

Two-Photon Double Ionization of H₂

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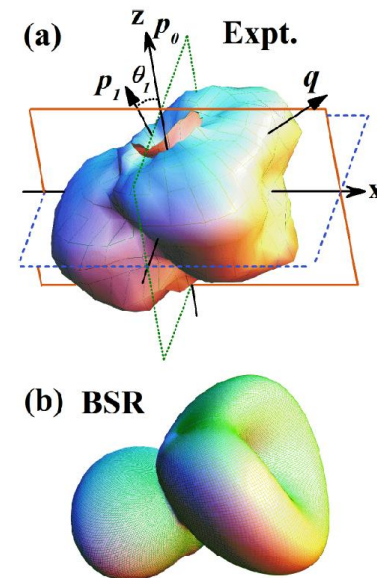
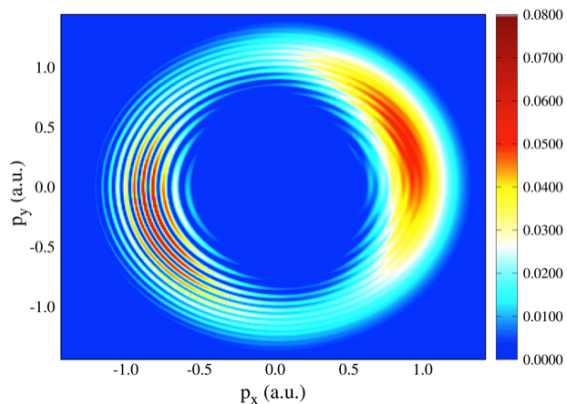
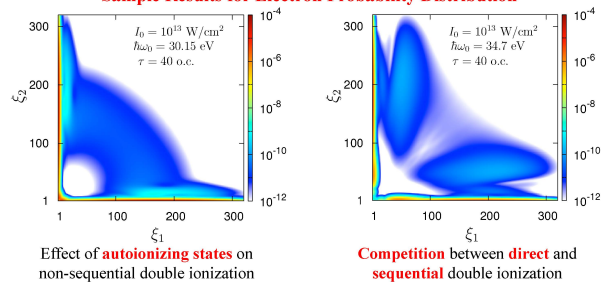
Goal: Resolve large discrepancies in previous calculations of this fundamental process.

Steps taken: 1) Optimized existing FEDVR code for Stampede
2) Sampled parameter space (photon energy, pulse duration) with about **100 runs (3000 cores and 10-20 hours of wallclock time each)**

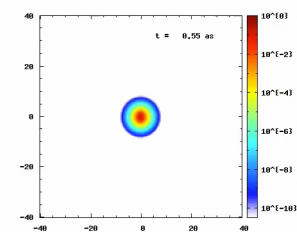
Findings: Discrepancies are due to surprisingly strong dependence of theoretical predictions on laser parameters and (previously unresolved) effect of autoionizing states.

Broad Impact: These calculations support/explain very expensive FEL experiments.

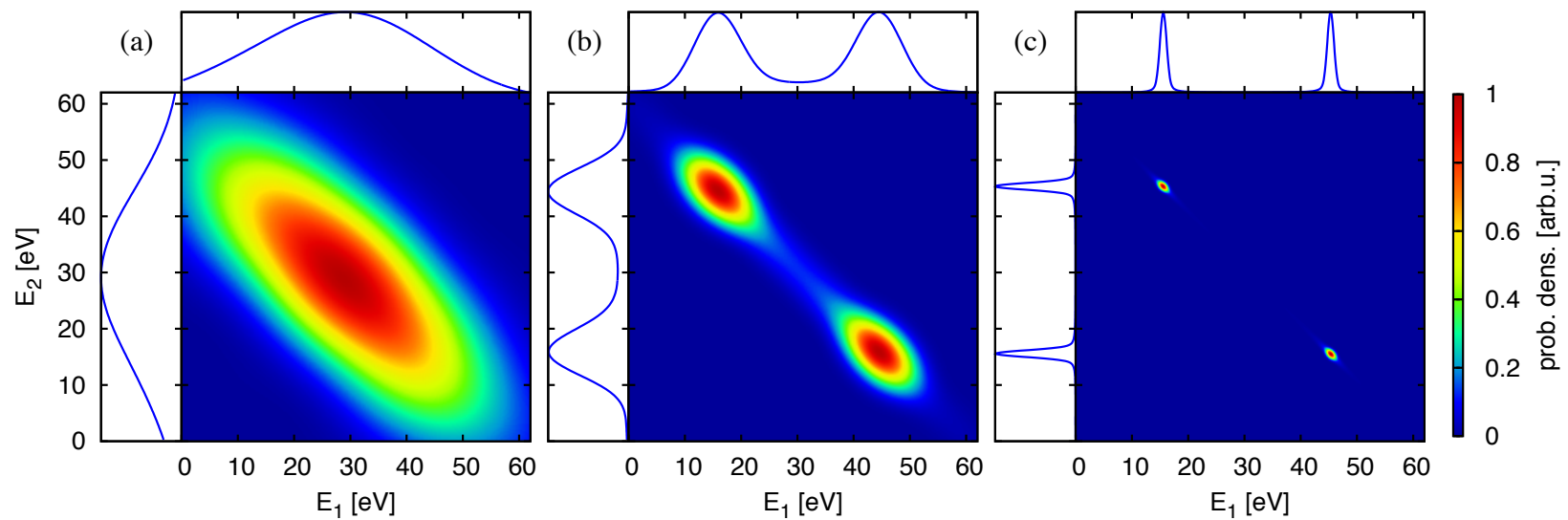
Sample Results for Electron Probability Distribution



Ionization of Ar(3d) by electron Impact:
Experiment(a) and Theory(b)



AMPGateway



Two Photon Double Ionization of He at 70 eV for Short(a) to Long Pulses(3) – Note How Sequential Ionization Breaks Down