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ARTICLES

A Lorentzian function based spectral filter for calculating the energy of excited bound states in quantum mechanics

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In this paper, we study a Lorentzian function based spectral filter suitable for computing highly excited bound states of a quantum system. Using this filter, we have derived an expression for spectral intensities and also implemented a filter diagonalization scheme. We have used a Chebyshev polynomial based series expansion of the filter operator, and this allows us to accomplish a partial resummation of the double series analytically when computing the necessary matrix elements; this saves considerable computational effort. The exponential damping term in the Lorentzian provides a convenient control over the resolution of the computed spectrum in the spectral intensity plot. As a numerical test, we have computed eigenvalues and spectral intensities of a model Hamiltonian in an arbitrary energy window. For situations where eigenvalues are distributed nonuniformly we suggest a computational protocol, which judiciously combines the spectral intensity information with the filter diagonalization method. This protocol is efficient only with the Lorentzian filter studied here. © *2003 American Institute of Physics.*
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I. INTRODUCTION

With the advent of new laser techniques, it has increasingly become possible to explore highly excited quantum states within a selected energy window of a molecular system.[1,2] A quantum mechanical understanding of such systems requires an accurate knowledge of the eigenspectrum of the corresponding Hamiltonian, in particular for the energy window of experimental interests. The realization that it may be possible to extract a small window from any region of the spectrum of the Hamiltonian, using a *spectral filter*, without having to solve the complete eigenvalue problem, has attracted considerable interest in recent years.[3–41] In this context, we have elaborated the idea of spectral filters, which originates from the basic propositions of the theory of measurement in quantum mechanics.[30,31] In spectral filter theory, the quantity of central importance is the *spectral density operator* (SDO), $\delta(E-\hat{H})$, where the filter energy, E, is within the spectral range of the Hamiltonian, $\hat{H}$, of the quantum system. As $\delta(E-\hat{H})$ is a projection onto the space of solutions of the homogeneous Schrödinger equation for scattering as well as bound states, its application on an arbitrary wave function (with appropriate boundary conditions), yields the eigenstates for the bound as well as scattering states.[8] Using this property of the SDO, one can obtain a *filter diagonalization* (FD) realization[11–37] of the spectral filter, suitable for computing the bound state spectrum in an arbitrary energy window. The SDO can also be used to obtain the spectral intensity of various peaks in a selected energy window. In this paper, we are concerned with an efficient implementation of the SDO for the purpose of computing spectral intensities and obtaining a convenient filter diagonalization scheme.

Since the SDO, $\delta(E-\hat{H})$, conceptually refers to a limiting process, it must be suitably approximated and represented before it can be applied numerically; and this is an important issue associated with the implementation of various spectral filter algorithms. In practical applications, it is often convenient to take the filter function as a prelimit expression of the SDO and express it as a convergent series, such that it separates the action of the filter energy, E, from that of the Hamiltonian. The choice of a prelimit expression of the SDO and its series expansion necessarily dictates the computational aspects of the resulting algorithm, and hence there have been several suggestions on this issue in the literature.[11–37] In particular, Kouri *et al.*[5–8] used a sinc function approximation of the SDO and obtained its series expansion in terms of Legendre and Chebyshev polynomials. A more general expansion of the SDO and Green's function in terms of Jacobi polynomials, of which Legendre and Chebyshev polynomials are special cases, has also been reported.[42] Hermite polynomials have also been used to obtain a series representation of the SDO, expressed as a Gaussian limiting process.[29] As we will explain later, a Lorentzian limiting expression of the SDO expressed in terms of Chebyshev polynomials offers a better choice for a spectral filter. Chebyshev polynomials are known to provide an uniformly convergent approximating scheme, and in the context of filter diagonalization they are very convenient for algebraic manipulations, leading to a compact set of equations.

The filter diagonalization method is conceptually well established and several important implementation schemes have been suggested in the literature,[11–37] differing mostly in the choice of the filter function, $\delta(E-\hat{H})$. Most earlier stud-

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ies have used either a sinc function or a prelimit Gaussian for the filter function, expressed in terms of the Chebyshev polynomials,[11–32] though some elaborate choices of the filter function have also been reported.[11,35] Specifically, the formulation of Neuhauser *et al.*[14] involved a prelimit Gaussian integral representation of the SDO, in conjunction with a Chebyshev polynomial expansion for the quantum time propagator.[43] We note that the use of a Gaussian integral representation, in conjunction with Chebyshev polynomials, does not allow certain time integrals to be done analytically and so the final expression for the SDO (and hence the relevant matrix elements, needed for diagonalization) is numerically inconvenient.[14] An efficient implementation of the FD method was later accomplished by Mandelshtam and Taylor,[18,19] who used a sinc function approximation of the spectral filter, expressed in terms of Chebyshev polynomials.[5–8] The use of the sinc function filter also appeared in other publications of FD method.[25–28,30–32] However, it is known that the oscillations in the sinc function are damped only slowly, and this damages its numerical efficacy for filter applications, particularly for computing spectral intensities.[30–32]

There is a crucial difference in the way the matrix elements have been computed in the Gaussian function based FD[14,29] as compared to the sinc function based FD, even though both used a Chebyshev polynomial exapnsion of the quantum time propagator. To simplify the expression for the matrix elements, the former studies have effectively used an identity, $\delta(E_m-\hat{H})\,\delta(E_n-\hat{H})=\delta(E_m-E_n)\,\delta(E_m-\hat{H})$, which is true in the exact limit of the delta function. This factorization, however, involves some error since a practical application uses only a finite number of terms in the series expansion of the filter function. On the other hand, the sinc function based FD methods[18,19,30] have used a direct multiplication of two truncated series, corresponding to $\delta(E_m-\hat{H})\,\delta(E_n-\hat{H})$, to simplify the expression for the matrix elements. In fact, a partial resummation of the double series could then be accomplished due to a special property of Chebyshev polynomials, not shared by other classical orthogonal polynomials. In the present study, we have followed the latter algebraic procedure.

