A Fresh Look at Metastable Electronic States: Equation-of-Motion Coupled-Cluster Based Approach

Thomas-C. Jagau and Anna I. Krylov

Department of Chemistry, University of Southern California, SSC 409, Los Angeles, CA 90089

Resonance states are important in diverse areas of science ranging from plasma physics to atmospheric chemistry and molecular biology. Such states are beyond the reach of standard quantum-chemical methods; they belong to the continuum part of the spectrum and are, thus, not L^2-integrable.

We present a production-level implementation of equation-of-motion coupled-cluster singles and doubles augmented by a complex absorbing potential (CAP-EOM-CCSD) that allows similar treatment of resonance states and bound states. A de-perturbative correction for resonance positions and lifetimes is introduced to study molecular resonances in a black-box manner. The usefulness of our protocol is discussed in light of the well-known challenges of resonance states such as pronounced basis-set dependence and difficulties when constructing potential energy surfaces.

[1] T.-C. Jagau, D. Zuev, K. B. Bravaya, E. Epifanovsky, and A. I. Krylov, *J. Phys. Chem. Lett.* **5**, 310 (2014).
[2] D. Zuev, T.-C. Jagau, K. B. Bravaya, E. Epifanovsky, Y. Shao, E. Sundstrom, M. Head-Gordon, and A. I. Krylov, *J. Chem. Phys.* **141**, 024102 (2014).
[3] T.-C. Jagau and A. I. Krylov, *J. Phys. Chem. Lett.* **5**, 3078 (2014).