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Spectral Description of Multi-Photon Processes in Quantized Many-Electron Systems Based on a Reduced-Density-Matrix Approach[1]
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— The frequency-dependent transition rates for multi-photon processes in quantized many-electron systems are evaluated using a reduced-density-matrix approach. We 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 in detailed evaluations of the spectral-line widths and shifts in the isolated-line and short-memory-time (Markov) approximations. The lowest-order contributions associated with environmental electron-photon and electron-phonon interactions are systematically taken into account. Our description is directly applicable to electromagnetic processes in a wide variety of semiconductor, photochemical, and biological systems, without premature approximations. In particular, our approach can be applied to investigate optical phenomena involving electrons in both bulk and nanoscale semiconductor materials entirely from first principles, using the density functional formalism and existing electronic structure codes.

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