In this paper, we propose the Lorentzian function as a filter. This choice overcomes all the limitations associated with the Gaussian and sinc function representations. We also show that this choice allows a compact and numerically convenient expression of the relevant matrix elements for the purpose of FD applications. The paper is organized as follows. In Sec. II, we discuss the idea and use of spectral filter and obtain a Chebyshev polynomial based series expansion of the Lorentzian filter operator. In Sec. III, we obtain a compact expression of relevant matrix elements for FD applications. We give the expression for the spectral intensity in Sec. IV. In Sec. V, we present numerical tests on a model Hamiltonian. Section VI contains a brief conclusion.

II. SPECTRAL FILTERS

Spectral filter methods use as a starting point

$$|\chi_{\epsilon,\zeta}\rangle=f(\epsilon-\hat{H};\zeta)|\psi\rangle=\sum_{\alpha}|\alpha\rangle f(\epsilon-E_{\alpha};\zeta)\langle\alpha|\psi\rangle, \quad (1)$$

where $|\chi_{\epsilon,\zeta}\rangle$ is the filtered state. Here $\hat{H}$ is the Hamiltonian of the system, the $|\alpha\rangle$ are the eigenstates of $\hat{H}$ with eigenvalues E_α, $|\psi\rangle$ is an arbitrary state with nonzero $\langle\alpha|\psi\rangle$, ϵ is an arbitrary energy but within the range of $\hat{H}$, and $f(X;\zeta)$ is a function that peaks at zero and has a width, ζ. We call $f(X;\zeta)$ a filter and examine here various possibilities for it, such as a Lorentzian, a Gaussian, and a sinc function, where $\mathrm{sinc}(x)=\sin(x)/x$.

As one can see from Eq. (1), the filtered state $|\chi_{\epsilon,\zeta}\rangle$ is a linear combination of energy eigenstates. The value of ϵ and ζ determine which eigenstates are included in this combination. A proper choice of these quantities (ζ small and ϵ close to E_α) can turn $|\chi_{\epsilon,\zeta}\rangle$ into an eigenstate $|\alpha\rangle$. If ζ is large, then $|\chi_{\epsilon,\zeta}\rangle$ is a linear combination of many eigenstates whose energies are in the vicinity of ϵ. It is thus clear that the filter, $f(X;\zeta)$, is a prelimit form of the spectral density operator, $\delta(E-\hat{H})$.

Equation (1) can be used in two ways. One is to take ζ smaller than the gap between the energy eigenvalues and vary ϵ through a preselected energy range, $[E_{\min},E_{\max}]$. When ϵ equals an eigenvalue, $|\chi_{\epsilon,\zeta}\rangle$ will peak and become equal to the corresponding energy eigenstate. Alternatively, one can calculate $|\chi_{\epsilon,\zeta}\rangle$ at each of a set of ϵ's ($E_{\min}\leqslant\epsilon_1,\epsilon_2,\ldots,\epsilon_L\leqslant E_{\max}$) and use these as an incomplete basis to diagonalize the Hamiltonian.[11–37] The eigenvalues obtained this way will lie in the range $[E_{\min},E_{\max}]$. The latter procedure, known as filter diagonalization,[11–14] is very attractive since the size of the filtered basis, L, is generally much smaller than the size of the full Hamiltonian matrix. An efficient implementation of either idea requires a bit of care and this is the subject of this paper. We survey briefly various pitfalls and present the strategy we recommend for avoiding them.

Since we plan to calculate $|\chi_{\epsilon,\zeta}\rangle$ for many values of ϵ in an energy window, it is important to have a recipe in which the calculation of a new value of ϵ is performed efficiently. We can achieve this in two steps. First, we represent $f(\epsilon-\hat{H};\zeta)$ as an integral transform over time:

$$f(\epsilon-\hat{H};\zeta)=\int_{-\infty}^{\infty}dt\tilde{f}(|t|;\zeta)e^{i\epsilon t}e^{-i\hat{H}t}. \quad (2)$$

This demands ϵ and $\hat{H}$ to be time independent, which is always satisfied for the conservative system. Thus we can represent $e^{-i\hat{H}t}$ by an expansion of the form[44]

$$e^{-i\hat{H}t}=\sum_{k=0}^{N}g_k(t)P_k(\hat{H}). \quad (3)$$

Here, $P_k(\hat{H})$ is an orthogonal polynomial of order k. For Hermitian $\hat{H}$, four such expansions have been used so far in quantum mechanics, in which P_k is a Chebyshev,[43] or a Legendre,[6,45] or a Gegenbauer,[42] or a Hermite polynomial.[29]

The function $g_k(t)$ depends on which polynomial is used, but in the first three cases, is proportional to a Bessel function.[5–8,42,43,45] This expansion is exact when N goes to infinity. We note that the argument of g_k and P_k should be dimensionless and hence $\hat{H}$ and t should be properly scaled. As Chebyshev, Legendre, and Gegenbauer polynomials are defined for the values of their argument in the range $[-1,1]$, one must scale the Hamiltonian such that $\hat{H}=\Delta\lambda\hat{H}_{sc}+\bar{\lambda}$, where $\Delta\lambda=(H_{max}-H_{min})/2$ and $\bar{\lambda}=(H_{max}+H_{min})/2$. The eigenvalues of $\hat{H}$ in the range $[H_{min},H_{max}]$ become eigenvalues of $\hat{H}_{sc}$ in the range $[-1,1]$. Also, $\Delta\lambda$ and $\bar{\lambda}$ have dimensions of energy, which renders $\hat{H}_{sc}$ dimensionless.

