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Relativistic Time-Dependent Configuration Interaction Singles Method

Attosecond physics aims to unravel the electron motion and coherence in atoms and molecules. Major contributions to this field are the real-time observations of the motion of electrons in ions and atoms through attosecond transient absorption spectroscopy (ATAS). Regarding the lack of a relativistic theory, our aim is to develop a general relativistic ATAS method for studying atoms far beyond the perturbative regime. Seeking a compromise between computational cost and accuracy, the relativistic time-dependent configuration interaction singles (RTDCIS) method is proposed. This novel method opens up the possibility to describe the electron spin dynamics by means of spin-resolved ATAS experiments far beyond the perturbative regime. Similarly, it can be applied to other strong-field processes, such as high-order harmonic generation, above-threshold ionization, laser-assisted photoionization, hole alignment, and the study of complex Rabi dynamics.

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