

Two-Photon Double Ionization of H_2

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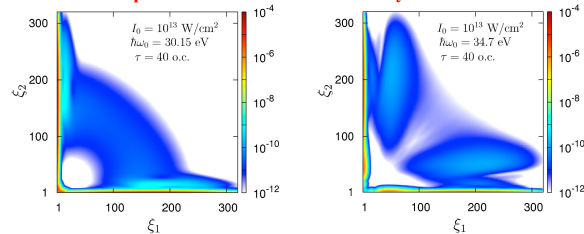
Goal: Resolve large discrepancies in previous calculations of this fundamental process.

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.

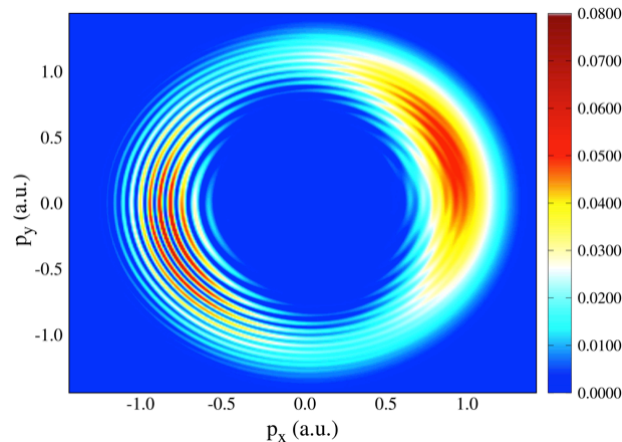
Broad Impact: These calculations support/explain very expensive FEL experiments.

Sample Results for Electron Probability Distribution

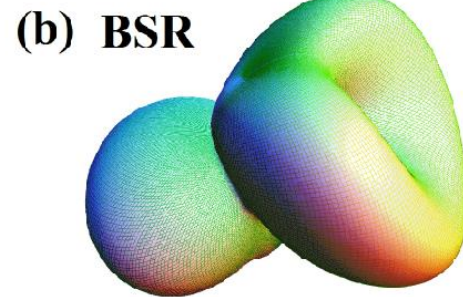
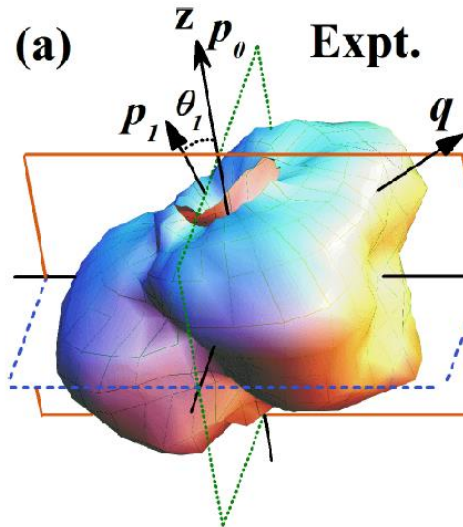


Effect of **autoionizing states** on non-sequential double ionization

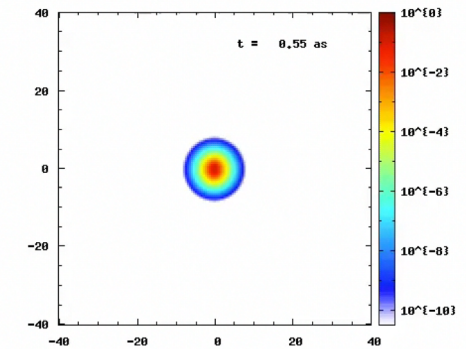
Competition between **direct** and **sequential** double ionization



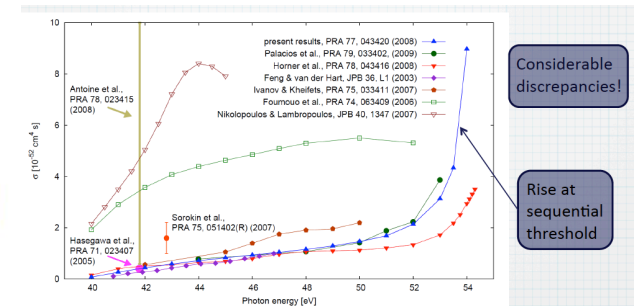
Photoelectron Momentum Distribution for Ar Ionization in Strong Electromagnetic Field



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



H_2^+ Ionization in strong, ultrafast electromagnetic field



Considerable discrepancies!

Rise at sequential threshold

2-Photon Double Ionization in He:
Approaching the Sequential Threshold