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

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We address the issues raised in the preceding comment by Mandelshtam and Carrington [Phys. Rev. E **65**, 028701 (2002)], concerning the eigenvalue determination by the spectral filter methods. We argue that the Fourier transformation is the building block of all currently known time-domain spectral filter algorithms, and, therefore, the time-energy uncertainty principle affects them all in a similar manner. We also explain the situation when the correlation function method may be less suitable, in comparison to the filter diagonalization method, for the determination of eigenvalues, even though both share the same fundamental principles.

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Measurement theory, which has been known since the inception of quantum mechanics, is based on the notion of the delta function as a limiting process taking place in the Hilbert space (which is assumed to be complete) and this notion is the fundamental thesis behind all currently known time-domain spectral filter algorithms, as popularized by the work of Wall and Neuhauser [1]. This fact, which was amply elaborated by us in Ref. [2], has been ignored by Mandelshtam and Carrington Jr. (MC) (preceding comment) [3], who prefer to dismiss the measurement analysis as a mere "philosophical" discourse and hence "controversial." This is unfortunate. In the following, we argue that the filter diagonalization method (FDM) is a straightforward implementation of the notion of the delta function as a selective measurement, contrary to the MC's claim of this being a purely signal fitting problem. In fact, MC's description of the FDM as a "harmonic inversion" problem, though conceptually correct, misses the real issues. MC also compare the performance of the FDM with the correlation function method (CFM), for the purpose of eigenvalue location. As we elaborate in the following, this comparison is misplaced as it completely glosses over the issue of spectral intensities. We also point out that the role of the time-energy uncertainty principle can be discussed separately for the FDM and the CFM, and there is no reason to mix them to address this issue. We first briefly summarize the principles behind the FDM and the CFM.

The FDM consists of two parts: (a) filtering a set of wave functions, $|\phi(x,E_m)\rangle$, from an arbitrary state, $|\psi(x,t=0)\rangle$, which is not orthogonal to the eigenstates of the Hamiltonian, and, (b) diagonalizing the Hamiltonian in the subspace of filtered wave functions, $|\phi(x,E_m)\rangle$, to finally compute the spectrum. In step (a), one employs the integral representation of a limiting approximation to the delta function, $\delta(E-\hat{H})$, where E and $\hat{H}$ are the filter energy and the system Hamiltonian, respectively. One example of this limiting approximation is $1/(\pi\zeta)\mathrm{sinc}([E-\hat{H}]/\zeta)$, where $\mathrm{sinc}(x)=\sin(x)/x$, in the limit $\zeta\to 0$. Thus we have

$$|\phi(x,E_m)\rangle=\delta(E_m-\hat{H})|\psi(x,0)\rangle = \lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{+T} dt\, e^{i(E_m-\hat{H})t}|\psi(x,0)\rangle. \quad (1)$$

The filtering step is accomplished in practice by using a Chebyshev polynomial expansion [4] for the time evolution operator in Eq. (1), $e^{-i\hat{H}t}$, interchanging the integration and the summation operations, and finally carrying out the integration over the time variable analytically [5]. This gives the following infinite series expansion for the filtered wave functions:

$$|\phi(x,E_m)\rangle=\frac{2}{\Delta\lambda}(1-\overline{E}_m)^{-1/2}\sum_{k=0}^{N\to\infty}(2-\delta_{k0})T_k(\overline{E}_m)T_k(\overline{H})|\psi(x,0)\rangle, \quad (2)$$

where $\overline{E}_m$ and $\overline{H}$ are the normalized filtered energy and Hamiltonian, respectively, and $\Delta\lambda$ is the scaling parameter. In this way, the overlap and the Hamiltonian matrix elements required for subspace diagonalization in step (b) involve a product of two infinite series [Eq. (2)] and it turns out that a partial summation of this double infinite series can be done analytically, leaving behind a single infinite series [2,6]. The final results are shown in Ref. [2]. Our analysis thus shows that the FDM is a Fourier transformation (FT), that is, Eq. (1), followed by diagonalization. We believe this is what has been called a "harmonic inversion" in the filter diagonalization literature as well as by MC in the preceding comment [3].

