Two-photon K-shell ionization cross sections for neutral atoms

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Synopsis The non-resonant two-photon K-shell ionization of neutral atoms has been studied within a fully relativistic framework, where many-electron effects have been accounted for by a screening potential. It is shown that both the relativistic and screening effects significantly alter the total as well as angle-differential cross section as compared to nonrelativistic calculation. Moreover, screening effects may lead to an elliptical dichroism in the photoelectron angular distribution.

Deep understanding of nonlinear processes became desirable with the recent development of bright and high-energetic free-electron laser sources. Two-photon ionization is one of the fundamental nonlinear processes, and a benchmark for studying the interaction of intense light with matter. Although recent experiments measured the two-photon K-shell ionization of mid-Z elements, the comparison of experiment with theory was based so far on the Schrödinger's nonrelativistic theory, and with little account of many-electron effects.

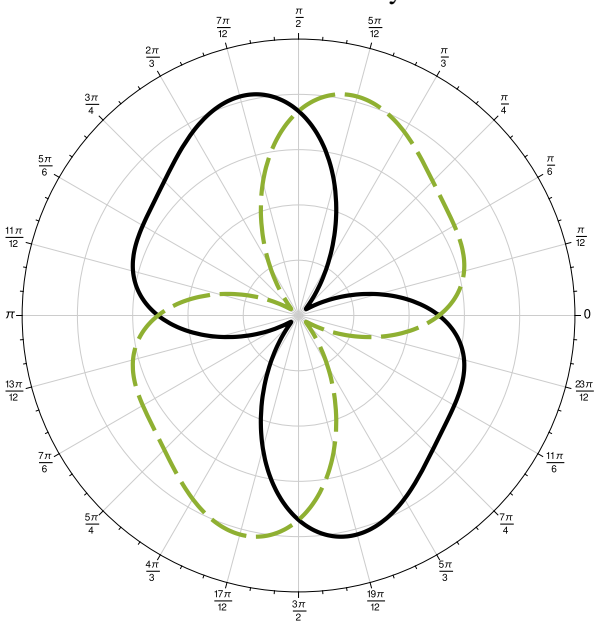

Figure 1. The elliptical dichroism in the non-resonant two-photon K-shell ionization of neutral Ne can be used to experimentally verify the importance screening effects.

To understand the interplay of relativistic and many-electron effects upon the two-photon K-shell ionization of mid- and high-Z elements, further theoretical effort had to be paid to this fundamental process. In our recent works [1, 2], we carried out relativistic computations for the two-photon ionization of neutral atoms, we applied the single-active electron approximation and accounted for all the other electrons by a screening potential in the interaction Hamiltonian. Within this framework, we analysed the importance of relativistic effects as well as the screening effects on the total cross section. We found, that relativistic effects may decrease the total cross section of ionization of heavy elements by a factor of up to three. Moreover, we analysed the individual relativistic contributions to the cross section. While the dominant contribution arises from the relativistic contraction of the K-shell orbital (direct relativistic effect), higher multipoles are less important. However, higher multipoles need to be incorporated into the calculations of the angle-differential cross section, as they significantly distort the electron distribution along the incident photon direction [3].

The screening of the active electron by all the other electrons results in an unexpected decrease of the total cross section for light atoms and near to the ionization threshold. A closer inspection of this behaviour reveals a more physical explanation of the drop in the cross section. For slow photoelectrons, in particular, the screened wavefunction of the dominant d-wave shifts away from the nucleus. As a consequence, the overlap integral of this dominant ionization channel is low, as well as, the total cross section is reduced. This influence occurs even more pronounced in the photoelectron angular distribution, where it leads to an elliptical dichroism in the photoelectron distribution, see Figure 1. As this effect is strongest for Ne atom, the detection of the dichroism is feasible and could serve for an experimental verification of the importance of screening effects.

References

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