Fully differential single photon double photoionization of atomic magnesium

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Synopsis The valence-shell double ionization of the $3s^2$ valence electrons of magnesium is calculated using a grid-based representation in the presence of a frozen-core configuration and compared with calculated results and experiment at $\omega =$ 55.49 eV.

Double photoionization, the mechanism of removing two electrons via a single photoabsorption, necessarily requires a correlated target, and the resulting angular distributions and possible energy sharings of the outgoing electrons from the Coulomb breakup problem requires an accurate non-perturbative treatment for theory and coincidence measurements of the fragments for experiment. The formalism we employ to study this process for targets with more than two electrons, here atomic magnesium, requires denoting the neon-like core occupancy of all but the valence electrons, which provide a closed-shell Coulomb and exchange interaction with the outer $3s^2$ electrons that feel the action of the photon towards the double continuum. The construction of atomic orbitals out of an underlying radial grid to represent these core electrons facilitates the approximation of holding them fixed in a configuration-interaction expansion and has been applied to other helium-like ns^2 atoms [1].

Within this frozen-core approximation, the problem then can be regarded as an effective two-electron problem involving a full CI of the $3s^2$ valence electrons of magnesium in the presence of the $1s^2 2s^2 2p^6$ core, the full Hamiltonian being $H = h(1) + h(2) + 1/r_{12}$, where the one-body operator h,

$$h = T - \frac{Z}{r} + \sum_{\rm occ} [2J_{\rm occ} - K_{\rm occ}], \qquad (1)$$

includes the interaction of fully occupied orbitals, $2J_{occ}$ and K_{occ}, felt by the $3s^3$ valence electrons.

Our results are presented with particular focus on the double ionization process at 55.49 eV, and compare with experimental measurements and theoretical calculations, such as the convergent close coupling (CCC) and time-dependent close coupling (TDCC) methods at this photon energy. Overall, we find good agreement with experiment and various theoretical treatments when comparing the fully-differential cross sections across different angular distributions and energy sharings. This particular photon energy is resonant with the state resulting from promotion of a $2p \rightarrow 3d$ electron embedded in the double continuum. The agreement of these results with other theoretical results, that do not take into account the resonant process is further explored. We propose a mechanism for the dominant structures of the angular distributions, which bear much in common with other non-resonant helium-like ns^2 photoabsorbtions.

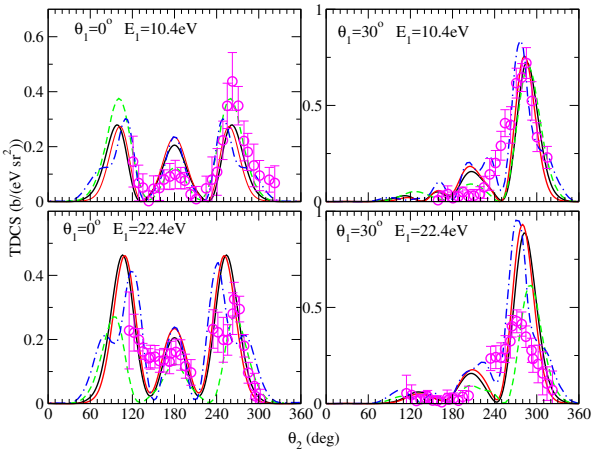

Figure 1. Fully-differential angular distributions of DPI from magnesium at various energy sharings, compared with other theoretical calculations, and experimental results.

References

[1] F.L.Yip, *et al.* 2010 *Phys. Rev. A* **81** 053407

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