Similarly, the CFM also consists of two parts: (a) filtering spectral intensities, $C(E_m)=\langle\psi(x,0)|\phi(x,E_m)\rangle$, (rather than wave functions as is done in FDM), and (b) location of zeroes of $dC(E)/dE$ to determine the eigenvalue positions. For step (a) we use the Fourier integral theorem as follows:

$$C(E_m)=\langle\psi(x,0)|\delta(E_m-\hat{H})|\psi(x,0)\rangle = \lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{+T}\langle\psi(x,0)|e^{i(E_m-\hat{H})t}|\psi(x,0)\rangle = \frac{4}{\Delta\lambda}(1-\overline{E}_m)^{-1/2}\sum_{k=0}^{N\to\infty}\left(1-\frac{\delta_{k0}}{2}\right)T_k(\overline{E}_m) \times\langle\psi(x,0)|T_k(\overline{H})|\psi(x,0)\rangle, \quad (3)$$

where in the last step we use a Chebyshev polynomial expansion [4] for the time evolution operator $e^{-i\hat{H}t}$, interchange the integration and the summation operations, and analytically integrate over the time variable [5]. In the CFM, we thus directly obtain the spectral intensities (as opposed to wave functions in the FDM) and the eigenvalue location is, therefore, a by product.

Now, in the absence of step (b) in the CFM, a ''stick spectrum,'' showing the exact location of eigenvalues, will appear only when the time goes to infinity, which reflects a limiting process involved in the Fourier transform. Likewise, in the absence of step (b) in the FDM, exact eigenfunctions will appear only when the time goes to infinity. In either case, we may stop the limiting process after a predetermined accuracy has been achieved. We thus see that the filtering step [i.e., step (a) in both cases], which is the most time-consuming step, is common in both methods because we use the same integral representation of the delta function in both cases. It is at this step where we need to discuss the issue of the time-energy uncertainty constraint. In the context of spectral determination, the time-energy uncertainty principle has mainly been discussed for the CFM route, where we strive only to separate all the peaks; and it has always been implicit that, after separating all peaks, finding the exact location of the eigenvalues will require the location of zeroes. Similarly, in the FDM we strive to precondition the basis by time propagation (or equivalently, Chebyshev recursions) just enough so that the eventual diagonalization will give the eigenvalue positions faithfully. Preconditioning may be considered as equivalent to separation of peaks in the CFM. Hence we make the comparison of ''just separation of peaks'' in the CFM to ''necessary and sufficient preconditioning of basis'' in the FDM, because the question of time-energy uncertainty only lies here.

Before we discuss the uncertainty principle, we clarify a practical limitation of the CFM for the purpose of eigenvalue location, as this was not sufficiently addressed in Ref. [2]. As we have used the sinc function to approximate the delta function and we do not exhaust the limiting process, the spectral intensities will have the features of the sinc function at the location of each eigenvalue. Now, if an eigenstate has a very small intensity compared to its close neighbors, its spectral features will be masked within the sinc structure of the neighboring peaks and thus it will not be identifiable. That is precisely what is reflected in Fig. 2 of Ref. [2], which has been reproduced in Fig. 1 of the preceding comment [3]. This means that the eigenvalue location by the CFM is critically dependent upon the choice of the initial wave function, and the best result would be obtained in the situation when the initial wave function has equal overlap with all the eigenstates of the Hamiltonian. In order to test this proposition, we have now purposefully selected the initial wave function such that it has equal overlap with all the eigenstates of the model Hamiltonian studied in Ref. [2], and this was accomplished by explicitly using the eigenvectors of the Hamiltonian. We present the computed spectrum in Fig. 1 here, which clearly shows all the eigenvalues in the window. This observation thus poses the question: Is it possible to ''precondition'' an initial arbitrary vector so that it has significant

