Resonances from short time complex-scaled cross-correlation probability amplitudes by the Filter-Diagonalization Method

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The Filter-Diagonalization Method is used to find the broad and even overlapping resonances of a 1D Hamiltonian used before as a test model for new resonance theories and computational methods. It is found that the use of several complex-scaled cross-correlation probability amplitudes from short time propagation enables the calculation of broad overlapping resonances, which can not be resolved from the amplitude of a single complex-scaled autocorrelation calculation.

Filter-Diagonalization was recently introduced by Neuhauser [1] and Neuhauser and Wall [2] as a general method to extract frequencies (poles) from a given signal. The approach has been extensively used to extract frequencies and poles in both quantum dynamics and general contexts, by several groups [3–5]. In this article, our goal is to investigate the performance of the method for a strict generic test-model of new approaches for extracting resonance poles. While a general filter can be used, in this derivation we follow Mandelshtam and Taylor who recently used very successfully the simple box filter [3]. First, the method is briefly reviewed.

For a given Hamiltonian, one wishes to obtain the spectrum in the energy interval, $E_{\min} < E < E_{\max}$. (This energy range can be much smaller than the total spectrum of the Hamiltonian; a power of the method is that it can be applied, with very small overhead, to many energy ranges, as explained below.) Let us first choose an initial state, $|\phi_1(0)\rangle$, which is randomly populated over the entire available phase space of the Hamiltonian. Then we calculate $|\phi_1(t)\rangle = \exp(-iHt/\hbar)|\phi_1(0)\rangle$ by any preferable propagation method up to time $t = T$. Of course, for long enough propagations when T is larger than the inverse of the smallest energy difference between adjacent eigenvalues of H, the spectrum can be resolved by carrying out a Fourier transform of the autocorrelation function $C_1(t) = \langle\phi_1(0)|\phi_1(t)\rangle$. There are, however, many motivations to avoid such long time propagations. For example: For multi dimensional systems the long time propagation is too expensive. There are also propagation methods which are efficient only for short time propagations. Moreover, broad resonances, which are associated with large imaginary parts of the complex eigenvalues of the Hamiltonian, have no contribution to the propagated wave packet when $t > 3M\hbar/\mathrm{Im}\,(E^{\mathrm{res}})$ where M is the number of digits of machine accuracy.

If we calculate the Fourier transform of $C_1(t)$ from $t = 0$ to T and the time interval is too short to resolve the spectrum, we will not get the eigenfunctions but we can construct an effective small basis set. Let us filter out from $\phi_1(t)$ the $\hbar\omega$ components at several frequencies ω:

$$|\Psi_\omega\rangle = \frac{1}{T}\int_0^T dt \exp(+i\omega t)\exp(-iHt/\hbar)|\phi_1(0)\rangle\,. \quad (1)$$

We can use the $|\Psi_\omega\rangle$ as a basis set to diagonalize the Hamiltonian in the desired range [2]; here we follow [3] and diagonalize instead the time evolution operator $U(\tau) = \exp(-iH\tau/\hbar)$ at time $t = \tau$. The eigenvalues of $U(\tau)$ are $\Lambda = \exp(-iE\tau/\hbar)$, where E are the exact eigenvalues of the studied Hamiltonian (Note that from Λ one gets only the eigenvalues E modulo $2\pi/(\hbar\tau)$. Therefore, τ is taken as a short time interval. The stability of the results is checked by varying $\tau = k\,dt; k = 1, 2, 3.$) The time evolution matrix element is $U(\omega', \omega) = \langle\Psi_{\omega'}|U(\tau)|\Psi_\omega\rangle$. It should be noted [2] that in the 'bra' we do *not* take the complex conjugate as usual [6]. The motivation for it will be clarified later. By inserting the definitions $|\Psi_\omega\rangle$ and $U(\tau)$ into the time evolution matrix elements, one immediately obtains

