Complex-variable coupled-cluster methods for autoionizing and Stark resonances

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Electron-molecule collisions and non-perturbative light-matter interactions often involve the formation of resonances that belong to the continuum and are beyond the reach of electronic-structure methods for bound states. An elegant treatment of resonances as quasistationary states with complex energy is possible by means of complex-variable (CV) techniques such as complex scaling or complex absorbing potentials.

In this talk, I will present recent advances in CV coupled-cluster (CC) methods [1] and discuss the suitability of different CV techniques for different types of resonances. In particular, I will focus on the differences between autoionizing resonances such as temporary anions and Stark resonances induced by external electric fields.

Exemplary applications to small molecules such as CO, O_2, and H_2O illustrate that an accurate treatment of electron correlation is of great importance even for a qualitative correct description of molecular Stark resonances and their strong-field ionization rates [2, 3]. An important advantage of the proposed CV-CC treatment of Stark resonances is that the computation of molecular properties is straightforward. The usefulness of molecular properties is illustrated by a simple criterion for distinguishing tunnel and above-barrier ionization in polyatomic molecules based on the second moment of the electronic charge distribution.

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[2] T.-C. Jagau, J. Chem. Phys. **145**, 204115 (2016).
[3] T.-C. Jagau, J. Chem. Phys., submitted (2018).