Comment on "Spectral filters in quantum mechanics: A measurement theory perspective"

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We criticize a paper by Vijay and Wyatt [Phys. Rev. E **63**, 4351 (2000)], in which the authors suggest that energy levels computed, from the same set of matrix-vector products, with the filter diagonalization method (FDM) and the Fourier spectral analysis using the same Chebyshev correlation function are of comparable accuracy. We explain why the FDM is superior and demonstrate it numerically, using the same test matrix as that employed in the above paper. We also compare the FDM with the Lanczos method, another commonly used iterative technique for computing eigenvalues. We find that eigenvalues in a low-density region near the middle of the spectrum converge more quickly with the FDM, but that the Lanczos method requires fewer matrix-vector products to converge all the eigenvalues.

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In a recent paper [1], Vijay and Wyatt (VW) presented a controversial interpretation of the filter diagonalization method (FDM) in terms of "measurement theory." In addition, the authors questioned previous statements that the FDM could "bypass the Fourier transform (FT) uncertainty principle" (e.g., in Refs. [2–5]), appealing to both "the fundamental principles of quantum mechanics" and their numerical calculations. We disagree with the interpretation by VW of their own numerical result, which led to the incorrect conclusions about the relative efficiencies of the FDM and FT spectral analysis. We avoid any philosophical discussion and concentrate on practical issues. We clarify the "bypass the FT uncertainty principle" statement and show that energy levels obtained from the FDM are clearly better than the FT results reported in Ref. [1], thus demonstrating the validity of the statement. In addition, we compare the FDM and the Cullum and Willoughby (CW) Lanczos approach [11].

The FDM is a high-resolution linear algebraic technique for spectral analysis of time signals. It is based on the solution of a harmonic inversion problem [2–4]. In [3], for a Hermitian $K\times K$ Hamiltonian matrix $\mathbf{H}$, it was shown how the FDM can be used to process a Chebyshev correlation function, $c_n=\langle\Phi|T_n(\mathbf{H})|\Phi\rangle$, by fitting it to the form

$$c_n=\sum_{k=1}^{K} d_k\cos(n\omega_k),\quad n=0,\ldots,N, \tag{1}$$

to extract amplitudes d_k and frequencies ω_k and thereby determine eigenvalues of $\mathbf{H}$. For convenience, without loss of generality, it is assumed here that the spectrum of the Hamiltonian matrix $\mathbf{H}$ is restricted to the interval $[-1,1]$. The frequencies yield the eigenvalues of $\mathbf{H}$ according to $E_k=\cos(\omega_k)$. To avoid missing eigenvalues, one usually uses a random starting vector Φ (unless some additional information about the system is available), for which it is unlikely that any of the d_k would be so small as to hinder the convergence of ω_k.

The spectral analysis of the same sequence $\{c_n\}$ can also be performed in the frequency domain by analyzing the finite FT spectrum [6,7],

$$\rho(E)=[1-\cos(\omega)]^{-1/2}\sum_{n=0}^{N}(1-\delta_{n0}/2)\cos(n\omega)c_n f_n,$$

$$E=\cos(\omega), \tag{2}$$

using an appropriate apodization function f_n (to remove the wiggles resulting from the truncation of the signal). If the assumption of Eq. (1) is satisfied (which is the case here), the FDM significantly outperforms the FT analysis for the problem of extracting the eigenvalues of $\mathbf{H}$. To be more quantitative, the spectral resolution of the finite FT is defined by the FT uncertainty principle,

$$\delta\omega\sim\pi N^{-1}\quad\text{or}\quad\delta E\sim\pi\sqrt{1-E^2}N^{-1}. \tag{3}$$

(Note that the spectral range of H is 2 and that the frequency is mapped to energy according to $E=\cos\omega$.) This restriction on the accuracy of the FT spectrum limits the accuracy of the eigenvalues E_k extracted from the positions of the maxima of $\rho(E)$.

