Double photoionization of atomic carbon and neon

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Synopsis We consider the double photoionization of the $2p^2$ valence electrons of atomic carbon, which provides for distinct final-state symmetries depending on the three possible angular momentum couplings (^3P, ^1D, and ^1S) of the initially-bound p^2 electrons that are ejected into the continuum by a single photon. Comparison of this process with neon provides an analogous case for the resulting final states within the treatment of the double photoionization proceeding with the ejected electrons influenced by the remaining bound electrons.

Double photoionization (DPI) events provide a sensitive probe of electron correlation and focus on few-electron targets continues to reveal the consequences of electron correlation for atoms and molecules that possess several electrons. Results previously calculated for neon and argon [1] agree well with experimental measurements [2, 3] for various final LS states. We apply the same methodology to compute the DPI cross section from atomic carbon. Removal of the valence p^2 electrons yields similar final state continua connected by a single photon. We focus our comparisons with neon in the ^3P symmetry.

To represent the frozen-core $1s$ and $2s$ electrons in carbon, a basis of orbitals is constructed from an FEM-DVR grid [4] which allows the evaluation of the Coulomb and exchange interactions with the core electrons. Using this orbital-DVR grid, we solve the first-order driven Schrodinger equation in an expansion appropriate for the atomic symmetry (coupled spherical harmonics).

Good agreement has been found for the total and energy sharing cross section with previous results for the total double photoionization cross section and the largest two contributions to the energy sharing (single) differential cross section of ^3P carbon [5]. Comparing the triple differential cross section (TDCS) relative sizes and features of the TDCS lobes for carbon and neon (Figure 1) has also been done for excess energies that are the same percentage of the DPI threshold. Future work will examine the cross sections of these targets in other symmetries.

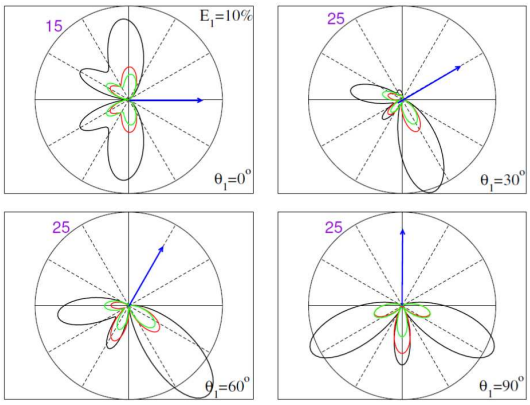

Figure 1. Triple differential cross sections (TDCS) for ^3P carbon (black curve) and neon (red and green curves) calculated in the velocity gauge. The carbon results and red neon curves are calculated at 10 eV excess photon energy (= 47.2 eV and = 76.0 eV, respectively), while the green neon result has the same percentage of excess energy in the fixed electron (= 83.7 eV) as the carbon black curve.

References

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