Using Eqs. (2) and (3) in Eq. (1) gives

$$|\chi_{\epsilon,\zeta}\rangle=f(\epsilon-\hat{H};\zeta)|\psi\rangle=\sum_{k=0}^{N} I(\epsilon,\zeta,k)P_k(\hat{H})|\psi\rangle \tag{4}$$

with

$$I(\epsilon,\zeta,k)=\int_{-\infty}^{\infty} dt\,\tilde{f}(|t|;\zeta)e^{i\epsilon t}g_k(t). \tag{5}$$

The sum in Eq. (4) may in practice have thousands of terms. For this reason it is important to perform the integral, $I(\epsilon,\zeta,k)$, analytically. This limits the choice of the filter operator, $f(\epsilon-\hat{H};\zeta)$, and the orthogonal polynomial [Eq. (3)]. We use the one in which P_k is a Chebyshev polynomial, T_k. The reasons for this choice will become clear later. There can be many forms of the filter operator, $f(\epsilon-\hat{H};\zeta)$, suitable for the purpose; however, with the choice of Chebyshev polynomials, we find that Eq. (5) can be evaluated analytically if $f(\epsilon-\hat{H};\zeta)$ is a Lorentzian or a sinc function,[5–8,42] but not for a Gaussian.[14] The Fourier transform of a sinc function is a step function, and this is known to be a bad filter due to the "Gibbs phenomenon."[46] For this reason, we use a Lorentzian.

The most important feature of Eq. (4) is that if we change ϵ and ζ we need not recompute $P_k(\hat{H})$, which is the most time-consuming part of the calculation. This is achieved because in Eq. (3), the functional dependence on t is separated from the dependence on $\hat{H}$.

With Chebyshev polynomials, T_k, for P_k, the function g_k in Eq. (3) is the Bessel function, $J_k(t\Delta\lambda)$.[43] The Lorentzian choice for the filter operator makes $\tilde{f}(t;\zeta)=\exp(-\zeta t)$. The integral in Eq. (5) can then be done analytically[5,42] and we can express Eq. (4) as follows:

$$|\chi_{\epsilon,\zeta}\rangle=f(\epsilon-\hat{H};\zeta)|\psi\rangle = \left(\frac{1}{\pi\Delta\lambda}\right)\sum_{k=0}^{N}(2-\delta_{k0})\mathrm{Re}[D(\epsilon)Z^k(\epsilon)]T_k(\hat{H}_{sc})|\psi\rangle, \tag{6}$$

where $D(\epsilon)^{-1}=[1-(\epsilon_{sc}+i\zeta_{sc})^2]^{1/2}$, $Z(\epsilon)=[(\epsilon_{sc}+i\zeta_{sc})-iD(\epsilon)^{-1}]$, $\zeta_{sc}=\zeta/\Delta\lambda$, and $\epsilon_{sc}=(\epsilon-\bar{\lambda})/\Delta\lambda$. Equation (6) is the final expression for the filtered state, which can be used either to obtain eigenstates and spectral intensities or as a basis to diagonalize the Hamiltonian in a selected energy window. We note that if we do not take the real part, Eq. (6) is the expansion of the causal Green's function, $(E-\hat{H}+i\zeta)^{-1}$, in terms of Chebyshev polynomials, known through the work of Kouri.[5] We have recently given a more general derivation of the Green's function, based on the ultraspherical polynomials, of which Eq. (6) is a special case.[42]

A comment concerning the convergence of the series in Eq. (6) is in order here. This series is composed of terms that oscillate faster with higher k, superimposed upon a k-dependent exponential damping factor. It is easy to verify the damping factor to be $\exp(-ky)$, where y is a positive number determined from the relation, $2\cosh^2 y=(1+\epsilon_{sc}^2+\zeta_{sc}^2)+[(1+\epsilon_{sc}^2+\zeta_{sc}^2)^2-4\epsilon_{sc}^2]^{1/2}$. The convergence is guaranteed here due to two factors: (1) summation of fast oscillating terms, and (2) the exponential damping. On the other hand, if we take the width of the Lorentzian, ζ, to be zero, y becomes zero and the damping term drops out. Then Eq. (6) will be transformed to the one obtained using a sinc function based spectral density operator,[5–8,42] and the convergence will depend entirely on the cancellation due to the summation of fast oscillating terms. We do not recommend taking this limit, as this would defeat the whole purpose of damping. We will later examine the role of this exponential damping in the computations of eigenvalues by FD and the spectral intensities.

III. FILTER DIAGONALIZATION

A FD method involves diagonalizing the Hamiltonian, expressed in the basis of filtered states, $|\chi_{\epsilon,\zeta}\rangle$, $\epsilon=\epsilon_1,\epsilon_2,\ldots,\epsilon_L$, in a given energy window.[11–37] We will later comment on the location and the length of the energy set, $\{\epsilon_m, m=1,L\}$ at which the filtering process should be carried out. At present, it may be considered as arbitrary. Since the filtered basis will not form an orthogonal set, we set up a generalized eigenvalue equation,[14] $HB=SBE$, where the vector B is defined through $|\alpha\rangle=\Sigma_{m=1}^{L} B_{\alpha,m}|\chi_{\epsilon_m,\zeta}\rangle$. H and S are the Hamiltonian and overlap matrices, respectively. In the basis of filtered states, a generic matrix element can be expressed as follows:

$$A_{m,n}^{(p)}=\langle\psi|f(\epsilon_m-\hat{H};\zeta)\hat{H}^p f(\epsilon_n-\hat{H};\zeta)|\psi\rangle \tag{7}$$

or equivalently,

$$A_{m,n}^{(p)}=\langle\chi_{\epsilon_m,\zeta}|\hat{H}^p|\chi_{\epsilon_n,\zeta}\rangle, \tag{8}$$

where $p=0$ gives the overlap matrix S, and $p=1$ gives the Hamiltonian, $\hat{H}$. As we explain in the following, although Eqs. (7) and (8) are formally equivalent they provide two alternate ways of deriving the final expression for the matrix elements. In the first approach, we can use the identity $f(\epsilon_m-\hat{H};\zeta)f(\epsilon_n-\hat{H};\zeta)=f(\epsilon_m-\epsilon_n;\zeta)f(\epsilon_m-\hat{H};\zeta)$ to factorize the product of two filter operators in Eq. (7) and formally obtain

$$A_{m,n}^{(p)}=f(\epsilon_m-\epsilon_n;\zeta)\langle\psi|f(\epsilon_m-\hat{H};\zeta)\hat{H}^p|\psi\rangle. \tag{9}$$

