vec{x}) \rangle.$$

A direct consequence of Eq. (1) is that

$$\Psi(\vec{x}, t) = e^{-i\hat{H}t} \Psi(\vec{x}, 0) = \hat{U}(t)\Psi(\vec{x}, 0),$$

with $\hat{U}(t) = e^{-i\hat{H}t}$ being the evolution operator.

[3] In fact this wave packet is not arbitrary, although it may be of a very general form (see section 5).

For the autocorrelation function

$$c(t) = \langle \Psi(\vec{x}, t) | \Psi(\vec{x}, 0) \rangle,$$

one obtains

$$c(t) = \sum |d_k|^2 \, e^{-i\epsilon_k t}. \tag{3}$$

Evidently

$$\langle \Psi(\vec{x}, t'') | \Psi(\vec{x}, t') \rangle = c(t'' - t').$$

Note that the correlation function might be computed at any point t directly from Eq. (1). Thus, instead of solving the original eigenvalue problem, one may consider another one, i.e., of computing the parameters $\{\epsilon_k, d_k\}$ which fit the set of correlation function values.

Nevertheless, to extract the eigenstates accurately, a long propagation time is required because of the energy-time uncertainty principle. In practice direct numerical solutions of the "simplified" problem stated above face severe difficulties, namely: it is often ill-conditioned and therefore requires some regularization; it is further "bulky" and should only be treated as a whole, i.e., the selective extraction of eigen-states at a certain energy range is not allowed.

An alternate indirect approach, the Filter Diagonalization Method was first proposed by Neuhaser (1990) and later developed and modified by Mandelstam, Taylor, and many others (see Belkić, 2001; Chen and Guo, 1996; Mandelshtam and Taylor, 1997; Pang and Neuhauser, 1996; Wall and Neuhauser, 1995; Yu and Smith, 1997, and the literature therein). In this method, one first has to construct the so-called filtered states, calculated at many energies within a selected range. The filtered states can be constructed by applying filter operators to an arbitrary initial reference state. The filter operator is designed to amplify the eigenstates near a given energy, while it suppresses the rest. A small Hamiltonian matrix is then evaluated on the basis of filtered functions, to yield the eigenvalues in the desired range. An attractive feature of this technique is that the spectral information is extracted from only a short segment of the correlation function; furthermore if only the spectrum is needed, one does not have to explicitly construct the filtered states.

The original problem of spectrum estimation is thus reduced to an algebraic one, with the resulting Hamiltonian matrix being diagonally dominant, i.e., with decaying off-diagonal elements. One can therefore, conveniently block diagonalize the matrices, avoiding the necessity to diagonalize very large matrices.

Still, in so doing it is practically impossible to estimate the numerical error caused by neglecting small off-diagonal elements. Another drawback is that the matrices dealt with are typically singular and need to be regularized before diagonalization. Also we note that the number of the eigenvalues, localized within the

range under consideration, is usually not known a priori, while at the same time the result of spectral estimation depends to a large extent on this preassumed number.

Below we will propose a modification of the approaches mentioned above, which both preserves the advantages of the filter diagonalization machinery and, at the same time, provides the automatic accuracy control at all computational stages, and results in matrices with purely zero off-diagonal elements escaping the necessity to diagonalize singular matrices. We will instead map the spectrum with a given resolution defined by an expected number of eigenvalues inside the interval of interest and simply enlarge the resolution of our mapping accordingly to see a more detailed picture. To proceed to our modification description, we need first to briefly consider the basic properties of the windowing functions employed, i.e., the zero-order prolate spheroidal wave functions.

3. PROLATE SPHEROIDAL WAVE FUNCTIONS AND FINITE FOURIER TRANSFORM

Let us consider eigenvalues and eigenfunctions of the finite Fourier transform:

$$\mu\psi(c, x) = \int_{-\sqrt{c}}^{\sqrt{c}} \exp(ixy)\psi(c, y)\, dy. \tag{4}$$

The eigenvalues μ_l, $l = 0, 1, \ldots$, are proved to be simple, while the corresponding eigenfunctions $\psi_l(c, x)$, $l = 0, 1, \ldots$, are orthogonal on I_c and constitute a complete set in $\mathcal{L}^2(I_c)$.

As is proved, $\sqrt{2\pi} > |\mu_0| > |\mu_1| > \cdots > 0$. In addition, as soon as l exceeds $2c/\pi$, the values of $|\mu_l|$ vanish exponentially fast with increasing l.

