

Abstract Submitted
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Hybrid Gaussian-discrete variable representation for continuum electrons in molecules¹ FRANK L. YIP, California Maritime Academy, C. WILLIAM MCCURDY, Lawrence Berkeley National Lab and U.C.Davis, THOMAS N. RESCIGNO, Lawrence Berkeley National Lab — A combined basis of analytic Gaussian functions and grid-based finite element discrete variable representation (FEM-DVR) with spherical harmonic expansion is specialized for description of continuum electron dynamics in the presence of electrons held fixed in core molecular orbitals. The applicability of this hybrid representation designed for general problems involving accurate determination of molecular continua wave functions is illustrated for photoionization of a second-row diatomic molecule, nitric oxide, NO. Accurate descriptions of such electron continuum dynamics are a necessary step towards analyzing correlated double continua photoejections. Examination of this hybrid method in comparison to a more computationally expensive pure grid-based single center expansion reveals several key advantages that by design make it attractive for describing processes involving one or more electrons moved to the continuum.

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