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Reduced-Density-Matrix Approach for the Spectral Description of Multi-Photon Processes in Quantized Many-Electron Systems[1] VERNE JACOBS, Naval Research Laboratory, ALEX KUTANA, Rice University — A reduced-density-matrix description is developed for the evaluation of the frequency-dependent transition rates for multi-photon processes in quantized many-electron systems. Our objective is to provide a fundamental foundation for systematic spectral simulations for atomic, molecular, and solid-state systems. A perturbation expansion of the frequency-domain Liouville-space self-energy operator is employed to evaluate the spectral-line widths and shifts in the isolated-line and short-memory-time (Markov) approximations. The lowest-order contributions from environmental electron-photon and electron-phonon interactions are systematically taken into account. The proposed description is directly applicable to dynamical processes in a variety of systems, including semiconductor, photochemical, and biological, without further approximations. In particular, our description can be applied to investigate the dynamical behavior of electrons in bulk and nanoscale semiconductor materials entirely from first principles, using the density functional formalism and existing electronic structure codes.

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