Eigenfunctions $\psi_l(c, x)$ can be continued analytically through the complex plane. Defined everywhere in $(-\infty, \infty)$, they compose an orthogonal basis in the class $\mathcal{B}$ of square integrable band limited functions, i.e., those representable as

$$f(x) = \frac{1}{2\pi} \int_{-\sqrt{c}}^{\sqrt{c}} \exp(ixy)\, F[f](y)\, dy. \tag{5}$$

Here and below $F[f]$ is the Fourier transform of f.

The eigenfunction $\psi_0(c, x)$, corresponding to μ_0, is the most concentrated inside I_c, among all functions f from $\mathcal{B}$, of a given total energy $\|f\|^2_\infty = \int_{-\infty}^{\infty} |f(x)|^2 dx$, i.e., has the largest fractional energy $\|\psi_0\|^2_c = \int_{-\sqrt{c}}^{\sqrt{c}} |\psi_0(c, x)|^2 dx$ in I_c:

$$\gamma_0 = \frac{|\mu_0|^2}{2\pi} = \frac{\|\psi_0\|^2_c}{\|\psi_0\|^2_\infty} = \max_{f\in\mathcal{B}} \frac{\|f\|^2_c}{\|f\|^2_\infty}. \tag{6}$$

Analogously, for any $l > 0$

$$\gamma_l = \frac{|\mu_l|^2}{2\pi} = \frac{\|\psi_l\|_c^2}{\|\psi_l\|_\infty^2} = \max_{f\in\mathcal{B}_l} \frac{\|f\|_c^2}{\|f\|_\infty^2}, \tag{7}$$

where $\mathcal{B}_l$ consists of all functions from $\mathcal{B}$ orthogonal to $\psi_0(c, x), \ldots, \psi_{l-1}(c, x)$.

As is well-known (Komarov *et al.*, 1976; Slepian and Pollak, 1961) $\psi_l(c, x)$ coincides up to a scaling factor with the angular prolate spheroidal wave function $S_{0l}(c, \eta)$ for $x \in I_c$, and the radial one $R_{0l}(c, \xi)$ for $x \notin I_c$, with η, ξ related to x by a simple scale change

$$x = \begin{cases} \sqrt{c}\eta & x \in I_c, \\ \sqrt{c}\xi & x \notin I_c. \end{cases}$$

The prolate spheroidal wave functions arise when variables are separated in the Helmholtz equation in prolate spheroidal coordinates (Komarov *et al.*, 1976; Morse and Feshbach, 1953).

Defined inside the interval $(-1, 1)$, the angular spheroidal functions $S_{ml}(\eta)$ are the eigenfunctions of the following selfadjoint Sturm–Liouville singular spectral problem with λ being an eigenvalue

$$\frac{d}{d\eta}(1-\eta^2)\frac{d}{d\eta}S + \left[\lambda + c^2(1-\eta^2) - \frac{m^2}{1-\eta^2}\right]S = 0,$$
$$-1 < \eta < 1, \quad m = 0, 1, \ldots, \tag{8}$$

posed on the set of functions bounded at the singular points $\eta = \pm 1$:

$$|S(\eta)| < \infty, \qquad \eta \to \pm(1-0). \tag{9}$$

These functions are usually normalized by

$$\int_{-1}^{1} S^2(\eta)\, d\eta = 1.$$

For a given number m the angular spheroidal functions $S_{ml}(\eta)$ are enumerated by the number of zeroes $l - m$ each one has inside $I_1 = (-1, 1)$. Hence $l = m, m + 1, \ldots$. In accordance with the parity of $l - m$, $S_{ml}(\eta)$ is either odd or even.

In the case $m = 0$ the solution to (8) bounded at $\eta = \pm 1$ behaves

$$S(\eta) \sim \text{const}, \qquad \text{as } \eta \to \pm(1-0).$$

Function S_{ml} has an analytical continuation, which up to a factor coincides with the radial prolate spheroidal wave function of the first kind—a solution to the equation

$$\frac{d}{d\xi}(\xi^2-1)\frac{d}{d\xi}R_{ml} + \left[c^2(\xi^2-1) - \lambda_{ml}(c) + \frac{m^2}{\xi^2-1}\right]R_{ml} = 0, \quad 1 < \xi < \infty, \tag{10}$$

bounded at $\xi = \pm 1$ and fixed by its asymptotic at infinity

$$R_{ml}^{(1)}(\xi) = \frac{1}{c\xi} \cos\left(c\xi - \frac{l+1}{2}\pi\right) + \mathrm{O}\left(\frac{1}{\xi^2}\right), \quad \xi \to \infty. \tag{11}$$

Like the angular function it is either odd or even depending on $l - m$: $R_{ml}^{(1)}(-\xi) = (-1)^{l-m} R_{ml}^{(1)}(\xi)$. (For more details, see, e.g., Landau and Pollak, 1961; Slepian, 1964; Slepian and Pollak, 1961, 1962, as well as the monographs, Komarov *et al.*, 1976; Morse and Feshbach, 1953, and the literature cited therein.)

