

Abstract Submitted
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Time-dependent photoionization of atomic and molecular systems using a hybrid Gaussian and Finite-elements discrete variable representation basis set¹ NICOLAS DOUGUET, University of Central Florida, HEMAN GHARIBNEJAD, BARRY SCHNEIDER, National Institute of Standards and Technology, LUCA ARGENTI, University of Central Florida — We present preliminary results of a computational method to solve the time-dependent Schrödinger equation for an atomic or molecular system interacting with a short laser pulse. The multi-electron system is described by combining the MESA (Molecular Electronic Structure Applications) quantum chemistry package with Gaussians functions and the Finite-Element Discrete Variable Representation (FEDVR) [1] basis. The matrix elements between bound-free and free-free functions are computed via the accurate 3-dimensional adaptive quadrature grid of Rescigno and McCurdy [2]. The method assumes a separable representation [2] and neglects exchange interactions involving FEDVR functions. The hybrid basis will be used to propagate an electronic wavepacket under the action of a short pulse. [1] T. N. Rescigno and C. W. McCurdy, Phys. Rev. A **62** 032706 (2000), [2] C. W. McCurdy and T. N. Rescigno, Phys. Rev. A **39** 4487 (1989).

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