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Role of initial-state correlation in one-photon double ionization of atoms and molecules[1] ROGER BELLO, Lawrence Berkeley National Laboratory, FRANK YIP, California State University Maritime Academy, THOMAS RESCIGNO, ROBERT LUCCHESE, Lawrence Berkeley National Laboratory, C. WILLIAM MCCURDY, University of California, Davis and Lawrence Berkeley National Laboratory — By decomposing the initial state wave function into its unique natural orbital expansion, as defined in the 1950s by Löwdin and used in modern studies of entanglement, we analyze the role of electron correlation in the initial state of an atom or molecule in determining the angular distribution of one-photon double ionization. Final state correlation of the two ejected electrons is treated completely in numerically accurate calculations and the initial states of He, H^- and H_2 are built up from correlating configurations in strict order of decreasing natural orbital occupations. In the two-electron atoms it is found that the initial state correlation plays a sometimes modest but generally measurable role. In striking contrast, for H_2 a large number of correlating configurations in the ground state is often necessary to produce angular distributions even approximately resembling the correct ones. One-photon double photoionization of oriented H_2 is found to be particularly sensitive to left-right correlation along the bond.

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