Large internuclear distance effects on photoionization of diatomic molecules \( \text{Li}_2^+ \) and \( \text{H}_2^+ \)

FRANK YIP, UC Berkeley and LBNL, THOMAS RESCIGNO, LBNL, C. WILLIAM MCCURDY, LBNL and UC Davis — The role of internuclear separation in diatomic molecules dramatically impacts the magnitude and angular distributions of single photoionization cross sections from these targets. We consider photoionization of \( \text{Li}_2^+ \), which has a large equilibrium bond distance at \( R = 5.86a_0 \), and the one-electron analog \( \text{H}_2^+ \) fixed at this internuclear distance. The highly non-spherical nature of such molecules causes higher angular momentum components to contribute more significantly compared to smaller diatomic bond distances even at low energies within 1eV of the photoionization threshold, resulting in angular distributions that appear to be \( f \)-wave dominated. At slightly higher energies, the photoelectron de Broglie wavelength becomes comparable with the bond distance, introducing interference effects in the resulting cross sections at energy ranges far lower than necessary for interference phenomena to appear with typical molecular bond distances.

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