

EXTRACTION OF ENERGY-DIFFERENTIAL IONIZATION CROSS SECTIONS FROM TIME-DEPENDENT CALCULATIONS

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OVERVIEW:

- I. Introduction: Temkin-Poet Model of e-H Collisions
- II. Extraction of Excitation and Ionization Cross Sections
- III. Results for Excitation and Ionization
- IV. Visualization
- V. Conclusions and Outlook

Temkin-Poet Model of e-H Collisions

- We solve the time-dependent Schrödinger Equation

$$i \frac{\partial P(r_1, r_2, t)}{\partial t} = \left[-\frac{1}{2} \left(\frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2} \right) - \frac{1}{r_<} \right] P(r_1, r_2, t)$$

by time-propagating the initial (singlet spin) state

$$P(r_1, r_2, 0) = [P_{1s}(r_1)G_{k_0}(r_2) + P_{1s}(r_2)G_{k_0}(r_1)] / \sqrt{2}$$

- **Excitation** cross sections for **discrete states** $2s, 3s, 4s, \dots, ns$ are obtained as

$$\sigma_{ns} \equiv \lim_{t \rightarrow \infty} \frac{\pi}{4k_0^2} 2 \cdot \int_0^\infty dr_2 |F_{ns}(r_2, t)|^2$$

where

$$F_{ns}(r_2, t) \equiv \int_0^\infty dr_1 P_{ns}(r_1) P(r_1, r_2, t)$$

- The **total ionization cross section** is obtained as

$$\sigma_{ion} = \frac{\pi}{4k_0^2} \left(1 - 2 \cdot \lim_{t \rightarrow \infty} \sum_{n=1}^{\infty} \int_0^\infty dr_2 |F_{ns}(r_2, t)|^2 \right)$$

Extension to Energy-Differential Ionization

- Replace $P_{ns}(r_1)$ by Coulomb functions:

$$F_{ks}(r_2, t) \equiv \int_0^\infty dr_1 P_{ks}(r_1) P(r_1, r_2, t),$$

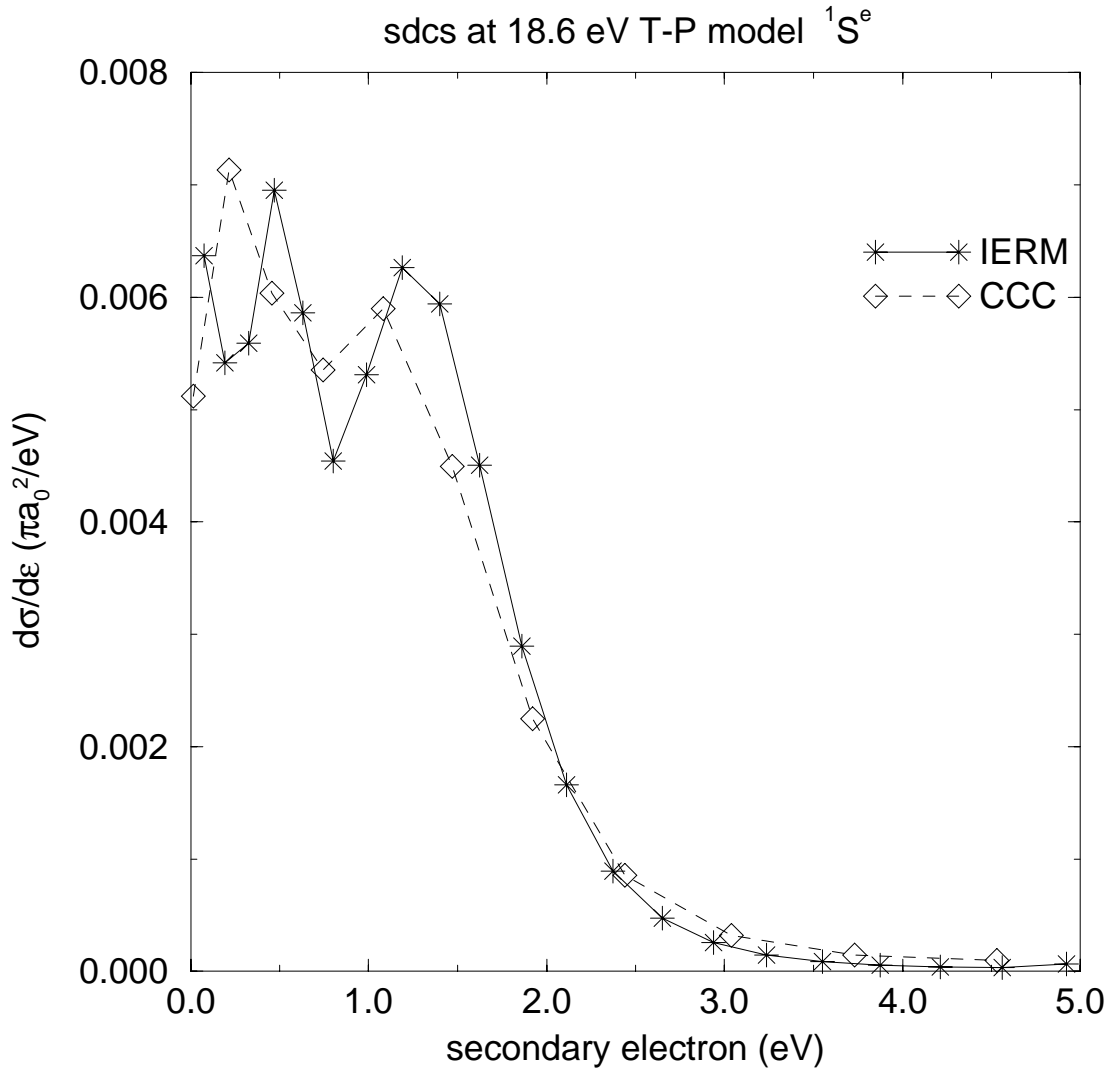
$$\bar{\sigma}_{ks} \equiv \lim_{t \rightarrow \infty} \frac{\pi}{4k_0^2} 2 \cdot \int_0^\infty dr_2 |F_{ks}(r_2, t)|^2.$$

