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Effective one-electron approaches to calculate high harmonic generation[1] NINA ROHRINGER, ROBIN SANTRA, Argonne National Laboratory, Argonne, IL 60439, USA — The single-active electron approach (SAE) is frequently applied to calculate high harmonic generation in atoms and consists in solving a one-particle Schrödinger equation in an appropriate model potential. As an ad hoc approach it is difficult to be systematically improved. Starting with the time-dependent configuration interaction singles (TDCIS) technique we derive a new class of effective one-electron approaches. The resulting one-electron equations are in general non-local and non-unitary. A local approximation to TDCIS can be derived by restricting the total many-body Hamiltonian to a local mean-field Hamiltonian (those usually used in SAE calculations). The resulting equations are similar to traditional SAE approaches but include an additional term which destroys the unitarity of the time-evolution. We show that this correction term is essential and improves on traditional SAE approaches. Numerical tests show that this improved SAE method gives dipole-moments in better agreement with exact results than time-dependent Hartree Fock. The test system is a one-dimensional model of helium which allows for a straightforward numerical solution and therefore provides a benchmark to assess the quality of the different approximations.

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Nina Rohringer
Argonne National Laboratory, Argonne, IL 60439, USA

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