Coherent excitation of shake-up states in rare gas atoms by attosecond xuv pulses

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Synopsis We present calculations on XUV-IR pump-probe setups to study the ionization dynamics of (coherently) excited shake-up states in neon and helium atoms. We investigate the role of coherent effects, electron-electron interaction, and the IR field in the shake-up process.

The rapid progress in the creation of attosecond pulses in the extreme ultraviolet (XUV) regime via high-harmonic generation paves the way towards time-resolved atomic physics (cf. [1] and references therein). Pump-probe setups exploiting these ultrashort pulses allow for the direct observation of ultrafast electronic dynamics.

In a recent experiment [2], Uiberacker *et al.* exposed neon atoms to a phase-stabilized few-cycle infrared (IR) laser field and a synchronized attosecond XUV pulse. The XUV pulse leads to single ionization of the Ne atom and the creation of excited (shake-up) states in the residual Ne^+ ion. The IR pulse can then further ionize the Ne^+ ion, thus serving as a probe for the quantum state of the singly ionized ion. By monitoring the yield of doubly charged Ne^{++} ions as a function of the time delay between the two pulses the (ionization) dynamics of the electronic wave packet created by the XUV pulse can thus be studied.

The overall stepwise structure of the resulting double ionization yield as a function of delay time results from tunneling of the excited shake-up states [2, 3]. The information accessible in such experiments beyond the step-wise incoherent tunneling ionization has remained an open question, triggered by the observation of a sequence of dips superimposed on the ionization signal. Those sub-structures point to additional coherent effects such as population transfer between the shake-up states or quantum beats, cf. [4]. The presence of the IR field might also significantly affect the shake-up process. In addition, electron-electron interactions could play an important role as well.

As a first step to identify the relevant mechanisms we calculate the response of the Ne^+ shake-up states to the IR field by solving the time-dependent Schrödinger equation in single-active electron (SAE) approximation. We find that the stepwise increase in the ion signal with superimposed dips is best reproduced when we chose the *same phases* for shake-up states of *same symmetry* (i.e., same angular quantum number l) and average over the phases of the remaining states. This is consistent with the sudden approximation for the shake-up process [5] which implies a monopole transition. The overall qualitative agreement with the experiment suggests that the experimental double ionization signal in an XUV-IR pump-probe setting contains evidence of the coherent excitation of shake-up wave packets.

In order to investigate the limitations of the SAE simulations, we also perform calculations for the complete XUV-IR pump-probe setup, however, instead of neon for *helium*, where the multi-electron dynamics can be solved *ab initio* without additional approximations [6]. We will present comparisons with SAE calculations for helium which will help to identify the predominant contributions to the resulting ionization yields.

References

[1] Krausz F and Ivanov M 2009 *Rev. Mod. Phys* **81** 163

[2] Uiberacker M *et al.* 2007 *Nature* **446** 627

[3] Yudin G L and Ivanov M Y 2001 *Phys. Rev. A* **64** 013409

[4] Kazansky A K, Kabachnik N M and Sazhina I P 2008 *Europhys. Lett.* **82** 13001

[5] Åberg T 1967 *Phys. Rev.* **156** 35

[6] Feist J, Nagele S, Pazourek R, Persson E, Schneider B I, Collins L A and Burgdörfer J 2008 *Phys. Rev. A* **77** 043420