We may then use Eq. (6) for the filter operator to finally obtain a single series for the matrix elements. This line of derivation has been implicit in some of the earlier studies.[14,29] As we pointed out in Sec. I, this factorization

holds only for an "exact" delta function. This assertion can easily be verified by using an integral representation, Eq. (2) of the Gaussian, sinc, or Lorentzian function. However, if one uses a series representation for the filter operator as given in Eq. (6), the above-mentioned factorization demands that $N\rightarrow\infty$, which is never realized in practice. For an arbitrarily truncated series approximation of the filter operator, as in Eq. (6), the above-mentioned factorization is not valid and represents a further unnecessary approximation. We have therefore avoided the use of this identity in the present work. Instead, we substitute a truncated series expansion (finite N) of the filtered state, Eq. (6), directly into Eq. (8) and obtain a double series for the generic matrix element, as follows:[47]

$$A_{m,n}^{(p)}=\frac{4}{(\pi\Delta\lambda)^2}\sum_{k=0}^{N}\sum_{k'=0}^{N}\left(1-\frac{\delta_{k0}}{2}\right)\left(1-\frac{\delta_{k'0}}{2}\right)\times \mathrm{Re}(D_m Z_m^k)\mathrm{Re}(D_n Z_n^{k'})\langle\psi|T_{k'}(\hat{H}_{\mathrm{sc}})\hat{H}^p T_k(\hat{H}_{\mathrm{sc}})|\psi\rangle \tag{10}$$

$$=\frac{1}{(\pi\Delta\lambda)^2}\sum_{k=0}^{N}\sum_{k'=0}^{N}\left(1-\frac{\delta_{k0}}{2}\right)\left(1-\frac{\delta_{k'0}}{2}\right)\times 2\,\mathrm{Re}(D_m Z_m^k)\mathrm{Re}(D_n Z_n^{k'})(c_{k+k'}^{(p)}+c_{|k-k'|}^{(p)}) \tag{11}$$

$$=\frac{1}{(\pi\Delta\lambda)^2}\mathrm{Re}\sum_{k=0}^{N}\sum_{k'=0}^{N}\left(1-\frac{\delta_{k0}}{2}\right)\left(1-\frac{\delta_{k'0}}{2}\right)\times(D_m D_n Z_m^k Z_n^{k'}+D_m D_n^{*} Z_m^k Z_n^{*k'})(c_{k+k'}^{(p)}+c_{|k-k'|}^{(p)}), \tag{12}$$

where $c_k^{(0)}=\langle\psi|T_k(\hat{H}_{\mathrm{sc}})|\psi\rangle$ and $c_k^{(p)}=(c_{k+p}^{(0)}+c_{|k-p|}^{(0)})/2$. To pass from Eq. (10) to (11), we have used a known identity of the product of Chebyshev polynomials, $2T_k(x)T_{k'}(x)=T_{k+k'}(x)+T_{|k-k'|}(x)$. As we explain in the following, this identity allows a partial resummation of the double series in Eq. (11), which turns into a single series. In this way we recover the computational advantage associated with the use of the factorization of the product of two filter functions as described previously. This line of derivation has been followed in some of the earlier studies.[18,30] No other orthogonal polynomial satisfies the above-mentioned property and this is one reason why we prefer Chebyshev polynomials. Moreover, Chebyshev polynomials are known to provide a uniform approximation scheme for the quantum time propagator.[43] To pass from Eq. (11) to (12), we have used the identity, $2\,\mathrm{Re}(X)\mathrm{Re}(Y)=\mathrm{Re}(XY)+\mathrm{Re}(XY^{*})$, noting $c_k^{(p)}$ to be real-valued.

We now discuss the resummation procedure used in the present study. We use a "Cauchy-type" expansion[48] of the double series, in which we collect all the terms for which $|k+k'|$ and $|k-k'|$ have the same values in Eq. (12) and then perform the summation of the resulting geometric series analytically.[18,30] This is possible because the series in Eq. (6) is absolutely convergent and it is presumed that the filtering process at a particular energy is complete after summing to N terms in Eq. (6). The essential result is

$$\begin{aligned}\sum_{k=0}^{N}\sum_{k'=0}^{N}&\left(1-\frac{\delta_{k0}}{2}\right)\left(1-\frac{\delta_{k'0}}{2}\right)Z_m^k Z_n^{k'}(c_{k+k'}^{(p)}+c_{|k-k'|}^{(p)})\\ &=\sum_{k=0}^{N}(1-\delta_{k0})c_{k+N}^{(p)}\left[\frac{Z_m^{N+1}Z_n^k-Z_m^k Z_n^{N+1}}{Z_m-Z_n}\right]+\left(1-\frac{\delta_{k0}}{2}\right)\\ &\quad\times c_k^{(p)}\left[\left(\frac{Z_m^{k+1}-Z_n^{k+1}}{Z_m-Z_n}\right)+\frac{Z_m Z_n}{1-Z_m Z_n}(Z_m^k+Z_n^k)\right.\\ &\quad\left.\times[1-(Z_m Z_n)^{N-k}]\right]\quad(Z_m\neq Z_n)\\ &=\sum_{k=0}^{N}\left(1-\frac{\delta_{k0}}{2}\right)\frac{c_k^{(p)}}{1-Z_m^2}[(k+1)Z_m^k-(k-1)Z_m^{k+2}\\ &\quad-2Z_m^{2N-k+2}]+(1-\delta_{k0})(N-k+1)c_{k+N}^{(p)}Z_m^{k+N}\\ &\quad(Z_m=Z_n).\end{aligned} \tag{13}$$

Equation (13) is the main result of the paper. It can be used to compute the matrix elements of the Hamiltonian, for an arbitrary energy window.