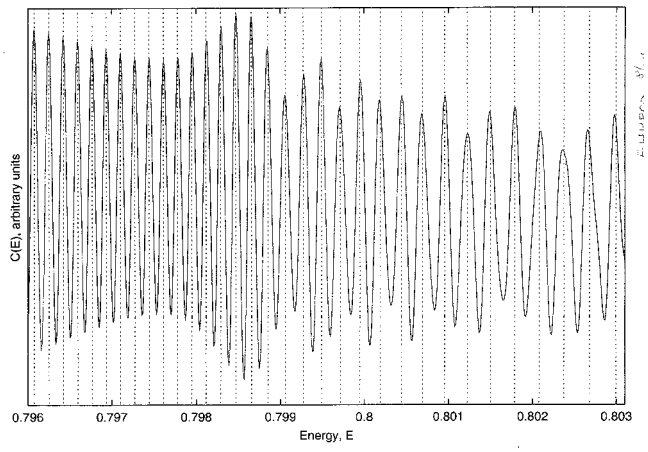

FIG. 1. The correlation amplitude, $C(E)$, as a function of energy E. The intensity is plotted in arbitrary units.

overlap with all the eigenstates of the Hamiltonian, hence allowing the CFM to give the best answer (for the purpose of just eigenvalue locations) in all situations? This is an open question and at present no general answer is known. However, this problem can be at least partly ameliorated by using a damping function (e.g., Gaussian damping) to suppress the sinc oscillations in the spectrum. Incorporation of a damping function is equivalent to approximating the delta function by the limiting form, other than the sinc function used here. On the other hand, the FDM or the Lanczos recursion is not dependent upon the initial wave function for the purpose of eigenvalue location, since the FDM filters the wave functions, as opposed to the spectral intensities, and finally computes the eigenvalues by explicit diagonalization. However, the spectral intensity may be difficult to compute by the FDM, if some states have very small overlap with the initial wave function. It is thus clear that step (b) in the FDM (which involves diagonalization) is more efficient for the eventual determination of eigenvalues than is step (b) in the CFM, which requires location of zeroes.

Now we come to the role of the time-energy uncertainty principle in the FDM and the CFM. We have already pointed out that the same prelimit integral representation of the delta function is used in both CFM and FDM. We thus ask the question: How many Chebyshev recursions are required in the CFM (assuming all the eigenstates in a given window have sufficient overlap with the initial wave function) to cleanly separate all the peaks so that the eigenvalues can be obtained by locating zeroes; and similarly, how many Chebyshev recursions are required in the FDM, so that the eventual location of eigenvalues can be accomplished by explicit diagonalization? The total number of Chebyshev recursions can be related to the total time propagation, as we know that the Chebyshev expansion of the time propagator, which has been used here in both the FDM and CFM, converges exponentially if the number of recursions is larger than the time-energy phase-space volume, $t\Delta\lambda$, where $\Delta\lambda$ $(=0.493\,222\,455$, for the Hamiltonian under study) is the parameter used for scaling the Hamiltonian. For further discussion, it is useful to define a quantity f, such that $(2\pi\Delta\lambda)f$ $=$ the number of Chebyshev recursions $\times$ eigenvalue spacing

in the window. Then f gives a measure of the relative phase an individual eigenstate receives in the computation, and $f = 1.0$ can roughly be taken as the time-energy uncertainty boundary. That is, if f is less than unity, the calculation has ''broken'' the uncertainty constraint. If there is a significant difference between the values of f with respect to the smallest and the largest eigenvalue spacing, the well-separated eigenvalues will converge faster than the denser region of the eigenvalue window. We have used $2N = 14\,000$ recursions in the CFM to compute the spectrum (0.796 to 0.803 energy window) shown in Fig. 1, and thus the total relative phases which the levels receive are about 0.98, 0.76, and 1.41 for the average, smallest, and the largest level spacings, respectively, in the window.