It is very well documented that the eigenfrequencies ω_k and, therefore, the eigenvalues E_k can, generally, be estimated much more accurately, from the same set of c_n's, using the FDM. This is true simply because by assuming the form of Eq. (1) one exploits important additional information about the signal, which is ignored in the FT spectral analysis. A simple algebraic analysis leads to the conclusion that there is no fundamental lower bound to the error in the eigenvalues determined from the solution of the harmonic inversion problem (1) by the FDM, provided the local average spacing of the eigenfrequencies ω_k or eigenvalues E_k satisfy the approximate relationships

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$$\langle \Delta\omega \rangle > 2\pi N^{-1} \quad \text{or} \quad \langle \Delta E \rangle > 2\pi\sqrt{1-E^2}N^{-1}. \tag{4}$$

This, in particular, means that the eigenvalues at the edges of the spectrum and in the sparse spectral regions will converge more quickly than those in the dense regions. The FDM computes eigenvalues in a subspace. The signal length N used in the spectral analysis implies an underlying Krylov basis size of $M=N/2$. Due to the subspace aspect, once an eigenvalue has started to converge, its error will decay exponentially as N increases, so just a slight increase of N can increase the accuracy by orders of magnitude [3]. This should be compared to the FT error estimate (3), that decays as slowly as N^{-1}. Of course, this unfavorable convergence rate cannot be bypassed by any accurate method to locate the maxima in the FT spectrum, as suggested without any verification by VW, because the ''information'' is already lost by implementing the truncated FT. However, in order to make a more accurate prediction of the rate of convergence one should take into account the actual distribution of the E_k's, roundoff errors, noise, the algorithm implementation, etc. For more details and numerical examples, we refer the reader to the literature (see, e.g., Refs. [2–5,8–10]).

Statements in previous papers claiming that the FDM bypasses the uncertainty principle were not meant to imply that a *single* filtered basis function had any properties that violated the uncertainty principle. Note that in the FDM, the individual filtered basis functions are only intermediate results, used as stepping stones to obtain eigenvalues. Instead, the statements were simply meant to indicate that, if one uses the FDM and the FT to compute the underlying frequencies and, in particular, the energy levels, from the same sequence $\{c_n\}$ (i.e., using the same number of matrix-vector products), the FDM estimates of the eigenvalues will always be more accurate. On the other hand, the FDM estimate of the infinite-time Fourier spectrum (i.e., a spectrum as a function of the real frequency) obtained from truncated time domain data will not always be better than the finite FT spectral estimate. In fact, there are published examples of signals that did not fit well with the form of the harmonic inversion problem (not the case here), for which a FT provided a better spectral estimate than that of the FDM (see, e.g., Ref. [10]). Note that there is no need to choose an artificial starting vector (e.g., one computed from eigenvectors of the Hamiltonian matrix) to obtain excellent results with the FDM.

To support our statements, we examine the numerical results reported by VW [1] and compare them with our own FDM calculations. We use their 2000×2000 test matrix. We use $C=0.04$ which is the value also used by VW (although $C=0.05$ is indicated in the paper). The eigenvalues of this matrix form 10 bands. Within each band, the eigenvalue gap is a smooth function of energy and can, therefore, be associated with the locally averaged spacing $\langle \Delta E \rangle$, except for the eigenvalues at the edges of the bands.

As far as we understand, the FDM version of Ref. [3] was rederived and used by VW in Appendix A of Ref. [1]. To use the FDM well, it is important to choose the width of the spectral window, $W=|\omega_{\max}-\omega_{\min}|$ (in the frequency domain), the number of Fourier basis functions in the window, L, consistently with the signal length N, and to ensure that converged results are obtained with as few matrix-vector products as possible. VW used the same values of L and W regardless of N. Instead, it is better to choose L and W so that they vary with N. The best performance is achieved when the following approximate condition for W, L, and N is satisfied [3]:

$$L/W \geqslant N/2\pi. \tag{5}$$

(It is usually safe to use $L/W=1.1N/2\pi$ if L is not too small. Also, note that L should not be chosen bigger than the size of the Krylov subspace $M=N/2$ to avoid the use of a linear-dependent basis.) When for a particular N the eigenvalues are not converged, N is increased. As long as Eq. (5) holds, one has some flexibility in choosing the parameters L and W, e.g., one can keep L fixed and decrease W, or fix W and increase L. It is also important to realize that, if condition (4) is nearly satisfied for a particular $N=N_0$, then increasing N substantially with Eq. (5) satisfied will result in a very ill-conditioned generalized eigenvalue problem, that must be handled with care. The approach used by VW (i.e., fix L and W and increase N) is very dangerous as well because for large values of N, when $L/W<N/2\pi$, it may lead to poorly converged or even missing eigenvalues.

