Abstract Submitted
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Overset grid implementation of the complex Kohn variational method for electron-polyatomic molecule scattering[1] C. WILLIAM MCCURDY, University of California, Davis and Lawrence Berkeley National Lab., ROBERT L. LUCCHESE, Texas A & M University, LOREN GREENMAN, University of California, Davis — The complex Kohn variational method, which represents the continuum wave function in each channel using a combination of Gaussians and Bessel or Coulomb functions, has been successful in numerous applications to electron-polyatomic molecule scattering and molecular photoionization. The hybrid basis representation limits it to relatively low energies (< 50 eV) , requires an approximation to exchange matrix elements involving continuum functions, and hampers its coupling to modern electronic structure codes for the description of correlated target states. We describe a successful implementation of the method using completely adaptive overset grids to describe continuum functions, in which spherical subgrids are placed on every atomic center to complement a spherical master grid that describes the behavior at large distances. An accurate method for applying the free-particle Greens function on the grid eliminates the need to operate explicitly with the kinetic energy, enabling a rapidly convergent Arnoldi algorithm for solving linear equations on the grid, and no approximations to exchange operators are made. Results for electron scattering from several polyatomic molecules will be presented.

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