We can also make an independent error estimate of the computed eigenvalues as

$$\begin{aligned}(\Delta E_\alpha)^2&=|\langle\alpha|(\hat{H}-E_\alpha)^2|\alpha\rangle|\\ &=|(B^t A^{(2)}B)_{mm}-\epsilon_m^2(B^t S B)_{mm}|.\end{aligned} \tag{14}$$

We note that Eq. (14) gives an upper bound to the error estimate. For a better error estimate, one may also use different variational principles, as suggested by Beck and Meyer,[35] and the extension of the present formulation would be straightforward.

We now comment on the numerical implementation of the present FD equations. The first step is to compute the scalar coefficients, $c_k^{(0)}=\langle\psi|T_k(\hat{H}_{\mathrm{sc}})|\psi\rangle$, using a three-term recurrence relation of the Chebyshev polynomials, $T_m(\hat{H}_{\mathrm{sc}})=2\hat{H}_{\mathrm{sc}}T_{m-1}(\hat{H}_{\mathrm{sc}})-T_{m-2}(\hat{H}_{\mathrm{sc}})$, acting on $|\psi\rangle$. The initial $|\psi\rangle$ is chosen randomly. Computing $c_k^{(0)}$'s is the most expensive step. However, N Chebyshev recursions are sufficient to generate $2N$ $c_k^{(0)}$'s as noted by Neuhauser.[14] In fact, using properties of Chebyshev polynomials it is straightforward to show that $c_{2m-1}^{(0)}=2\langle\phi_{m-1}|\phi_m\rangle-c_1^{(0)}$ and $c_{2m}^{(0)}=2\langle\phi_m|\phi_m\rangle-c_0^{(0)}$, where $|\phi_m\rangle=T_m(\hat{H}_{\mathrm{sc}})|\psi\rangle$. In the next step, we use these $c_k^{(0)}$'s to compute the overlap and Hamiltonian matrices [Eqs. (12) and (13)] for a preselected energy window and solve the general eigenvalue problem by the method of singular value decomposition.[14,49] The same $c_k^{(0)}$'s can also be used to obtain an error estimate of the computed eigenvalues [Eq. (14)]. One may use overlapping energy windows for efficient computation of a broad range of eigenvalues, as suggested by Neuhauser.[14]

How does the present FD method compare with earlier ones? We first note that the computation of $c_k^{(0)}$s, which is the most expensive step, is a step commonly shared by all Chebyshev polynomial based FD methods in the literature,[14,18,25,30] and so the most important issue here is how many terms, N in Eqs. (6) and (13), are required to obtain converged eigenvalues in a given energy window. We will analyze this and other related issues in Sec. V. The present FD method closely resembles the sinc function based

TABLE I. A comparison of the present FD method and exact eigenvalues for the energy window, 0.5001–0.5021, of the model Hamiltonian. The value of ζ is 2×10^{-4}.

(6000/18)[a]		*(6000/20)*[a]		*(6500/20)*[a]		*(7000/20)*[a]		Exact
0.500 160	(2.384)	0.500 157	(2.649)	0.500 158	(0.877)	0.500 161	(0.305)	0.500 162
0.500 416	(4.872)	0.500 400	(5.223)	0.500 400	(1.901)	0.500 407	(0.232)	0.500 409
0.500 665	(0.912)	0.500 664	(1.442)	0.500 663	(0.609)	0.500 664	(0.221)	0.500 664
0.501 143	(14.311)	0.501 019	(18.042)	0.500 868	(5.140)	0.500 914	(0.809)	0.500 925
0.501 221	(10.929)	0.501 199	(4.016)	0.501 194	(0.388)	0.501 194	(0.246)	0.501 194
0.501 470	(0.787)	0.501 470	(0.602)	0.501 470	(0.130)	0.501 470	(0.088)	0.501 470
0.501 755	(1.213)	0.501 754	(1.244)	0.501 753	(0.262)	0.501 753	(0.248)	0.501 753
0.502 044	(1.041)	0.502 044	(1.044)	0.502 043	(0.326)	0.502 041	(1.403)	0.502 043

[a](N/L) refers to the number of Chebyshev recursions and the number of filtered states. N Chebyshev recursions are sufficient to generate $2N$ terms, and $2N$ $c_k^{(p)}$'s were finally used in Eq. (13). The error estimate, $(\Delta E_\alpha)^2 \times 10^3$ [Eq. (14)], is given in parentheses.

FD method discussed in earlier studies.[18,19,30–32] However, the expression for the matrix elements here [Eqs. (12) and (13)] differs from the one obtained by the sinc function based methods. Presumably, this may have a different convergence behavior for eigenvalues. We will analyze this further in Sec. V. In any case, the numerical effort necessary to compute the matrix elements by the present method, and also the storage requirement, is similar to that of the sinc function based method.

IV. SPECTRAL INTENSITY

The spectral intensity gives the contribution of an individual eigenstate, $|\alpha\rangle$, to the initial wave packet, $|\psi\rangle$, and it is defined as $|A(E_\alpha)|^2=|\langle\psi|\alpha\rangle|^2$. In principle, one could compute the spectral intensities in a given energy window by using the coefficients, $c_k^{(0)}$ and the eigenvectors obtained by filter diagonalization. However, it is computationally favorable to use a more direct approach. Using Eq. (6), the spectral intensity at energy E can be computed as

$$|A(E)|^2=\langle\psi|f(E-\hat{H};\zeta)|\psi\rangle = \left(\frac{1}{\pi\Delta\lambda}\right)\sum_{k=0}^{N}(2-\delta_{k0})\mathrm{Re}[D(E)Z^k(E)]c_k^{(0)}. \quad (15)$$

If ζ is small enough, for finite N, Eq. (15) will give a Lorentzian spectrum, with peaks whenever E equals an eigenvalue, E_α. An important feature of Eq. (15) is that it provides a complementary way of identifying the spectrum in a given energy window. If we take the parameter ζ as zero, Eq. (15) will transform to the one obtained by the sinc function based method.[7,8,18,30,31] We do not recommend this approach here.

