

Abstract Submitted
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Virtual detector methods for efficiently computing momentum-resolved dissociation and ionization spectra¹ ALEX KRAMER, UWE THUMM, Kansas State University — We discuss a class of window-transform-based “virtual detector” methods for computing momentum-resolved dissociation and ionization spectra by numerically analyzing the motion of nuclear or electronic quantum-mechanical wavepackets at the periphery of their numerical grids. While prior applications of such surface-flux methods considered semi-classical limits to derive ionization [1] and dissociation [2] spectra, we systematically include quantum-mechanical corrections and extensions to higher dimensions, discussing numerical convergence properties and the computational efficiency of our method in comparison with alternative schemes for obtaining momentum distributions. Using the example of atomic ionization by co- and counter-rotating circularly polarized laser pulses [3], we scrutinize the efficiency of common finite-difference schemes for solving the time-dependent Schrödinger equation in virtual detection and standard Fourier-transformation methods for extracting momentum spectra. [1] B. Feuerstein and U. Thumm, J. Phys B **36**, 707 (2003). [2] M. Magrakvelidze, C. M. Aikens, and U. Thumm, Phys. Rev. A **86**,023402 (2012). [3] D. B. Milosovic, et al., Phys. Rev. A **61**,063403 (2000).

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