$$\begin{aligned}U(\,\omega'\,,\omega) &= \frac{1}{T}\int_0^T dt' \mathrm{e}^{+i\omega' t'} \times \\ &\quad \frac{1}{T}\int_0^T dt\, \mathrm{e}^{+i\omega t}\langle\phi_1(0)|\,\mathrm{e}^{-iH(t+t'+\tau)/\hbar}|\phi_1(0)\rangle \\ &= \frac{1}{T}\int_0^T dt' \mathrm{e}^{+i\omega' t'}\frac{1}{T}\int_0^T dt \mathrm{e}^{+i\omega t}C_1(t+t'+\tau) \\ &= \frac{1}{2T^2}\int_0^{2T} dt_+ C(t_+ + \tau)\int_{-\Delta}^{\Delta} dt_- \mathrm{e}^{i(\omega_+ t_+ + \omega_- t_-)} \quad (2)\end{aligned}$$

with $t_\pm = t \pm t'$, $\omega_\pm = (\omega \pm \omega')/2$ and $\Delta = T - |T - t_+|$.

As one can see from Eq. (2), the 2D Fourier transform is reduced to a 1D Fourier transform and the time evolution matrix elements are given by

$$U(\omega', \omega) =$$

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$$\frac{1}{T^2\omega_-}\int_0^{2T} dt_+ \sin(\omega_-\Delta(t_+))\, e^{i\omega_+ t_+} C_1(t_+ + \tau)\,. \qquad (3)$$

For $\omega' = \omega$, the term $\sin(\omega_-\Delta(t_+))/\omega_-$ in the above expression should be replaced by $\Delta(t_+)$. The overlap matrix elements, $S(\omega',\omega) = \langle\Psi_{\omega'}|\Psi_\omega\rangle$, are immediately obtained by inserting $\tau = 0$ in (3).

It is clear that if we would have used the usual scalar product instead of the c-product [6], then: (a) we would need to calculate $\langle\phi_1(0)|\exp[-iH(t-t'+\tau)/\hbar]|\phi_1(0)\rangle$, which implies backward propagation in time (Note that H is the complex scaled Hamiltonian and therefore $C_1(-t) \neq C_1^*(t)$); (b) we would not be able to replace the 2D transform Fourier by a 1D one.

In addition, we should stress that as $T \to \infty$, the overlap matrix S becomes diagonal. For finite values of T, the Ψ_ω form a non orthogonal basis set. This basis can be a relatively small one and yet filter out the eigenvalues within the desired energy interval if discrete values for ω are chosen. For example, we choose

$$\omega_j = \frac{1}{\hbar}\left(E_{\min} + (E_{\max} - E_{\min})\,\frac{j}{N_\omega}\right), \qquad (4)$$

$j = 0, 1, 2, \ldots, N_\omega$, where $N_\omega{+}1$ needs to be chosen somewhat bigger than the the number of chosen frequencies in the studied range (which can be much smaller than the total number of frequencies in the spectrum of the Hamiltonian).

We used this method to calculate the complex poles of the 1D model Hamiltonian that has been used for many years as a test-case for new theoretical and computational approaches [7]:

$$H = \frac{1}{2}\,p_x^2 + \left(\frac{1}{2}\,x^2 - 0.8\right) e^{-0.1x^2} + 0.8\,. \qquad (5)$$

By using 700 particle-in-a-box basis functions, with a box size of $L = 40$ and $\hbar = 1$, and by rotating the coordinate x into the complex coordinate plane by the angle $\theta = 0.75$ (i.e., we scale x by $\exp(i\theta)$) we calculate the first 20 complex poles which are closest to the real axis in more then six digits of accuracy and 20 more in less accuracy. The first seven ones are isolated resonances but only the first two are narrow resonances ($E_1^{\rm res} = 1.4209709 - i\,0.5826663\cdot 10^{-4}$, $E_2^{\rm res} = 2.1271971 - i\,0.015447319$). All the others are broad resonances. For example the 7-th one is equal to $E_7^{\rm res} = 3.8243295 - i\,2.4874462$. Between 3.0 to 4.5 there are nine poles with widths which vary from about 10 to 20 (note that $-2\,{\rm Im}(E^{\rm res}) = \Gamma$). Since we are interested in the calculation of the short lived resonances we choose $E_{\min} = 3.0$ and $E_{\max} = 4.5$. Note that there are overlapping resonances which have about the same position and are very different with respect to their widths.