V. RESULTS AND DISCUSSION

To test the numerical performance of the present theory, we have selected a model Hamiltonian due to Wyatt,[40] which was studied earlier with the sinc function based FD method.[30–32] The model system consists of n_b bands of states, with n_s states in each band. The Hamiltonian matrix elements are as follows: For diagonal matrix elements, $H_{ij,ij}=(i-1)\Delta+(j-1)\delta$; for intraband coupling, $H_{ij,ij'}=C\exp(-|j-j'|)$; and for interband coupling, $H_{ij,i'j'}=[C/(n_{od}|i-i'|+1)]\exp(-|j-j'|)$, where i denotes the band index, $i=1,2,\ldots,n_b$, and j denotes the index for states in this band, $j=1,2,\ldots,n_s$. The model has six parameters, for which we choose the following values: $n_b=10$, $n_s=200$, $C=0.04$, $\Delta=0.1$, $\delta=0.0001$, and $n_{od}=5$. For comparison, we obtained the exact eigenvalues for this model 2000×2000 matrix by explicit diagonalization. All the eigenvalues fall between 0 and 1. In order to test the present filter diagonalization scheme, we have generated $|\psi\rangle$ by taking random real amplitudes on a spatial grid, and then normalizing. We looked at several energy windows but we show only representative results here.

The present scheme, for a given energy window, involves three parameters: the number of terms N [Eq. (6)], the number of filtered basis functions L, and the damping parameter ζ. A judicious choice of these parameters should give good accuracy in the calculations. Obviously, ζ should be smaller than the expected smallest eigenvalue gap in the window. If ζ is large, not all eigenvalues in the window may be resolved, particularly when we compute the spectral intensities. We will comment on the number and location of filtered basis later.

As an example, we first show the results for a small window, with energy range 0.5001–0.5021 in Table I. This window contains eight eigenvalues. The results shown in Table I have used basis functions filtered at an equidistant energy grid within the energy window. The starting initial vector, $|\psi\rangle$, was chosen as random. It is pleasing to note that the results computed by the present method are in good agreement with the exact values. We point out some notable features. First, L should be as large as the number of eigenvalues expected in the window. The parameters N and L are coupled for lower values of L. For a fixed value of N, the results are more or less insensitive to L beyond a certain value ($L\equiv20$ in the present case). We see a significant improvement in increasing L from 18 to 20 here. With L fixed, as N increases, the computed results improve and approach the exact results. Second, it is also clear from Table I that the well-separated eigenvalues (at the edge of the window) converge before those that lie closer together. Third, the error estimate provides reliable guidance for identifying spurious (if any) eigenvalues in the calculations. We have also computed the eigenvalues using the sinc function based FD method[18,19,30] for the same energy window and set of parameters. We show the results in Table II. We do not find any

TABLE II. A comparison of the sinc function based FD[a] and exact eigenvalues for the model Hamiltonian.

(6000/18)[b]		*(6000/20)*[b]		*(6500/20)*[b]		*(7000/20)*[b]		Exact
0.500 156	(2.514)	0.500 156	(2.512)	0.500 159	(0.941)	0.500 162	(0.214)	0.500 162
0.500 401	(4.743)	0.500 401	(4.743)	0.500 400	(1.802)	0.500 409	(0.376)	0.500 409
0.500 664	(1.352)	0.500 664	(1.352)	0.500 663	(0.671)	0.500 664	(0.123)	0.500 664
0.501 084	(17.288)	0.501 085	(17.316)	0.500 867	(5.034)	0.500 923	(1.202)	0.500 925
0.501 197	(3.617)	0.501 197	(3.653)	0.501 194	(0.326)	0.501 194	(0.098)	0.501 194
0.501 470	(0.760)	0.501 470	(0.764)	0.501 470	(0.155)	0.501 470	(0.047)	0.501 470
0.501 753	(0.683)	0.501 753	(0.687)	0.501 753	(0.268)	0.501 753	(0.080)	0.501 753
0.502 046	(1.531)	0.502 046	(1.533)	0.502 039	(3.027)	0.502 043	(0.489)	0.502 043

[a]See Refs. 18 and 30.

[b](N/L) refers to the number of Chebyshev recursions and the number of filtered states. N Chebyshev recursions are sufficient to generate $2N$ terms, and $2N$ $c_k^{(p)}$'s were finally used in Eq. (13). The error estimate, $(\Delta E_\alpha)^2 \times 10^3$ [Eq. (14)], is given in parentheses.

significant difference between the two methods for this example.

We now address the role of the time-energy uncertainty principle within spectral filter methods. This issue has been debated in the earlier studies on the sinc function based methods.[18,19,30–32] We first note that the uncertainty principle becomes relevant here only due to the use of an integral transform of the filter function over time, Eq. (2), and that this step is inevitable in the derivation of spectral filters. We have also seen that the same spectral filter is used in the derivation of FD as in the expression for the spectral intensities. Traditionally, the uncertainty principle has been discussed only in the context of spectral intensities, wherein the spectral resolution is constrained by the relation $\Delta E = 2\pi/T$, where ΔE is the eigenvalue gap and T is the total length of time propagation. T is related to the number of Chebyshev recursions. The question naturally arises: Is the FD method also limited by this uncertainty constraint? Specifically, is it possible to resolve the spectrum, by computing spectral intensities, with the same numerical effort (that is, the number of Hamiltonian operations on the wave function) as that required in the FD method? As we explain in the following, the answer is yes, but there is no conflict between the two approaches of obtaining the spectrum. In fact, as we explain in the following it turns out that the FD and spectral intensities play complementary roles here, and a judicious use of both offers us a faithful computational protocol for spectral prediction.

