# Extracting complex resonance energies from real calculations.

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Two complementary approaches are presented to demonstrate how the resonance energies and widths can be computed with a good accuracy by using standard quantum chemistry codes. The first approach is the analytic continuation in coupling constants (ACCC) method [1, 2]. The complex resonance energy is obtained from Padé approximation of the $k(\lambda) = \sqrt{E(\lambda)}$ function, where $\lambda$ is the parameter of an attractive perturbation $V(\lambda)$, that may be an additional nuclear charge or a coordinate-dependent potential. Successful applications to atomic anions and negative amino acid ions will be presented.

The second approach is based on a unified formulation of the quantum theory of unstable states and of their dynamics [3]. The method has a simple and rigorous mathematical framework and is based on non-Hermitian changes of representation of the dynamics and on the analytical properties of the Fourier-Laplace transformation [4]. A hybrid computational scheme borrows from both the Hermitian stabilization methods and the non-Hermitian approaches using complex absorbing potentials. Real energies depending on a real parameter $\lambda$ provided by real ab initio (or model) calculations are by the transformation $\lambda \to -\imath\lambda$ converted into the complex energies of the resonances, similarly as in the ACCC method. The advantages and drawbacks of the second approach will be presented on two models, spherical potential and Fano model.

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