Because of their extremal properties as well as their double orthogonality, *prolates* are of special importance in signal, data, and image processing. Nevertheless, they are often reported as functions too difficult to handle numerically. In fact, as far back as in the late eighties in Abramov *et al.* (1984, 1991) a numerical technique was developed, which allowed the computation of both spheroidal wave functions and various functionals of them for arbitrary value m in a wide range of parameter values. In Levitina and Brändas (2001) this technique received a new development.

4. PROLATES FOR FILTER DIAGONALIZATION

We will now proceed with an analysis of the Fourier transform of the autocorrelation function $c(t) = \langle \Psi(\vec{x}, t) | \Psi(\vec{x}, 0) \rangle$. According to (3)

$$F^{-1}[c(t)] = \sum_{k=0}^{\infty} |d_k|^2 \delta(\omega - \epsilon_k). \tag{12}$$

Such a formal representation seems at first useless for practical computations, therefore one usually carries out some kind of a regularization or smoothing in practice, like, e.g., applying the Discrete Fourier Transform instead of (12) (see, e.g., Mandelshtam, 2001). As the next step the filtering process is introduced, which extracts the eigenstates of energies located within a selected interval, say $(\omega - \Omega, \omega + \Omega)$, by suppressing the eigenstates outside this interval.

Up to now we have more or less reviewed existing procedures and numerical techniques. To begin with some new ideas and suggestions, we introduce the function $C_i(\omega)$ as

$$C_l(\omega) = F^{-1}[c(t)] * \theta_l(\omega), \tag{13}$$

where

$$\theta_l(\omega) = \begin{cases} S_{0l}\left(T\Omega, \frac{\omega}{\Omega}\right), & \omega \in (-\Omega, \Omega), \\ 0, & \omega \in (-\infty, -\Omega) \cup (\Omega, \infty). \end{cases} \tag{14}$$

Let further $\Theta_l(t)$ be defined by

$$\Theta_l(t) = \begin{cases} S_{0l}\left(T\Omega, \frac{t}{T}\right), & t \in (-T, T), \\ \rho_l R_{0l}^{(1)}\left(T\Omega, \frac{t}{T}\right), & t \in (-\infty, -T) \cup (T, \infty). \end{cases}$$

Above the radial function $R_{ol}^{(1)}(\cdot)$ is multiplied by the factor ρ_l to make it the analytical continuation of the angular part. Then, according to (4), we obtain the relations

$$F[\theta_l(w)] = (-1)^l \mu_l \sqrt{\frac{\Omega}{T}} \Theta_l(t) \quad F^{-1}[\theta_l(\omega)] = \frac{\mu_l}{2\pi} \sqrt{\frac{\Omega}{T}} \Theta_l(t) \tag{15}$$

(we remind that the parity both of $\theta_l(\omega)$ and $\Theta_l(t)$ is defined by that of l). Hence, one can compute $C_l(\omega)$ as

$$C_l(\omega) = F^{-1}[c(t)F[\theta_l(\omega)]] = \frac{(-1)^l}{2\pi} \mu_l \sqrt{\frac{\Omega}{T}} \int_{-\infty}^{\infty} e^{i\omega t} c(t) \Theta_l(t)\, dt. \tag{16}$$

We emphasize that the right-hand side of (16) may be evaluated as accurate as desired, with the numerical technique, advertised in Levitina and Brändas (2001), provided $c(t)$ is known at an arbitrary time t. Furthermore, for $l < 2T\Omega/\pi$ the integral there might be approximated by

$$\int_{-T}^{T} e^{i\omega t} c(t) \Theta_l(t)\, dt.$$

It follows from (6) and (7) that the error made by this approximation is majorated by

$$\max_{t \in \mathcal{R}} |c(t)| \left\{ \int_{-\infty}^{\infty} |\Theta_l(t)|^2\, dt - \int_{-T}^{T} |\Theta_l(t)|^2\, dt \right\}^{1/2} \leq \max_{t \in \mathcal{R}} |c(t)| \sqrt{T} \left\{ \frac{1 - \gamma_l}{\gamma_l} \right\}^{1/2}. \tag{17}$$

With increasing $T\Omega$, this value becomes negligibly small for $l < 2T\Omega/\pi$ and almost infinite otherwise. Thus, to achieve a good accuracy in the calculation of $C_l(\omega)$ is easier in the case of relatively large values of $T\Omega$.