To fairly compare the performance of the FDM and FT, one must compare eigenvalues computed with both methods to numerically exact eigenvalues. According to Table III of Ref. [1], the FDM results for most of the eigenvalues in a small energy window consisting of 33 eigenvalues are converged to at least eight figures if one uses a signal of length $N=13\,000$ ($M=6500$ matrix-vector products). Of course, eigenvalues in sparser regions and at the edges of the energy bands converge more quickly. Also, note that it is often unnecessary to compute eigenvalues to this accuracy. Our FDM results (see below) indicate that most energy levels in this window can be computed with fewer matrix-vector products. According to Eq. (3), to calculate the eigenvalues to (a more reasonable), say, six digit, accuracy by FT spectral analysis, one would need, roughly, $N\sim10^6$ or $N\sim10^5$ (both estimates are much larger than the N required to obtain converged eigenvalues with the FDM).

In their Fig. 2, VW show the spectrum $\rho(E)$ computed from Eq. (2) with $f_n=1$ and using $N=13\,000$. The authors claim that their figure has 35 peaks. In addition, they claim that first and second derivative plots reveal that two peaks are spurious and conclude that the FT spectrum correctly estimates the eigenvalues and that the performance of the FDM and FT is similar. In Fig. 1, we reproduce the upper panel of Fig. 2 of Ref. [1] and superimpose the exact eigenenergies from Table III of Ref. [1]. Clearly, the positions of only several of the largest peaks correspond to accurate eigenvalues. The other peaks (more than two) are spurious. Where the spectrum is dense there are fewer peaks than eigenvalues, while where the spectrum is sparse, there are extra peaks. Some of the ''spurious FT peaks'' are quite large, even larger than the true unresolved peaks, and that is why the latter are not seen. These spurious peaks are caused by the sinc wiggles of the strong peaks resulting from the truncation of the Fourier series in Eq. (2). We note that with

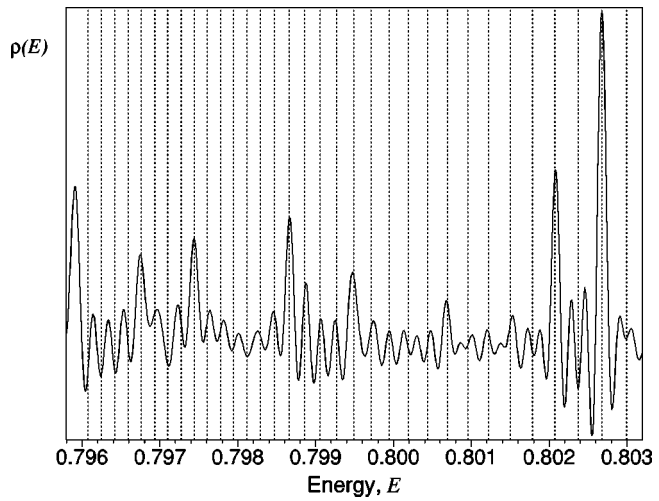

FIG. 1. The finite FT spectrum (solid line) of a Chebyshev correlation function reproduced from Fig. 2 of Ref. [1]. It was computed by Eq. (2) with $f_n=1$ and $N=13\,000$ ($M=6500$ matrix-vector products). The dotted lines show the positions of the exact eigenenergies. The latter could be computed to eight digit accuracy for most eigenvalues in this window using the FDM.

a more appropriate apodization function f_n (e.g., Gaussian) the sinc wiggles could be suppressed and fewer (than 33) peaks would appear in the spectrum. In this case, it would become apparent that, unless an artificial starting vector is used, a much longer signal would be required to reproduce even the right number of eigenvalues. Note that when comparing the number of matrix-vector products required to compute energy levels by extracting them from $\rho(E)$ and by using the FDM, it is essential to compare energy levels of similar accuracy. It would, for example, be misleading to compare the number of matrix-vector products required to reproduce the right number of peaks in $\rho(E)$ with the number of matrix-vector products required using the FDM to compute eigenvalues to eight significant figures.

