Double Photoionization of Atomic Oxygen: Feshbach Resonances in the Two-Electron Continuum

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Synopsis We present a joint theoretical and experimental analysis of double ionization of atomic oxygen due to single photon absorption. The theoretical cross sections were calculated using an R-matrix with pseudostates (RMPS) method, and the experimental measurements were performed at the Advanced Light Source (ALS).

Double photoionization processes proceed only via higher-order electron correlation processes and thus provide a sensitive measure of the inter-electron interactions in the atom. The pseudostates method [1] for theoretically treating double ionization processes was first realized within an R-matrix methodology for He [2, 3, 4], and a more recent RMPS calculation on He [5] demonstrated convergence of the pseudostate basis expansion. Similar convergence has been achieved for other quasi-two-electron systems, but no RMPS calculations have been reported for systems involving more than two active electrons.

Several experiments for double photoionization of the simpler, two-electron He atom have likewise been carried out. However, except for the rare gases, there has been relatively little experimental attention paid to other atomic photoionization cases since most elements are difficult to isolate from their natural molecular gas form. One exception is oxygen, which has been isolated and studied in atomic form for single photoionization [6], and for earlier, low-resolution double photoionization measurements [7].

In this study, we present new double photoionization calculations for oxygen, the first RMPS calculation treating more than two active electrons, and also new, high-resolution experimental measurements, which were undertaken at the ALS. Preliminary results are presented in Fig. 1, showing overall good agreement between RMPS and experimental results. However, the sharper resonance features observed in the measurements, attributed to excitation-plus-ionization Feshbach-resonances embedded in the double ionization continuum, were not reproduced in these preliminary RMPS calculations, indicating an additional difficulty inherent in using a discrete set of pseudostates to span a two-electron final ionized state.

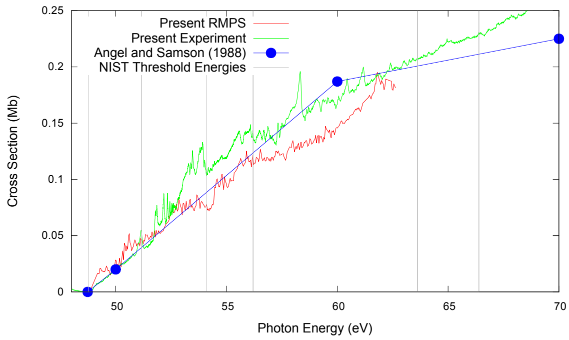

Figure 1. Double photoionization of atomic oxygen: Present RMPS results (red); present ALS experimental results (green); earlier experimental results [7] (magenta); NIST O^{2+} threshold values (grey).

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