Obtained directly from (12) and (13), $C_l(\omega)$ is

$$C_l(\omega) = \sum_{\epsilon_k \in (\omega - \Omega, \omega + \Omega)} |d_k|^2 \theta_l(\omega - \epsilon_k). \tag{18}$$

By the definition (14) the function $\theta_l(\omega)$ is of finite support, and therefore the equality (18) is exact, compare the treatment in Mandelshtam (2001).

In the present approach one can "play" with two characteristic parrameters and their respective intervals of interest namely time and frequency. The smaller the value of Ω is, the smaller is the number of eigenstates located inside $(\omega - \Omega, \omega + \Omega)$. If the eigenvalues are separated by some constant distance, Ω may

be chosen so that every interval $(\omega - \Omega, \omega + \Omega)$ contains at most one eigenvalue. Suppose inside a particular interval $(\omega - \Omega, \omega + \Omega)$ there is a unique eigenvalue ϵ_K. To find its precise location, a single value $C_l(\omega)$ of a particular index l is not enough. Instead it may be obtained from $e^{-i\epsilon_K}$, which is expressed in terms of $C_l(\omega)$, $l = 0, 1, \ldots$. In view of (15) and (16) one can now compute at an arbitrary $t_* \neq 0$:

$$e^{i(\omega-\epsilon_K)t_*} = \frac{1}{\sqrt{T\Omega}} \sum_{l=0}^{\infty} \mu_l \theta_l(\omega - \epsilon_K)\Theta_l(t_*) = \frac{1}{\sqrt{T\Omega}|d_K|^2} \sum_{l=0}^{\infty} \mu_l C_l(\omega)\Theta_l(t_*). \tag{19}$$

Therefore $|d_K|$ and ϵ_K can be readily extracted from the absolute value and the argument of the sum $\sum_{l=0}^{\infty} \mu_l C_l(\omega)\Theta_l(t_*)$, respectively.

It may, however, happen in the computations that $e^{i(\omega-\epsilon_K)t_*} \approx 1$; then to avoid ambiguity in determining ϵ_K the basic frequency can be shifted a little. Note that, if the shifted interval $(\omega' - \Omega, \omega' + \Omega)$ contains the same eigenvalue as $(\omega - \Omega, \omega + \Omega)$, then

$$\frac{\sum_{l=0}^{\infty} \mu_l C_l(\omega)\Theta_l(t_*)}{\sum_{l=0}^{\infty} \mu_l C_l(\omega')\Theta_l(t_*)} = e^{i(\omega-\omega')t_*}. \tag{20}$$

At this point we remind the readers that the only sources of in-accuracies are the numerical integration in the right side of (16) and the truncation of the infinite series (19) by summing the first terms of $l \leq \frac{2T\Omega}{\pi}$. In both cases the error may be easily estimated a priori and expressed through the parameters $\|\hat{H}\|$, T, Ω, uniformly in ω. However in practice a very narrow interval Ω might be required to localize a single eigenvalue. Therefore, to preserve the accuracy, one has to enlarge T respectively (see above).

Alternatively one can treat the interval $\omega_{\min}$, $\omega_{\max}$, containing several eigenvalues ϵ_k, $k = K, K+1, \ldots, K+p$. The problem at hand is then reducible to a linear one (see, e.g., the details in Mandelshtam, 2001). Let $\omega_{\min} + \Omega = \omega_1, < \omega_2 < \cdots < \omega_M = \omega_{\max} - \Omega$, where the number M should be selected so that the linear system to be considered below is resolvable (see Mandelshtam, 2001).