The quantity f was also computed to determine the influence of uncertainty in the FDM calculations and the representative results were shown in Ref. [2]. We note that the FDM involves two parameters: the number of Chebyshev recursions, $2N$, and the number of filtered states, L, for an arbitrary selected window. Evidently, the parameter L should be at least as large as the total number of the eigenstates in the window, and this number is *a priori* unknown. We have also pointed out in Ref. [2] that N and L are not totally independent parameters and thus there is some latitude (though not a great deal) in their choice. The preceding comment [3] highlights this point once again. In our experience, the FDM becomes dependent only on N, once we have chosen L to be sufficiently larger than the number of eigenstates in the window. MC also proposes the size of the selected energy window (W, in the preceding comment [3]) to be variable, and not arbitrary [3], the advantage of which is not clear for a general situation, including the present one. In any case, we reconsider the results shown in the preceding comment [3]. For the window with eigenvalue range, 0.796 to 0.803, MC report that all eigenvalues converge with $N = 6500$, though they have not reported the exact value of L in their calculations. We have also obtained converged results for $N = 6500$ in Ref. [2]. The observation that the widely separated eigenvalues converge faster than those in the denser region is not surprising and this can also be understood from the parameter f, which, for $N = 6500$, is 0.91, 0.71, and 1.31 for the average, smallest, and the largest level spacings, respectively. This observation was not explicitly pointed out in Ref. [2], as we had then concentrated on obtaining all the eigenvalues in the window.

Comparing FDM to CFM, we thus see that the parameter f is not very different for the same spectral window (0.796 to 0.803) in the two methods. This leads to the conclusion that *the time-energy uncertainty principle affects both FDM and CFM in a similar manner*. However, the FDM is better suited to practical calculations, particularly in a situation where the spectral intensity distribution in the initial wave function is not favorable (*vide supra*). For the window with eigenvalue range 0.644 to 0.682, MC report $N = 3000$, compared to $N = 3500$ in Ref. [2]; however, they have not reported the value of L used in their calculations. Even with $N = 3000$, the individual levels in this window receive a phase, f, of about 2.21, 0.68, and 28.44 for the average, smallest, and largest level spacings, respectively. As there is a large difference in f for the smallest and the largest level spacings, it is not surprising that the widely separated eigenvalues converge much faster than the denser ones here.

The preceding comment [3] compares the FDM with only step (a) of the CFM (which is filteration accomplished by the FT) and justifies the statement that the FDM bypasses the uncertainty regime. This is unfair, since it is clear that the FDM is a FT followed by diagonalization, whereas CFM is a FT followed by location of zeroes (*vide supra*). Thus, the numerical efficiency of the FDM for eigenvalue determination, can be compared with that of the CFM, only after the location of zeroes have been performed. As the notion of the uncertainty principle comes from the FT and the filteration step in both methods [step (a)] also utilizes the FT, this step can be unambiguously compared, as we have explained above.

We now point out the source of convergence for spectral filters, which is valid for FDM as well as CFM. In the present formulation, we have utilized a Chebyshev expansion for the time propagator [4] in Eqs. (1) and (3). This includes a Bessel function in the series, whose argument is the time-energy phase-space volume, $t\Delta\lambda$, and it is well known that the Bessel function exponentially goes to zero, if its order is greater than its argument. This provides the necessary convergence for the Chebyshev series. MC, on the other hand, suggest this convergence due to the ''subspace'' aspect of the problem. This is only partly true, as the nature of subspace is determined by the matrix-vector recursion procedure, which is different for different polynomials utilized to expand the time propagator. In fact, the series expansion of the time propagator with other orthogonal polynomials (e.g., Hermite [7]) have different rate of convergence.

We now remark on the Lanczos recursion method as it has been discussed in the preceding comment [3], even though we did not make such a comparison in Ref. [2]. We first note that the FDM shares many operational details with the Lanczos recursion method and thus it makes sense to compare their numerical efficiencies. Now, since the eigenvalue is a time-independent concept, it is not mandatory to utilize time-dependent methods like the FDM. Therefore, there is no *a priori* limit on the efficiency of any algorithm that it has to satisfy the uncertainty principle, as long as we do not invoke the Fourier transformation in its derivation. As the Lanczos method is based on the principle that a matrix satisfies its own polynomial, it is expected that one has to carry out at least M matrix-vector products for a $M \times M$ matrix, in order to faithfully recover the whole spectrum. This point is further confirmed in the preceding comment [3]. It is also well known that the well-separated eigenvalues converge much faster in the Lanczos recursion method. Further, it is important to note the observation in the preceding comment that the Lanczos method provides eigenvalues more efficiently than the FDM for the present model Hamiltonian [3].

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