Double photoionization of quasi two-electron atoms

Frank L. Yip[*1]

[*] Department of Sciences and Mathematics, California State University-Maritime Academy, Vallejo, CA 94590, USA

Synopsis Moving beyond helium in double ionization studies of more complicated targets requires an accounting of any electrons that remain attached to the atomic (or molecular) fragments. The grid-based *ab initio* approach of including these interactions for core and valence electrons that remain bound and interact with the continuum electrons will be discussed, including application to several other systems, both helium-like in their initial state configuration (ns^2), as well as open-shell fragments that result (neon and argon).

The removal of two electrons from a target atom or molecule via a single photoabsorption, provides a direct and sensitive probe of electron correlation in gas phase matter. In double ionization studies, a complete accounting of the fully differential energy sharing and angular distributions that result when photoejecting two electrons in a Coulomb breakup problem requires an accurate non-perturbative treatment for theory and coincidence measurements of the fragments for experiment. The study of this process for the simplest target, atomic helium, has seen several theories accurately agree with each other with experiment. To advance beyond simple two-electron targets, it is necessary to consider the influence and impact of any remaining electrons that remain bound to the target fragment(s) on the continuum electrons.

Our work over the past few years to expand computational grid-based *ab initio* methods to be able to treat targets with core electrons has led to analogous studies of double ionization processes in atomic targets that also possess more than two electrons. 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 atomic targets with more than two electrons using both in a time-independent and time-dependent framework. Within this frozen-core approximation, the problem then can be regarded as an effective two-electron problem involving the outgoing (valence) electrons in the presence of the core occupancy that requires additional consideration of the ionic fragment that remains. For a closed-shell fragment, the outgoing electrons experience a one-body interaction with the target

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

This approach is equivalent to a limited configuration interaction with the core occupancy held fixed, but full CI in terms of the continuum electrons [1]. These methods have also been applied to calculate the triply-differential cross sections for DPI from neon and argon that agree well with experiment [3], and may provide the means to compare with more complicated and experimentally suitable targets to further probe electron correlation.

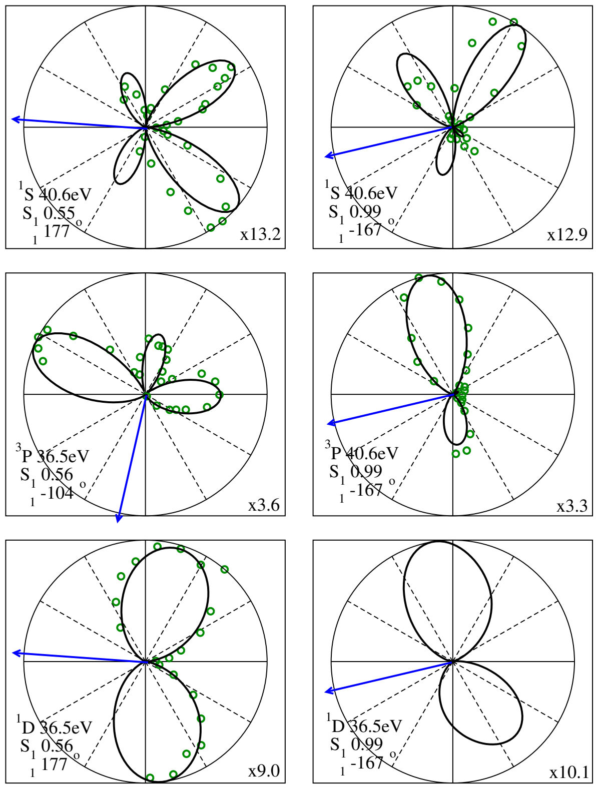

Figure 1. Fully-differential angular distributions of DPI from neon [2], which can result in several final-state symmetries with remaining (open-shell) electrons, compared to experimental results [3]

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References

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[1]E-mail: fyip.csum.edu