Abstract Submitted
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Multiphoton ionization and RABBITT in H_2 studied by the molecular "R-matrix with time" method JAKUB BENDA, Charles University, Prague, Czech Republic, GREG ARMSTRONG, ANDREW BROWN, DANIEL CLARKE, Queen's University Belfast, UK, JIMENA GORFINKIEL, The Open University, Milton Keynes, UK, HUGO VAN DER HART, Queen's University Belfast, UK, ZDENEK MASIN, Charles University, Prague, Czech Republic — We have developed the molecular R-matrix method with time [1] (RMT), a variational ab initio multi-electron method for solution of the time-dependent Schrödinger equation for arbitrarily polarized and shaped electric fields. This approach is based on the well established atomic code which has recently undergone a significant upgrade. The molecular strand is interfaced with the mature UKRmol+ [2] time-independent multi-configurational R-matrix codes. The method and the codes are applicable to general polyatomic molecules. As the first application of the molecular RMT code we have decided to study ultrafast laser-induced processes in H_2 (multi-photon ionization and RABBITT) for which accurate results are available. In the case of multi-photon ionization of H_2 we demonstrate agreement with earlier calculations based on the R-matrix Floquet approach in the limit of long pulses, as well as with results from perturbation method for weak field limit. For the same molecule we also calculate photoionization time delays for several orientations of the molecule using simulated RABBITT interference and compare our results with other ab-initio calculations. [1] A. C. Brown et al, Comput. Phys. Commun., 2020, in press [2] Z. Mašín et al, Comput. Phys. Comm. 249 (2020) 1070

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