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K-Shell Photoionization of Oxygen

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Synopsis R-matrix calculations of the $1s$ photoionization in oxygen are reported. Proper treatment of spectator Auger broadening, relaxation, pseudoresonace elimination, and shake-up/shake-off are addressed.

K-shell photoionization calculations are complicated by the need to account for spectator Auger decay of resonances, on the one hand, and relaxation effects, on the other. These can be accounted for within the R-matrix method via an optical potential [1], for the former, and a pseudoorbital basis, for the latter. This approach was used in an earlier study of oxygen photoionization [2], where the experimental resonance spectrum [3] was reproduced fairly well. However, the computed oscillator strengths were too large, and the cross section above threshold was inconsistent with independent experimental results [4].

Inaccuracies in the earlier R-matrix calculations [2] are found to be due to unphysical pseudoresonance structure. A proper treatment to eliminate this spurious structure [5] reveals that further shake-up and shake-off contributions, amounting to 20%, are needed above threshold as a result of substantial relaxation effects.

These issues are addressed in the various stages of Fig. 1. Use of a single set of atomic orbitals fails to account for relaxation effects, and the threshold energy position and cross section are both grossly overestimated (see the blue curve in the upper panel). By introducing additional pseudoorbitals (see the red curve in all panels), relaxation is properly treated, and the resonance oscillator strengths and threshold cross sections are in excellent agreement with experiment [3, 4]. Failure to eliminate pseudoresonances [5] gives an unphysically enhanced cross section (blue curve in the middle panel), which was the cause of the earlier overestimation [2].

The correct R-matrix results approach only 80% of the independent-particle (IP) asymptote, due to relaxation effects, and the remaining 20% contribution is computed using both shake approximation and R-matrix with pseudostates [6] methods. Preliminary results are shown as the blue curve in the lower panel.

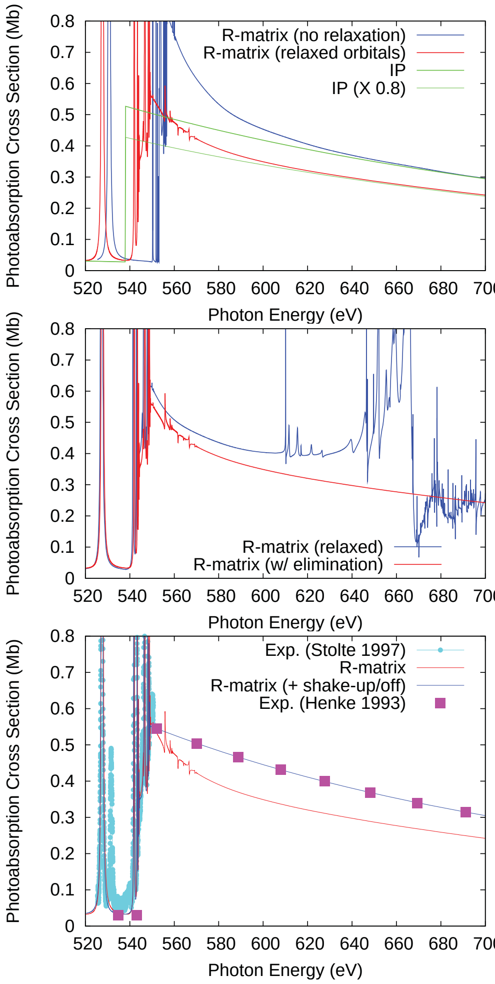

Figure 1. R-matrix cross sections vs. experimental and independent-particle (IP) results.

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