To proceed, we introduce an analogue of the Fourier basis considered in Mandelshtam (2001). For any $s \leq M$ and $l \leq L \leq \frac{2T\Omega}{\pi}$ we define[4]

$$\Phi_{sl}(\vec{x}) = F^{-1}[\Psi(\vec{x}, t)] * \theta_l(\omega)|_{\omega=\omega_s}.$$

As can be readily seen

$$\Phi_{sl}(\vec{x}) = \frac{(-1)^l}{2\pi} \mu_l \sqrt{\frac{\Omega}{T}} \int_{-\infty}^{\infty} e^{i\omega_s t} \Psi(\vec{x}, t)\Theta_l(t)\, dt.$$

[4] Here and below we keep both indexes s, l in order to emphasize the possibility to vary any of parameters M, L. In actual calculations one has first to enumerate the Fourier basis elements sequentially.

and therefore with the initial wave package $\Psi(\vec{x}, 0)$ we obtain

$$\langle \Phi_{sl}(\vec{x}) | \Psi(\vec{x}, 0) \rangle = \frac{(-1)^l}{2\pi} \mu_l \sqrt{\frac{\Omega}{T}} \int_{-\infty}^{\infty} e^{i\omega_s t} c(t) \Theta_l(t)\, dt = C_l(\omega_s).$$

At the same time

$$\Phi_{sl}(\vec{x}) = \sum_{k=K}^{K+p} |d_k|^2 \theta_l(\omega_s - \epsilon_k) \Psi_k(\vec{x}), \tag{21}$$

which means that $\Phi_{sl}(\vec{x})$ is a linear combination of eigenfunctions $\Psi_k(\vec{x})$, $k = K, K+1, \ldots, K+p$. Again we note that the above equality is exact. Let the matrix B of elements b_q^{sl} establish the inverse relation

$$\Psi_q(\vec{x}) = \sum_{\substack{s \le M \\ l \le L}} b_q^{sl} \Phi_{sl}(\vec{x}).$$

Then for any arbitrary t

$$\hat{U}(t) \Psi_q(\vec{x}) = \sum_{\substack{s \le M \\ l \le L}} b_q^{sl} \hat{U}(t) \Phi_{sl}(\vec{x}) = e^{i\epsilon_q t} \Psi_q(\vec{x}) = e^{i\epsilon_q t} \sum_{\substack{s \le M \\ l \le L}} b_q^{sl} \Phi_{sl}(\vec{x})$$

and multiplying the relation by Φ_{rp}, we obtain the generalized eigen-value problem

$$\sum_{\substack{s \le M \\ l \le L}} b_q^{sl} U_{sl}^{rp} = e^{i\epsilon_q t} \sum_{\substack{s \le M \\ l \le L}} b_q^{sl} W_{sl}^{rp}. \tag{22}$$

Here $\vec{b}_q = (\ldots, b_q^{sl}, \ldots)^T$ stands for the q^{th} eigenvector, corresponding to the eigenvalue $e^{i\epsilon_q t}$, and the matrix elements U_{sl}^{rp}, W_{sl}^{rp} are computed by the formulas

$$\begin{aligned} U_{sl}^{rp} &= \langle \Phi_{rp}(\vec{x}) | \hat{U}(t) | \Phi_{sl}(\vec{x}) \rangle = \frac{(-1)^{l+p}}{4\pi^2} \mu_l \mu_p \frac{\Omega}{T} \\ &\quad \times \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i\omega_r t'} \Theta_p(t')\, e^{-i\omega_s t''} \Theta_l(t'') c(t' - t'')\, dt'\, dt'', \\ W_{sl}^{rp} &= \langle \Phi_{rp}(\vec{x}) | \Phi_{sl}(\vec{x}) \rangle = \frac{(-1)^{l+p}}{4\pi^2} \mu_l \mu_p \frac{\Omega}{T} \\ &\quad \times \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i\omega_r t'} \Theta_p(t')\, e^{-i\omega_s t''} \Theta_l(t'') c(t' - t'')\, dt'\, dt''. \end{aligned}$$

The above integrals may be truncated and approximated by the integrals over the domain $[-T, T] \times [-T, T]$; the truncation error estimate is obtained then in a similar way as in (17).

Since the system (22) is exact, the only source of inaccuracy is the numerical evaluation of the matrix elements. However, the latter procedure may constitute

an essential difficulty, even if the machinery presented in Levitina and Brandas (2001) is applied.

To avoid this, we will concentrate on the Eqs. (18)–(20). After evaluating $C_l(\omega_s)$ according to (16), we combine them as

$$C(\omega_s) = \sum_{t=0}^{\infty} \mu_l C_l(\omega_s) \Theta_l(t_*), \tag{23}$$

which is nothing but

$$\begin{aligned} C(\omega_s) &= \sqrt{T\Omega} \sum_{\epsilon_k \in (\omega_s - \Omega, \omega_s - \Omega)} |d_k|^2 \, e^{i(\omega_s - \epsilon_k)t_*} \\ &= \sqrt{T\Omega}\, e^{i\omega_s t_*} \sum_{\epsilon_k \in (\omega_s - \Omega, \omega_s - \Omega)} |d_k|^2 \, e^{-i\epsilon_k t_*}. \end{aligned} \tag{24}$$

One can offer various approaches to extract eigenvalues from (24). What we present below is certainly not yet optimal.

