Time delay in photoionization of half-filled shell atoms

V. K. Dolmatov*[1], A. S. Kheifets†, S. T. Manson‡ and P. C. Deshmukh§

* Department of Physics and Earth Science, University of North Alabama, Florence, Alabama 35632, U.S.A.
† Research School of Physics and Engineering, Australian National University, Canberra ACT 0200, Australia
‡ Department of Physics and Astronomy, Georgia State University, Atlanta, Georgia 30303, U.S.A.
§ Department of Physics, Indian Institute of Technology Madras, Chennai-600036, India

Synopsis Time delay in photoionization of a half-filled shell atom is predicted to be strongly term-dependent and subject to the dramatic impact of a giant autoionization resonance. Photoionization of the Mn atom is chosen as a case study.

Time delay in photoelectron emission from atoms [1] has become a hot topic of modern studies. To date, however, neither the significance of autoionization resonances in photoionization time delay has been established, nor features in time delay brought about by the configuration of open-shell atoms have been uncovered.

In this work, we discuss the 3d- and 4s-photoionization of the Mn(...$3p^6 3d^5 4s^2$, ^6S) atom which has a $3d^5$ half-filled subshell in its configuration, as a convenient case study. In Mn, the resonance excitation from a $3p^6$ subshell to the half-filled $3d^5$ subshell occurs at $\hbar\omega_r \approx$ 50 eV, autoionizes primarily into 3d $\to$ f and 3d $\to$ p continua and has a big resonance width $\gamma \approx 2$ eV at a half-maximum of the 3d-photoionization cross section ($\sigma_{3d}^{max} > 50$ Mb) [2, 3] (and references therein). Furthermore, the removal of a 4s-electron from Mn results in the ion-remainder in the state with a term $Mn^+(4s^1, {}^5S)$ or $Mn^+(4s^1, {}^7S)$.

In the present study, we use the "spin-polarized" random phase approximation with exchange (SPRPAE) [3] to calculate the τ_{3d}, $\tau_{4s}(^5S)$ and $\tau_{4s}(^7S)$ time delays for Mn 3d- and 4s-photoionization in the photon energy region which encompasses the 3p $\to$ 3d resonance. Calculated data are plotted in figure 1. Note how remarkably big all calculated time delays are, especially the τ_{3d} time delay, due to the impact of the 3p $\to$ 3d giant resonance. And τ_{3d}, obtained by accounting for both the 3d $\to$ f and 3d $\to$ p photoionization channels in the calculation (marked as the "3d, two-channel time delay" in figure 1), differs dramatically from τ_{3d} when only the dominant 3d $\to$ f continuum was accounted for [marked as the "3d, single-channel (3d − f) time delay" in figure 1]. Note also that $\tau_{4s}(^5S)$ and $\tau_{4s}(^7S)$ differ strongly from each other, thereby revealing significant term-dependence in photoionization time delay in the half-filled shell Mn atom. These remarkable effects, elucidated above, should be general features of photoionization time delay in other half-filled shell atoms as well.

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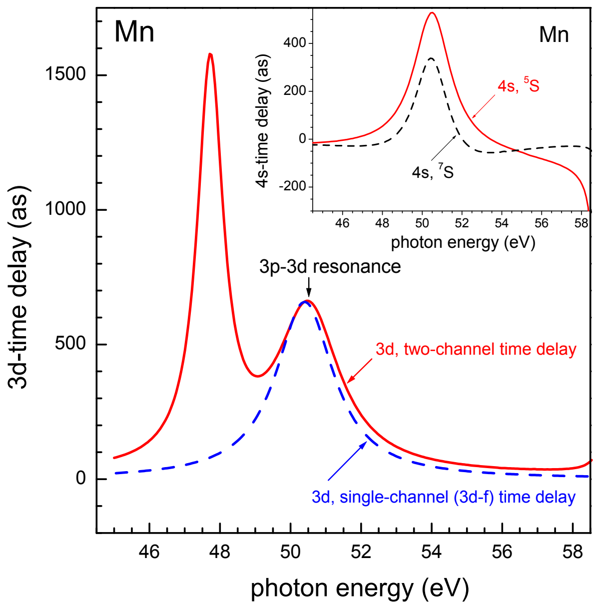

Figure 1. Calculated SPRPAE data for the τ_{3d}, $\tau_{4s}(^5S)$ and $\tau_{4s}(^7S)$ time delays upon the photoionization of Mn, as marked.

References

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[1]E-mail: vkdolmatov@una.edu

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