First, we discuss the computation of spectral intensities, using Eq. (15). We have selected an energy window ranging from 0.796 to 0.803. Within this window, the smallest eigenvalue gap is 0.000 168 09, which should be the upper limit for the damping parameter, ζ, for a faithful spectral identification by the spectral intensity method. In fact, the choice of ζ dictates the resolution in the final computed spectrum. In Fig. 1, we show the computed spectrum for $\zeta=0.000\,05$ and for $\zeta=0.000\,20$, along with the location of exact eigenvalues in this window. For this purpose, we have used $N=16\,000$; due to a special property of Chebyshev polynomials, only 8000 recursions are necessary in Eq. (15). It is clear from Fig. 1 that the spectral resolution is markedly improved with the decrease in ζ. The larger value of ζ is able to resolve only high intensity peaks, whereas a majority of eigenvalues are easily identifiable with the smaller value of ζ. We note, however, that a few peaks of very low intensity are still not fully resolved here, which can be improved. In general, we observe a systematic improvement in the spectral resolution as we decrease the value of ζ with fixed N, and high intensity

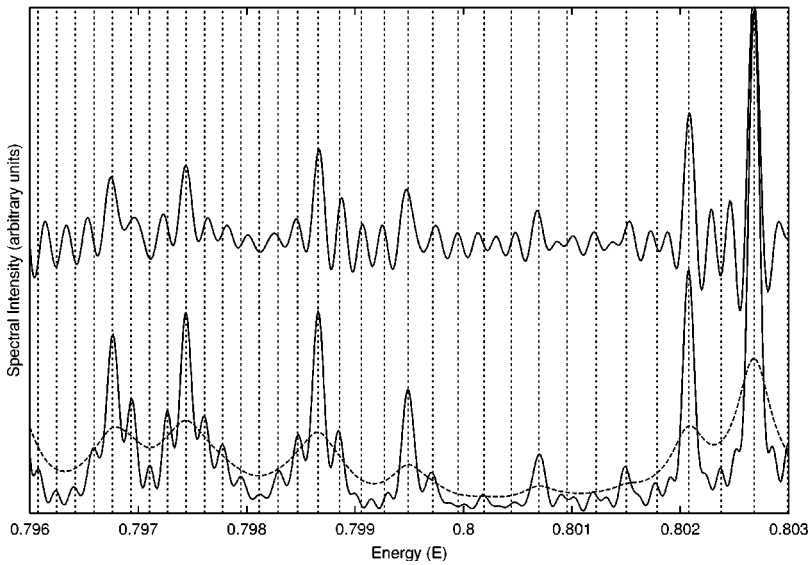

FIG. 1. The spectral intensity as a function of energy. The intensity is plotted in arbitrary units. The lower lines show results obtained using the present method [Eq. (15)]: the continuous line refers to $\zeta=0.000\,05$ and the broken line refers to $\zeta=0.000\,20$. The upper continuous line shows the result obtained using the sinc function based method (see Refs. 30–32). The locations of the exact eigenvalues are indicated by vertical dotted lines.

TABLE III. A comparison of the present FD method and exact eigenvalues for the energy window, 0.796–0.803, of the model Hamiltonian. The value of ζ is 0.00017.

(6500/50)[a]		*(7000/50)*[a]		*(7500/50)*[a]		Exact
0.796 037 59	(5.139 90)	0.796 061 43	(1.583 87)	0.796 066 37	(1.370 78)	0.796 075 29
0.796 176 59	(5.818 79)	0.796 244 00	(0.318 03)	0.796 243 40	(0.325 19)	0.796 248 08
0.796 408 56	(2.279 04)	0.796 419 11	(0.293 05)	0.796 419 24	(0.212 22)	0.796 420 28
0.796 589 59	(1.185 50)	0.796 591 77	(0.033 24)	0.796 591 76	(0.032 58)	0.796 591 88
0.796 762 37	(0.645 10)	0.796 762 88	(0.033 22)	0.796 762 88	(0.021 47)	0.796 762 90
0.796 932 38	(0.998 11)	0.796 933 32	(0.020 24)	0.796 933 32	(0.019 00)	0.796 933 36
0.797 097 06	(2.748 28)	0.797 103 01	(0.088 90)	0.797 103 01	(0.057 95)	0.797 103 26
0.797 271 76	(1.154 10)	0.797 272 57	(0.020 28)	0.797 272 57	(0.018 50)	0.797 272 60
0.797 441 16	(0.762 10)	0.797 441 41	(0.016 76)	0.797 441 41	(0.011 48)	0.797 441 42
0.797 609 11	(1.560 29)	0.797 609 75	(0.019 01)	0.797 609 75	(0.016 58)	0.797 609 77
0.797 776 77	(3.182 64)	0.797 777 83	(0.026 86)	0.797 777 83	(0.019 23)	0.797 777 86
0.797 887 80	(32.165 21)					
0.797 948 41	(6.184 31)	0.797 946 26	(0.033 05)	0.797 946 25	(0.027 15)	0.797 946 31
0.798 117 33	(2.221 77)	0.798 116 29	(0.082 32)	0.798 116 29	(0.060 31)	0.798 116 53
0.798 290 69	(0.303 91)	0.798 290 65	(0.031 12)	0.798 290 65	(0.023 98)	0.798 290 68
0.798 470 92	(0.077 29)	0.798 470 92	(0.024 02)	0.798 470 92	(0.017 44)	0.798 470 94
0.798 658 68	(0.018 73)	0.798 658 68	(0.012 89)	0.798 658 68	(0.009 37)	0.798 658 69
0.798 854 43	(0.018 42)	0.798 854 43	(0.025 14)	0.798 854 43	(0.017 58)	0.798 854 44
0.799 055 94	(0.227 05)	0.799 055 49	(0.346 07)	0.799 055 53	(0.237 34)	0.799 058 20
0.799 269 25	(0.104 35)	0.799 269 15	(0.179 05)	0.799 269 17	(0.118 31)	0.799 269 77
0.799 488 92	(0.011 33)	0.799 488 92	(0.019 69)	0.799 488 92	(0.012 61)	0.799 488 93
0.799 715 47	(0.023 16)	0.799 715 47	(0.042 85)	0.799 715 47	(0.026 32)	0.799 715 49
0.799 949 15	(0.076 12)	0.799 949 09	(0.146 68)	0.799 949 11	(0.086 34)	0.799 949 33
0.800 190 30	(0.036 01)	0.800 190 29	(0.074 20)	0.800 190 30	(0.041 58)	0.800 190 34
0.800 438 36	(0.071 47)	0.800 438 31	(0.157 98)	0.800 438 33	(0.083 70)	0.800 438 47
0.800 693 68	(0.018 65)	0.800 693 67	(0.045 04)	0.800 693 68	(0.022 41)	0.800 693 68
0.800 955 96	(0.039 84)	0.800 955 94	(0.106 84)	0.800 955 95	(0.049 38)	0.800 955 98
0.801 225 35	(0.039 23)	0.801 225 33	(0.119 34)	0.801 225 34	(0.050 48)	0.801 225 36
0.801 501 85	(0.024 80)	0.801 501 84	(0.088 03)	0.801 501 85	(0.033 43)	0.801 501 86
0.801 785 50	(0.042 25)	0.801 785 47	(0.180 98)	0.801 785 50	(0.059 83)	0.801 785 50
0.802 076 35	(0.011 08)	0.802 076 35	(0.059 51)	0.802 076 35	(0.016 34)	0.802 076 35
0.802 374 47	(0.048 58)	0.802 374 39	(0.330 56)	0.802 374 49	(0.068 89)	0.802 374 46
0.802 679 89	(0.012 90)	0.802 679 88	(0.091 10)	0.802 679 89	(0.012 20)	0.802 679 89
0.802 992 71	(0.217 36)	0.802 992 49	(0.691 55)	0.802 992 73	(0.037 02)	0.802 992 71

