Atomic and molecular suite of R-matrix codes for ultrafast dynamics in strong laser fields and electron/positron scattering

Journal Item

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Synopsis We describe and illustrate a number of recent developments of the atomic and molecular ab initio R-matrix suites for both time-dependent calculations of ultrafast laser-induced dynamics and time-independent calculations of photoionization and electron scattering.

The field of attosecond science has presented computational physics with a set of new challenges to describe the dynamics of matter in strong femtosecond lasers. The recent move to study complex multielectron systems makes the need for a matching ab initio theoretical description even more pressing. In the more mature field of electron-molecule collisions, the need to study more complex targets has also required software improvements. Our R-matrix suites of codes [**?**, **?**] have recently undergone a major upgrade and been made available to the community.

A set of atomic and the molecular time-independent codes form their core. On the atomic side these are the well-established RMATRXI and RMATRXII codes: both use a B-spline representation of the continuum; RMATRXI allows the inclusion of relativistic (Breit-Pauli) corrections. On the molecular side, a major development has led to the release of UKRmol+, based on code originally developed for electron/positron - molecule scattering. This suite has been extended to enable photoionization calculations and to include B-splines in the representation of the continuum via the new GBTOlib integral library. Significant improvements in performance of the molecular codes have been achieved developing a new parallel Hamiltonian build algorithm and a parallelized version of the R-matrix propagator.

The second layer of the R-matrix suite comprises R-matrix with time (RMT) [**?**] codes which can now be used to propagate in time both the atomic and molecular (in the fixed-nuclei approximation) wavefunctions. Recent developments allow the use of arbitrary polarized light and interfacing with the atomic RMATRXI suite thus enabling studies of spin-orbit dynamics in ultrafast laser fields.

The recent developments will be described, including illustrations of the results on generation of electron vortices from argon atoms, relativistic effects in the vicinity of the giant resonance in Xenon and validation tests of molecular RMT on photoionization of water. The benefits for the electron-molecule scattering community will be illustrated with the results for inelastic electron scattering from thiophene.

References

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