Abstract Submitted
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Time-independent and time-dependent calculations on one and two-photon ionization of diatomic molecules with a grid-based method in prolate spheroidal coordinates[1] LIANG TAO, LBNL, C.W. MCCURDY, LBNL and UCDavis, T.N. RESCIGNO, LBNL — We show how to combine finite elements and the discrete variable representation in prolate spheroidal coordinates to develop a grid-based approach for quantum mechanical studies involving diatomic molecular targets. The use of exterior complex scaling in the present implementation allows for a transparently simple way of enforcing Coulomb boundary conditions and therefore straightforward application to electronic continuum problems. The time-independent and time-dependent calculations of photoionizaton cross sections for H_2^+, as well as time-independent results for the two-electron H_2 target, show that the efficiency and accuracy of the present approach offers distinct advantages over methods based on single-center expansions.

[1]Work performed under auspices of USDOE by LBNL.

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