[a](N/L) refers to the number of Chebyshev recursions and the number of filtered states. N Chebyshev recursions are sufficient to generate $2N$ terms, and $2N$ $c_k^{(p)}$'s were finally used in Eq. (13). The error estimate, $(\Delta E_\alpha)^2 \times 10^3$ [Eq. (14)], is given in parentheses.

peaks are resolved before those with lower intensity. This means that either small or large values of ζ may be useful depending on the situation: for example, one could choose a ζ consistent with the resolution of an experimental result.

For comparison, Fig. 1 also shows the spectral intensities obtained by the sinc method.[30–32] It is clear that the spectral resolution is much better with the present Lorentzian filter than that obtained with the sinc method. In fact, only the present method is able to identify the peak locations correctly. This is not surprising, since for the sinc method, it is well known that if an eigenstate has a very small intensity compared to its neighbors, its spectral features get masked by the sinc structure of the neighboring peaks and therefore is not identifiable.[31] By definition, the present method does not suffer from this difficulty.

We have used the present FD method to compute the eigenvalues for the same spectral window (0.796–0.803), as shown in Table III. We have performed the filtering on a uniform energy grid in the window. The number of Chebyshev recursion required to obtain the eigenvalues faithfully by the present method can vary (though not a great deal) with the choice of number and energies of the filtered basis vectors, and the damping parameter, ζ. However, Table III shows typical results. We find that the present FD method is reliable, and for the present model it requires about 6500–7000 Chebyshev recursions to produce the spectrum reliably, which is similar to what has been noted for the sinc method.[30–32]

The above-described numerical experiments reveal that the number of Chebyshev recursions required to resolve the spectrum by computing spectral intensities can be expected to be similar to the number needed to compute the eigenvalues by the FD method. This suggests an useful computational protocol for studying quantum bound state problems. First, we calculate the coefficients, $\{c_k^{(0)}, k=1,N\}$, by Chebyshev recursions and store them. Using these $c_k^{(0)}$'s, we calculate the spectral intensities using Eq. (15) by varying the damping parameter, ζ, to identify tentative eigenvalues. We then use these estimated eigenvalues as the energies at which we filter the states for the purpose of filter diagonalization. We do not need to filter states in regions where there are no peaks. We have then obtained a very compact representation of Hamiltonian for the selected energy window. This proto-

col does not excessively suffer from the overcompleteness problem occurring in the overlap matrix, S, which of course is taken care of by the SVD algorithm.[49] The diagonalization step of the FD method (to obtain the exact location of eigenvalues) is then very efficient.

We have tested this protocol here. In the present example, we have found that two energies within each peak seen on the spectral intensity plot are sufficient in the filter diagonalization. After finding the exact location of eigenvalues in this way by the FD method, we may compute the corresponding intensity again using Eq. (15).

We thus see that the information obtained by the intensity plot—as illustrated in Fig. 1—can be used as complementary to the FD method presented here. We envision this protocol to be useful for the situation when some eigenvalues are very close together while the others are well spaced. In particular, the spectral intensity plot gives us an idea as to how to position the energy window. We then need to sample the filtered basis only in the region where we have seen that there are eigenstates present. We wish to emphasize that this protocol is less feasible with the sinc function, as the latter has difficulty in resolving peaks in the intensity plot, and generate spurious peaks where there are no eigenvalues.[31,32]

VI. CONCLUSIONS

In this paper, we have clarified the notion and use of spectral filtering in quantum mechanics. It appears that the Lorentzian function based filter developed here offers the best protocol at the present time. It has an advantage over the Gaussian function based method because within the Chebyshev polynomial framework, it allows all the relevant integrals to be solved analytically and obtain a very efficient expression for the relevant matrix elements. It must, however, be admitted that a Lorentzian function displays a slower falloff than a Gaussian and is hence expected to be somewhat less efficient in the filtering process.

The present FD method is conceptually similar to the one based on the sinc function. From the numerical applications in the present study, it appears that the computational efficiency of the Lorentzian based filter diagonalization is similar to that of the sinc function. However, the Lorentzian filter is more reliable in computing spectral intensities. We have thus shown that the present implementation has been able to resolve difficulties faced by other methods. To conclude, the Lorentzian function based spectral filter method derived here allows us to faithfully study bound state problems in nonrelativistic quantum mechanics.

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