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Localization of S-matrix poles in the complex energy plane using the molecular R-matrix method[1] ZDENEK MASIN, Institute of Theoretical Physics, Charles University, Prague, Czech Republic — Identification of resonances in computed cross sections is one of the main goals of ab initio scattering calculations. A common approach involves fitting of the data computed for real scattering energies to the Breit-Wigner form (in case of eigenphase sums) or the Lorentzian form (in case of time-delays), see e.g. [1-2]. While this approach works well for narrow resonances, it becomes unreliable especially for very wide resonances and core-excited resonances appearing in electronically inelastic calculations. In this contribution we resurrect an approach for localization of resonant S-matrix poles using the diatomic R-matrix method [3]. The exact energy factorization of the R-matrix approach is ideally suited for finding the Siegert solutions of the Schrödinger equation in the complex plane. We describe our implementation within the polyatomic UKRmol+ codes, study its numerical properties and apply it to localization of resonances in low-energy electron collisions with pyrrole including their dependence on nuclear geometry.
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