As has been clarified and re-demonstrated in the present paper, the FDM is an efficient tool for calculating energy levels. It does enable one to calculate energy levels with fewer matrix-vector products than would be required if one used an FT. It is the diagonalization aspect that enables the FDM to ''bypass the Fourier transform uncertainty principle.'' Each vector of the FDM subspace is a linear combination of the Krylov vectors $\mathbf{v_0}, \mathbf{v_1}, \ldots, \mathbf{v_M}$, where $\mathbf{v_k} = \mathbf{H^k\Phi}$ and $\mathbf{\Phi}$ is a starting vector. With exact arithmetic (i.e., no roundoff errors) and with $M \geqslant L \geqslant K$, where K is the size of $\mathbf{H}$, the FDM eigenvalues are exact even if $M=N/2$ is smaller than that defined by condition (4). In practice, to reduce the size of the matrix whose eigenvalues are computed and make the method more numerically stable, one chooses $L \ll K$ and chooses M using Eq. (4). This makes the FDM numerically stable at the price of slowing down the convergence (as compared to the unrealistic case of a calculation in exact arithmetic with a larger value of L and a smaller value of M).

The Lanczos method extracts eigenvalues of $\mathbf{H}$ from the same set of Krylov vectors. In the Lanczos method, the Kry-

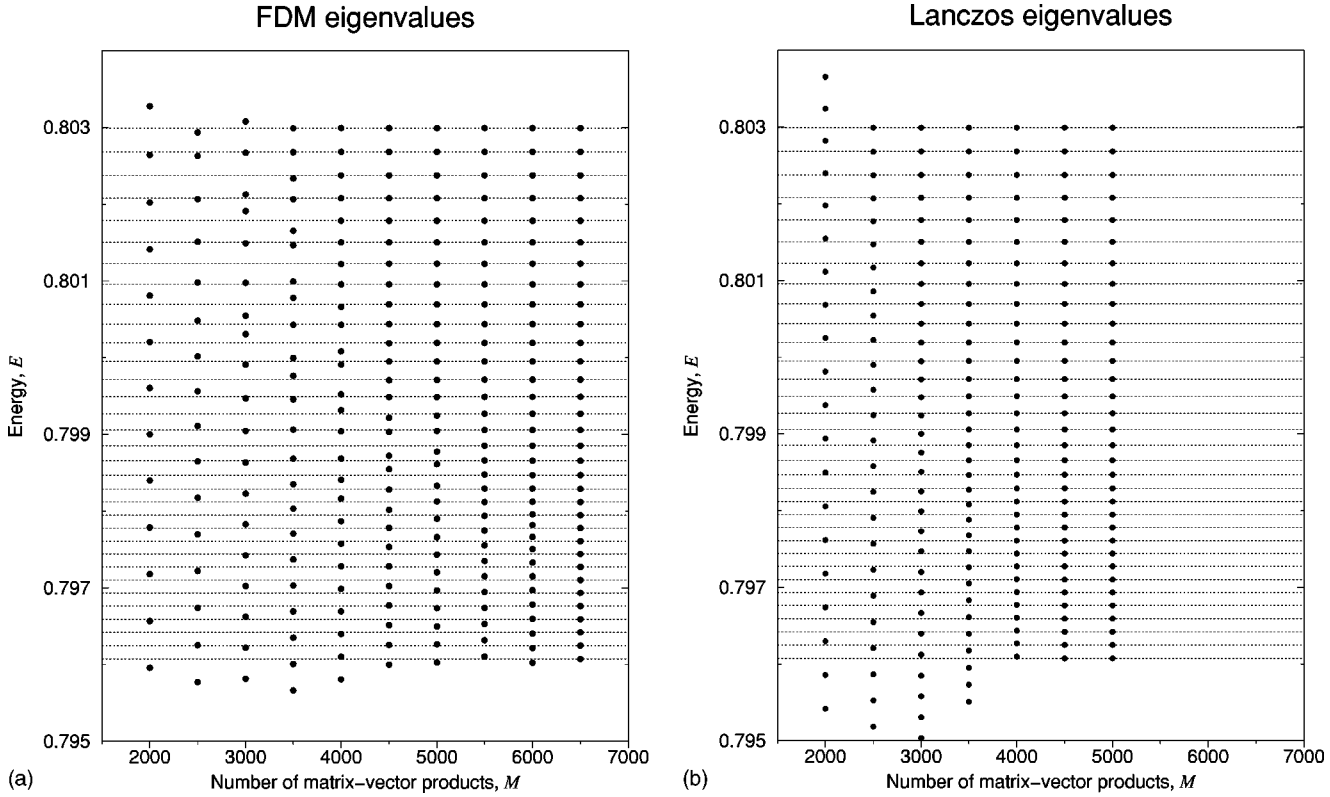

FIG. 2. Convergence behavior of the FDM and the Lanczos method for the energy window of Fig. 1. The exact eigenvalues are shown with dotted lines.