We suggest to repeat the computation twice: first for the interval $\omega_s \pm \Omega$, and a second time for $\omega_{s+1} \pm (\Omega - \Delta\omega)$, where $\Delta\omega = \omega_{s+1} - \omega_s$ is a characteristic grid-size. Then the difference $\Delta_s = e^{-i\omega_s t_*} C_\Omega(\omega_s) - e^{-i\omega_{s+1} t_*} C_{\Omega - \Delta\omega}(\omega_{s+1})$ reveals the eigenvalues enclosed in $I_s = (\omega_s - \Omega, \omega_{s+2} - \Omega)$.

Let us for instance assume that $2 \times \Delta\omega$ is smaller than a typical distance between two eigenvalues. Suppose the residue Δ_s is not zero within the given accuracy of computations. (The opposite would mean that there are no eigenvalues within I_s, or more accurate, that no knowledge on the eigenvalues inside I_s is contained in $c(t)$, see section 5.) Then the eigenvalue $\epsilon_k \in I_s$ is to be extracted from the phase of Δ_s, while the asociated coefficient d_k follows from its argument. Like in Mandelshtam (2001), there is no necessity to explicitly construct the filtered states, if only the spectrum is sought.

On the contrary, if needed, the corresponding eigenfunction Ψ_k may be expressed in terms of Φ_{sl} from Eq. (22).

The proposed technique resembles cartography. The considered interval is split into small subintervals—cells. Each cell is inspected to contain eigenvalues. Those containing eigenvalues may be treated as "eigencells." The associated eigenvectors are linear combinations of actual eigenvectors, corresponding to the eigenvalues hidden inside the cell. When increasing the resolution, i.e., splitting the interval into smaller cells, we get more accurate knowledge about the eigenvalue location. Under the given assumptions on the Hamitonian, we necessarily gain such a resolution that each cell contains at most one eigenvalue, i.e., more resolution would add no new eigenvalues. As a result, as usual, the block of the Hamiltonian matrix corresponding to the spectrum laying inside the interval in hand is diagonalized.

5. DISCUSSION AND CONCLUSIONS

We present a practical procedure for the description of computing eigenvalues and eigenfunctions for a selfadjoint operator of a general nature. The present approach is based on the Filter Diagonalization technique, with prolate spheroidal wave functions being employed for the filtering. Exclusive properties of prolates, investigated by Slepian *et al*. (Landau and Pollak, 1961; Slepian, 1964; Slepian and Pollak, 1961, 1962), as well as the relevant numerical machinery, invented by Abramov *et al.* (1984, 1991) and further developed by Levitina and Brändas (2001), enable efficient extraction of eigenvalues and eigenfunctions, at the same time keeping check on the accuracy at any computational stage.

The spectrum of the operator is assumed to consist of simple eigenvalues but, as appears from the above description, this condition is only used locally inside the interval under study.

It is also clear that the presented approach allows the detection of multiple eigenvalues, albeit with no opportunity to determine their multiplicity. From a computational viewpoint, closely situated and coinciding (multiple) eigenvalues are undistinguishable for lack of resolution and the present procedure treats them as single simple eigenvalues. Note however that this drawback occurs in all other known analogous, employing the autocorrelation function.

The point is here that the autocorrelation function involves no other "information" on the spectrum than that presented in the initial wave packet. It is therefore not possible to extract from (21) an eigenstate orthogonal to the initial wave packet from its propagation: only those eigenvalues will be detected, which have nonzero expansion coefficients, i.e., $d_k \neq 0$. Ideally, the initial packet should be a generating element for the operator $\hat{H}$. To accurately extract a multiple eigenvalue a single wave packet propagation is not enough; a so-called generating basis is needed (see Naimark, 1967).

Nevertheless our suggestions lead us to a new approach where one may increase the resolution practically without any severe limitations from, e.g., the uncertainty principle. Namely the latter restricts the product $T\Omega$, while the resolution is defined by the grid-size $\Delta\omega$. The former knowledge, i.e., that corresponding to, let us say, the parameters M and Ω, remains valid for computational purposes with $2M$ and/or $\Omega/2$.

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