Resonance excited states energies and life-times: Suite of complex scaled EOM-CCSD methods

Dmitry Zuev, Ksenia B. Bravaya, Anna I. Krylov
University of Southern California, Los Angeles, CA

Resonance states are ubiquitous in Nature: they encounter in atomic and molecular systems, in plasma and in radioactive isotopes. We present a new suite of *ab initio* methods for calculation of autoionizing electronically excited states (both positions and lifetimes) – complex scaled equation-of-motion coupled-cluster (cs-EOM-EE-CCSD and cs-EOM-EA-CCSD) theories combined with complex scaled coupled cluster (cs-CCSD) and complex scaled Hartree-Fock (cs-HF). The problem in description of this phenomenon lies in the exponentially divergent character of the resonance wave-function. These states can not be described using conventional *ab initio* methods and special techniques have to be used. An elegant solution is provided by complex scaling formalism in which resonance wave-function is naturally obtained as a square-integrable eigenfunction of the complex-scaled Hamiltonian, and real and imaginary parts of the complex eigenvalue correspond to the resonance position and life-time, respectively [1-3]. This technique enables description of the resonance states with the same methods and algorithms one usually uses to describe bound states. We present an implementation of the cs-EOM-EE-CCSD and cs-EOM-EA-CCSD methods, which combine ideas of the complex scaling method for treating resonance states with state-of-the-art quantum chemistry description of the excited states and electron-attached states (EOM-EE-CCSD and EOM-EA-CCSD, [4]). Ground state obtained by cs-HF and cs-CCSD is a suitable reference for cs-EOM-CCSD calculations. Our test calculations of atomic resonances on two (H-, He) and many electron (Be) systems give accurate values of both resonance position and lifetime [5-6]. The methods can be universally applied to both Feshbach and shape type of resonances.

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