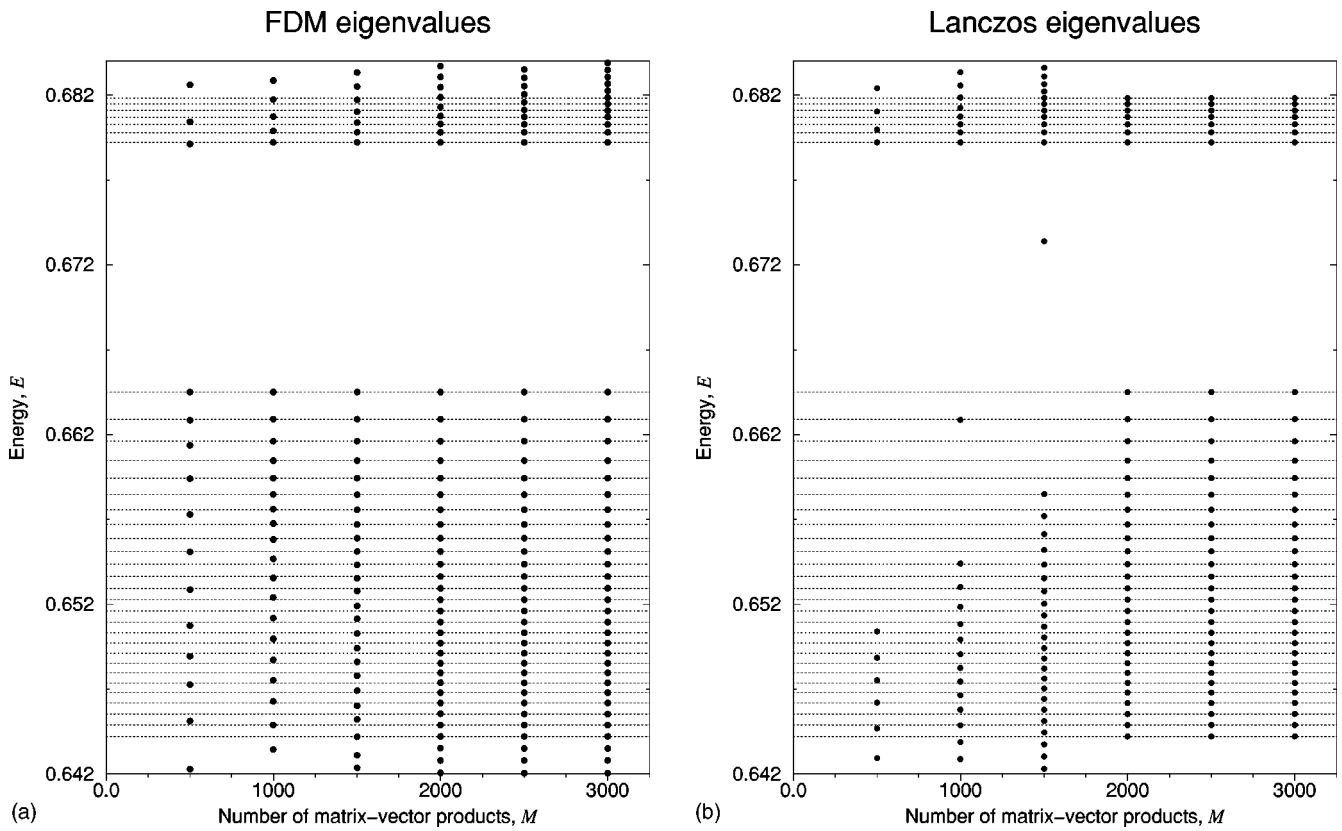

FIG. 3. Same as Fig. 2, but for another energy window, corresponding to Table IV of Ref. [1]. Note that the eigenvalue distribution is much less uniform here.

lov vectors are combined to yield (formally) orthogonal Lanczos vectors. From the Lanczos vectors, one computes the nonzero elements of a tridiagonal matrix $\mathbf{T_M}$, some of whose eigenvalues are also eigenvalues of **H**. Although, in practice, the orthogonality of the Lanczos vectors is lost because of roundoff errors, it is still possible to compute numerically exact eigenvalues of **H** by calculating eigenvalues of $\mathbf{T_M}$ [11]. The FDM and the Lanczos method, therefore, share many advantages. Both require only evaluating matrix-vector products and both can be implemented by storing only a few vectors. The FDM and the Lanczos method obtain eigenvalues from the same Krylov subspace but they exploit different strategies for reducing the matrix representation in the Krylov basis to something manageable. The subspace spanned by the Lanczos vectors is larger than the subspace spanned by the filtered vectors in the FDM. Therefore, in exact arithmetic (or when the roundoff errors are irrelevant) the Lanczos algorithm would always yield more accurate eigenvalues. With finite arithmetic it is not obvious whether the FDM or the Lanczos strategy will be better. Some results indicate that the Lanczos method is sometimes more efficient [12,13].

For the matrix considered by VW, we have compared the FDM and the Lanczos algorithm. Spurious eigenvalues of $\mathbf{T_M}$ are detected and removed using the test of CW [11]. The results for two representative energy windows are shown in Figs. 2 and 3 corresponding to, respectively, Tables III (and Fig. 1 here) and IV of Ref. [1]. For each figure, when changing N we implemented a fixed energy window with the size by about 