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Reply

Reply to Comment on 'Time delays in molecular photoionization'

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In a comment on our article *Time delays in molecular photoionization* [1], Baykusheva and Wörner [2] state that, to calculate photoionization time delays, the transition dipole matrix elements from the bound state to the continuum state must be included. We agree with this point, and that standard photoionization theory is correct; indeed the transition dipole matrix elements are included in our calculations. Perhaps the confusion arose from our simplified notation in section 2, where the transition dipoles are implicitly included in the final scattering wavefunction. However, as is clear from our section 3, and the online material referred to in section 3[4], the dipole matrix elements are included. In fact, in the additional work cited by Baykusheva and Wörner [3], they use the same software suite as we do to perform the photoionization calculations, namely ePolyScat [4–6], which is well-tested for photoionization problems and clearly contains the complete canonical photoionization physics [7]. Furthermore, without the transition dipole matrix elements, our results (e.g. figures 1 and 2 in the original manuscript) would not exhibit the detailed energy and angular structure that is apparent.

In sum, we can reassure readers that the formalism we applied is indeed canonical scattering and photoionization theory. Baykusheva and Wörner's concern is, therefore, unfounded.

For interested readers, we note that a detailed, technical response, prepared by some of the present authors, is also available [8].

[4] To view this online material please visit https://doi.org/10.6084/m9.figshare.2007486.

References

[1] Hockett P, Frumker E, Villeneuve D M and Corkum P B 2016 Time delays in molecular photoionization *J. Phys. B: At. Mol. Opt. Phys.* **49** 0956
[2] Baykusheva D and Wörner H J 2016 Comment on 'Time delays in molecular photoionization' *J. Phys. B: At. Mol. Phys.* **50** 078001
[3] Huppert M, Jordan I, Baykusheva D, von Conta A and Jakob Wörner H 2016 Attosecond delays in molecular photoionization *Phys. Rev. Lett.* **117** 093001
[4] Gianturco F A, Lucchese R R and Sanna N 1994 Calculation of low-energy elastic cross sections for electron-CF_4 scattering *J. Chem. Phys.* **100** 6464
[5] Natalense A P P and Lucchese R R 1999 Cross section and asymmetry parameter calculation for sulfur 1s photoionization of SF_6 *J. Chem. Phys.* **111** 5344
[6] Lucchese R R 2015 Lucchese Group Website (http://chem.tamu.edu/rgroup/lucchese/)
[7] Toffoli D, Lucchese R R, Lebech M, Houver J C and Dowek D 2007 Molecular frame and recoil frame photoelectron angular distributions from dissociative photoionization of NO_2 *J. Chem. Phys.* **126** 054307
[8] Hockett P and Frumker E 2016 Response to 'Comment on "Time delays in molecular photoionization"': extended discussion and technical notes arXiv: 1612.00481

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