Simulating the time-dependent non-equilibrium dynamics of many-electron systems

Stefan Donsa, Isabella Floss, Valerie Smejkal, Fabian Lackner, Christoph Lemell, Iva Březinová, Joachim Burgdörfer

Institute for Theoretical Physics, TU Wien

We investigate the correlated non-equilibrium multi-electron dynamics of bosonic and fermionic systems initiated and driven by time-dependent perturbations. The accurate description of these processes requires powerful numerical resources in terms of memory as well as computational performance. We use a broad variety of different techniques ranging from directly solving the time-dependent Schrödinger equation over advanced multi-electron methods (e.g. multi-configurational time-dependent Hartree-Fock, two-particle reduced density matrix method) to effective mean-field theories like time-dependent density functional theory (TDDFT) and the Gross-Pitaevskii equation.

Recent results obtained using the Vienna Scientific Cluster include:

- **Electron dynamics in helium:** Mapping the absorption time of photons to the angular distribution of electrons emitted by two-photon double ionization by using an ultrashort XUV-XUV pump-probe sequence with elliptically polarized laser pulses [1].
- **Anderson localization of an interacting many-body system:** Understanding the role of particle-particle interactions within the expansion dynamics of a Bose-Einstein condensate in a shallow disorder potential [2].
- **Non-linear electron dynamics in dielectrics:** Understanding the influence of mesoscopic effects (pulse propagation inside the medium, inhomogeneous pulse profile) in high-harmonic generation in dielectrics and insulators (e.g. diamond) [3].

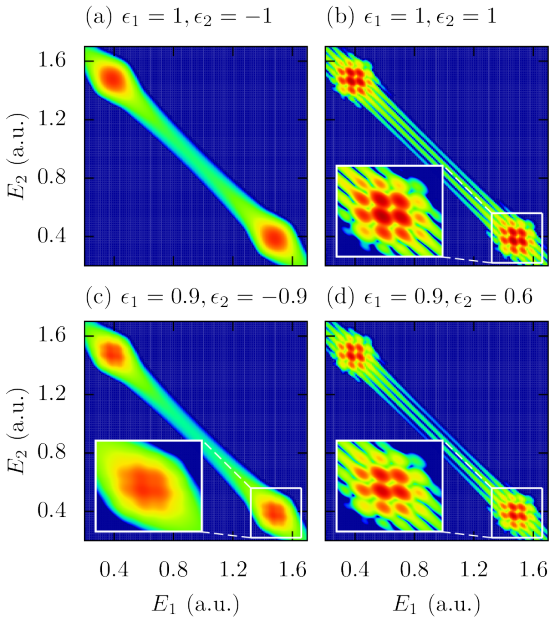

Fig. 1: Double-ionization spectrum of atomic helium after ionization by an ultrashort XUV-XUV sequence with different ellipticities ϵ_1, ϵ_2.

References

[1] Donsa, S. et al., arXiv:1811.09110

[2] Donsa, S. et al., Phys. Rev. A **96**, 0463630 (2017)

[3] Floss, I. et al., Phys. Rev. A **97**, 011401(R) (2018)