10% bigger than that reported by VW (to exclude the poorly converged eigenvalues at the edges of the window) and using $L=1.1WN/2\pi$ according to Eq. (5). First, note that the number of matrix-vector products required to converge the eigenvalues using the FDM is, indeed, approximately inversely proportional to the locally averaged energy gap. Therefore, the statements by VW in Ref. [1], that the eigenvalues in Table III (Fig. 2 here) required $M=6500$ and in Table IV (Fig. 3 here) $M=3500$ for the FDM to converge, are quite misleading. It is well known that widely spaced eigenvalues and eigenvalues closer to the top (or bottom) of the spectrum generally converge with fewer Lanczos iterations [11]. Apparently, the FDM also follows this rule. The eigenvalues of Fig. 3 are more widely spaced and, therefore, converge more quickly by both methods than the eigenvalues of Fig. 2. Convergence is more sudden when using the Lanczos method. Note that some FDM eigenvalues in the sparse energy region near the middle of the spectrum (see Fig. 3) were converged with fewer matrix-vector products than their Lanczos counterparts. However, the Lanczos method converged at $M\sim4500$ for all the 2000 eigenvalues of this matrix, while $M\sim6500$ was needed to converge all the eigenvalues by the FDM.

To conclude, we have clarified the issue of the relative efficiency of spectral analyses by the FDM and FT and demonstrated for the test matrix of Ref. [1] that the FDM is substantially more efficient. We have also compared the FDM and the Lanczos method. The convergence of the FDM is more uniform and predictable and may be faster for certain

eigenvalues in the sparse spectral regions of the test matrix considered, while to converge all the eigenvalues of this matrix, the Lanczos method required less matrix-vector products than FDM.

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