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Three-Step Model for High-Harmonic Generation in Many-Electron Systems[1] ROBIN SANTRA, Argonne National Laboratory, Argonne, IL 60439, ARIEL GORDON, Research Laboratory of Electronics, Massachusetts Institute of Technology, 77 Massachusetts Ave., Cambridge, MA 02139 — The three-step model (TSM) of high-harmonic generation (HHG) is generalized to atomic and molecular many-electron systems. Using many-body perturbation theory, corrections to the standard TSM due to exchange and electron–electron correlations are derived. It is shown that canonical Hartree-Fock orbitals represent the most appropriate set of one-electron states for calculating the HHG spectrum. To zeroth order in many-body perturbation theory, a HHG experiment allows direct access in general to a combination of occupied Hartree-Fock orbitals rather than to the highest occupied molecular orbital by itself.

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