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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. A major contribution to this field was the real-time observation of the motion of valance-shell electrons in krypton ions made by Goulielmakis et al. in 2010 [1]. Since then, ATAS has been widely used in different scenarios [2]. Despite the great success of ATAS, all studies so far are based on non-relativistic ATAS theory [3], although the importance of spin-orbit coupling was demonstrated already by the first ATAS experiment [1]. Regarding the lack of a relativistic theory, our aim is to develop a general relativistic attosecond transient absorption spectroscopy method for studying atoms far beyond the perturbative regime [4].

In order to achive our goal, the N-electron time-dependent Dirac equation (TDDE) must be solved. As a compromise between computational cost and accuracy, the relativistic time-dependent configuration interaction singles (RTDCIS) method is proposed as an efficient option to solve this complicated task [5]. In oder to validate RTDCIS, different observables has been computed for krypton and xenon, such as the photoionization cross sections. RTDCIS results have been compared with other relativistic calculations and experimental data. As expected, RTDCIS results are similar to RRPA within the Tamm-Dancoff approximation (RRPA(TD)). This novel method opens the possibility to describe the electron spin dynamics by means of spin-resolved ATAS experiments far beyond the perturbative regime.

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Authors: Dr ZAPATA ABELLAN, Felipe (Lund University); Mr LJUNGDAHL, Anton (Stockholm University); Mr VINBLADH, Jimmy (Stockholm University); Prof. LINDROTH, Eva (Stockholm University); Dr DAHLSTRÖM, Jan Marcus (Lund University)

Presenter: Dr ZAPATA ABELLAN, Felipe (Lund University)

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