Spectral Analysis of Time Correlation Functions by the Filter Diagonalization Method

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Abstract

The Filter Diagonalization Method (FDM) for spectral analysis of time signals, first introduced by Neuhauser, has extensively been developed and applied by several groups to various problems in physics and chemistry. I will review some interesting developments and applications of FDM in the area of quantum dynamics calculations and semiclassical quantization.

FDM is designed to solve the Harmonic Inversion Problem which corresponds to fitting a (time) signal by a sum of damped sinusoids. Formally being nonlinear it has though a unique solution that can be obtained by FDM. In the most efficient version FDM allows to extract the maximum information contained in the time signal of question. To optimally utilize this property one wants to produce signals (e.g., quantum time correlation function) with minimum amount of noise. For a quantum scattering problem this is complicated by the need to implement an optical potential to localize the propagated wave function, as all existing numerical schemes for the time propagators with optical potentials are approximate and therefore always introduce some noise. Interestingly, Chebyshev correlation function is conceptually similar to the time correlation function, but has the advantage of being both very accurate (i.e., zero noise) and easy to evaluate numerically. Moreover, it can be modified with absorbing boundary conditions which correspond to introducing an effective complex optical potential. The resulting Chebyshev correlation function can be shown to be exactly a sum of damped sinusoids which is ideal for FDM. this method allows to compute very accurately hundreds of resonances with moderate numerical effort.

Exactly the same method of harmonic inversion can be used in the very straight forward way to invert semiclassical signals, for instance, a Gutzwiller periodic orbit sum to yield semiclassical both resonance and bound state energies.