The complex-scaled autocorrelation amplitude probability, $C_1(t)$, was calculated for an initial state that was constructed of a random complex superposition of all eigenstates of the complex scaled Hamiltonian (not only the poles) with energy above unity. This was done to simplify the calculations and it is equivalent to populate randomly the phase space from $E = 1$ to $E = 5$. (Equivalently, a completely random initial wavefunction made of all eigenstates could be taken.)

The results presented in Fig.1 show that only the most narrow isolated pole is accurately obtained (six significant digits for the position and four for the width), whereas the three others were obtained in much less accuracy. $N_\omega = 30$ filter basis functions were found to provide stable results in this calculation (for large value of N_ω the overlap matrix becomes singular and needs to be handled [2] with singular value decomposition). The time step was $dt = \pi/10$. We have made no effort here to study the required number of time steps, so that a large number of steps (860) was taken.

In order to increase the accuracy of the results obtained from the filter diagonalization calculations, we replaced (following [2]) the autocorrelation probability amplitude $C_1(t)$ by the cross-correlation probability amplitudes, $C^{[n',n]}(t) = \langle\phi_{n'}(0)|\phi_n(t)\rangle$; $n, n' = 1, \ldots, N$. Let us first describe the motivation for this. The filter basis functions obtained from the autocorrelation probability calculations are assigned two indices, ω and $n = 1, 2, \ldots$, the latter associated with the selected initial condition. For example we can choose N different initial wave packets that are randomly distributed in the available phase space. The filter basis functions are now $|\Psi_{\omega,n}\rangle$; $n = 1, 2, \ldots, N$ rather than $|\Psi_{\omega,1}\rangle$ used above. The time evolution matrix element $U(\omega',\omega)$ is denoted by two more indices, n and n': $U(\omega', n', \omega, n)$. When discrete values for ω are taken, we will replace the notation of ω by $\omega_j = \omega_{\min} + j\,d\omega$ and of ω' by $\omega_{j'} = \omega_{\min} + j'd\omega$. Therefore the matrices $\mathbf{U}$ and $\mathbf{S}$ are constructed from the sub-matrices $\mathbf{U}^{[n'n]}$ and $\mathbf{S}^{[n'n]}$. Since the integration over time is carried out on a grid, $t_k = k\,dt$; $k = 0, 1, \ldots, N_t$, we may replace the integrals in Eq. (3) by a summation. The matrix elements of the sub-matrices of the time evolution operator and of the overlap between two filter basis functions are given by

$$U_{j',j}^{[n',n]} = \sum_{k=0}^{2N_t} F_{j',j}(k) \exp(i\,dt\,k(\omega_{j'} + \omega_j))\, C_{k+1}^{[n',n]} \qquad (6)$$

$$S_{j',j}^{[n',n]} = \sum_{k=0}^{2N_t} F_{j',j}(k) \exp(i\,dt\,k(\omega_{j'} + \omega_j))\, C_k^{[n',n]} \qquad (7)$$

with

$$F_{j',j}(k) = \sin((T - |T - dt\,k|)(\omega_{j'} - \omega_j))/(\omega_{j'} - \omega_j) \quad (8)$$

for $j' \neq j$ and

$$F_{j,j}(k) = T - |T - dt\,k|\,. \qquad (9)$$

Note that the cross-correlation probability amplitude $C_k^{[n',n]}$ is equal to $\langle\phi_{n'}(0)|\phi_n(t=t_k)\rangle$; $t_k = k\,dt$. The desired spectrum, $E_\ell = i(\hbar/\tau)\ln\Lambda_\ell$, is obtained by solving the generalized eigenvalue problem $\mathbf{U}\Psi_\ell = \Lambda_\ell\mathbf{S}\Psi_\ell$, where $\ell = 1, 2, \ldots, NN_\omega$.

The results shown in Figs. 2–3 are obtained for four and eight initial states, respectively, which randomly populate the eigenstates of the Hamiltonian with energies larger then 1.4. Both the real and the imaginary parts of the linear coefficients were randomly obtained. The $A_{n',n} = \langle\phi_{n'}(0)|\phi_n(0)\rangle$ was c-normalized to unity for $n' = n$ and, for $n' = 2, n = 1$, $|A_{1,2}|^2 = 0.00475$, and $|A_{1,3}|^2 = 0.1221$, $|A_{1,4}|^2 = 0.1845$, $|A_{2,3}|^2 = 0.0127$, $|A_{2,4}|^2 = 0.000538$, $|A_{3,4}|^2 = 0.06035$.