- If $\lim_{r \rightarrow \infty} P_{ks}(r_1) = k^{-1/2} \times \sin(kr\dots)$, then $\bar{\sigma}_{ks}$ is proportional to the SDCS at the energy $k^2/2$ and can be normalized by using the total ionization cross section.

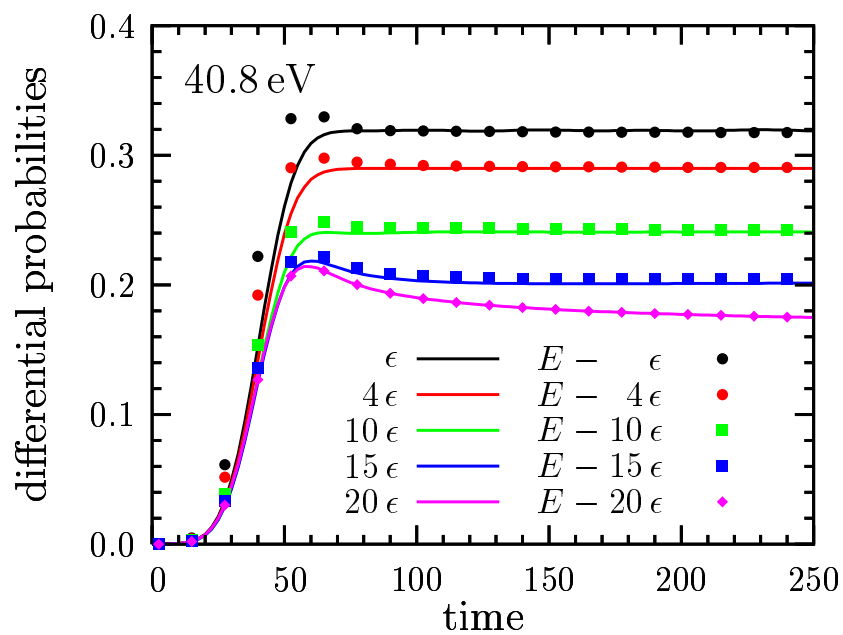
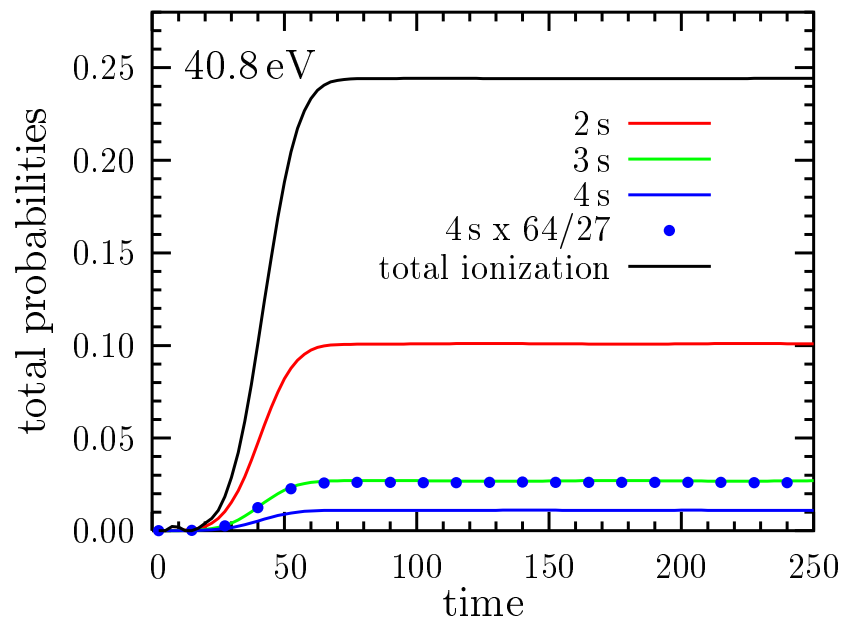
[A similar idea was suggested by Colgan, Pindzola, and Robicieux.]

