

Abstract Submitted
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Dipole-Forbidden Transitions in Numerical Solutions of the Time-Dependent Schrödinger Equation¹ DUSTIN URSREY, BRETT ESRY, J.R. Macdonald Laboratory, Kansas State University, Manhattan, KS 66506, USA — Theoretical studies of atoms and molecules in intense, ultrafast laser pulses require numerical solutions of the time-dependent Schrodinger equation (TDSE). Such numerical solutions necessarily introduce approximations to the exact wavefunction, and - if care is not taken -, these approximations can produce results that do not accurately describe the physics predicted by the TDSE. Here we present one such non-physical result that can occur in numerical solutions. Specifically, we show that seemingly dipole-forbidden transitions can be found for dissociation of D_2^+ , excitation of a hydrogen atom, and excitation of a model three-level system. Moreover, we show that these non-physical excitations occur for a variety of spatial representations of the wavefunction (both finite-differencing and a finite-element discrete variable representation) and time propagation techniques (Crank-Nicholson and Runge-Kutta). We show that these non-physical excitations are caused by the way electric field is turned on in the code, and propose methods for eliminating such excitations without increasing the computation time required to solve the TDSE.

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