Ab Initio Approach To The Study Of Transient States And Ultra-Fast Processes

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Abstract. Recent advances in attosecond XUV pulse generation pave the way for time-resolved investigation and control of electron wave-packets [1]. The interpretation of this as well as of similar experiments often relies on single-particle models where the interaction of the photoelectron with the remaining electrons in the atom is approximated by a local static potential. The assumptions at the basis of these models, however, come with two major limitations: they do not account for the underlying many-electron processes that unfold on the same time-scale as the photoelectron emission, and they do not properly enforce the exclusion principle.

In this contribution, we report on the development of a package that aims at integrating the Time-Dependent Schrödinger Equation (TDSE) including many-body effects, as well as providing reliable ab initio data of use in atomic attophysics, e.g. photoelectron phases – which relate to so-called photoionization time delays –, multi-photon ionization cross-sections, and resonnance properties. We follow a configuration interaction approach with orbitals expended on B-spline basis sets. For dealing with the complicated angular integration involved in computing matrix elements, we use the Atomic Structure Package (ATSP2K) [2]. In order to avoid problems due to the finite box, in time independent computations, we solve the many-body problem along complex radial coordinates, i.e. using the (exterior) complex scaling method.

Photoionization cross-sections and resonnance widths are reported using (i) time-independent perturbation theory combined with complex scaling, and (ii) integration of the TDSE. We also present photoelectron phases obtained using exterior compex scaling.

1. F. Krausz and M. Ivanov, *Rev. Mod. Phys.* **81**, 163 (2009)
2. C. Froese Fischer *et al.*, *Comp. Phys. Comm.* **176**, 559 (2007)