The comparison between Figs. 1,2 and 3 shows very clearly that the use of cross-correlation functions not only increases the accuracy of the calculations but also enables us to obtain from short time dependent calculations broad overlapping poles. For example, the fifth pole has an imaginary part which is equal to -1.1111 and its contribution to the evolution in time of the propagated wave packet decays to zero much before 860 time steps of propagation (i.e. $\exp(-\mathrm{Im}E^{\mathrm{res}}t/\hbar) \sim \exp(-300)$, after 860 time steps). Since the main point of this illustrative numerical example is in the comparison between the best results one can get out of the time autocorrelation probability amplitude and the results obtained when several cross-correlation functions are calculated, we did not try to find out what is actually the minimal length of the time propagation one can use.

We believe that the proposed method, which is a combination of complex scaling and Filter-Diagonalization, will be found to be useful for calculating the resonances of other systems. The major new point we address in this communication is that the energy spectra (not only broad resonances but also narrow ones and bound states) can be obtained from short time propagations of several randomly selected initial wave packets and by calculating the corresponding cross-correlation probability amplitudes.

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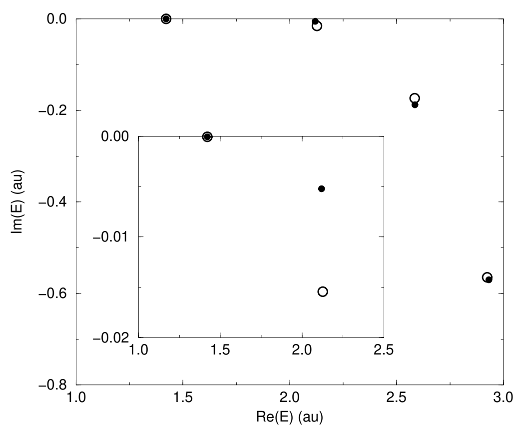

FIG. 1. The poles obtained from the autocorrelation probability amplitude, $C_1(t)$, (full circles) in comparison with the exact numerical results (open circles). The insert shows a magnification of the first two low lying resonances.

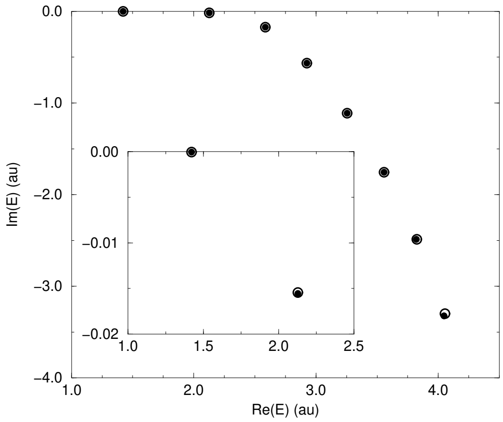

FIG. 2. The resonance poles as obtained by the filter-diagonalization method from four cross-correlation amplitude probabilities. The four initial states were taken at $t = 0$ as random superposition of all eigenstates of the complex scaled Hamiltonian above the threshold. 30 energy filter points were used ($N_\omega = 30$ and $\omega_{\min} = 3$ and $\omega_{\max} = 4.5$).

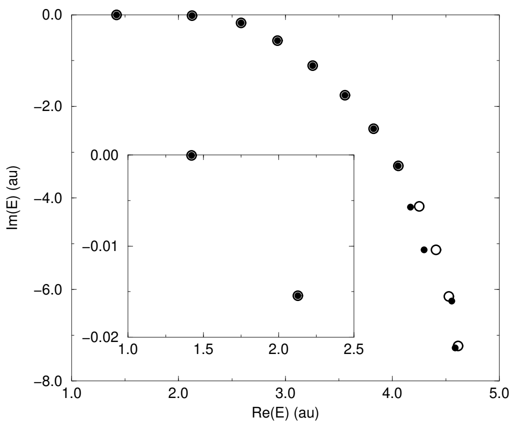

FIG. 3. As in Fig. 2, but eight cross-correlation amplitude probabilities were used in the generation of the filter basis set.