Goals of the Project

- Visualization of $|F_{ks}(r_2, t)|^2$
- Is $\bar{\sigma}_{ks}$ symmetric around half the excess energy $E/2$?
- Many pseudo-state methods, such as CCC, RMPS, IERM produce **non-symmetric** “raw” results!
- Example: TP model at 18.6 eV (from M.P. Scott)

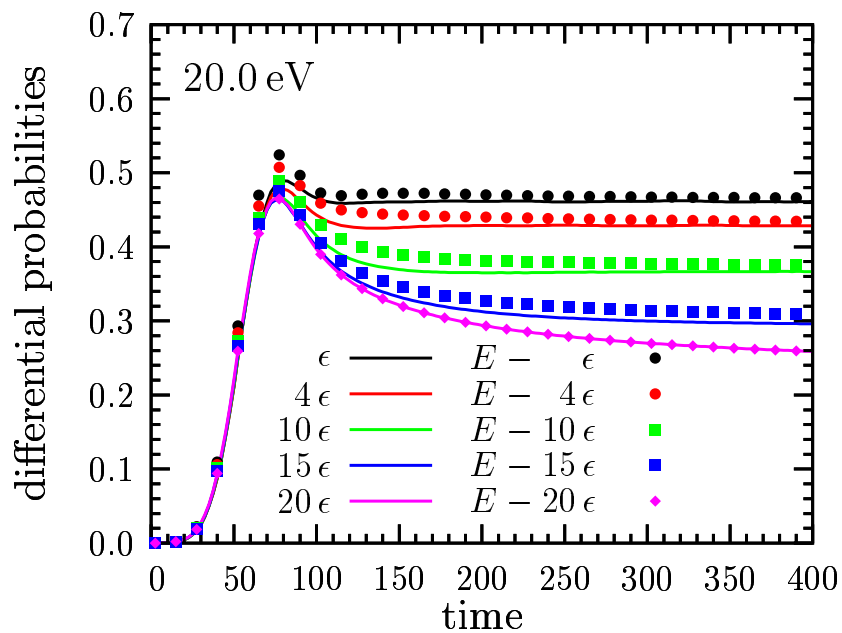
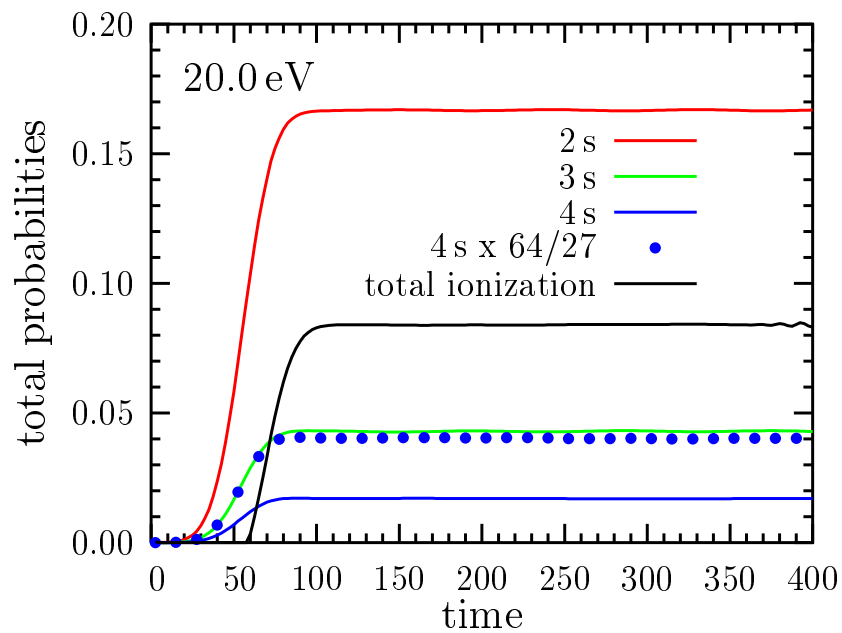


Excitation and Ionization Probabilities at 40.8 eV



- Note the symmetry in the ionization probabilities around $E/2$!
($\epsilon = E/40$.)

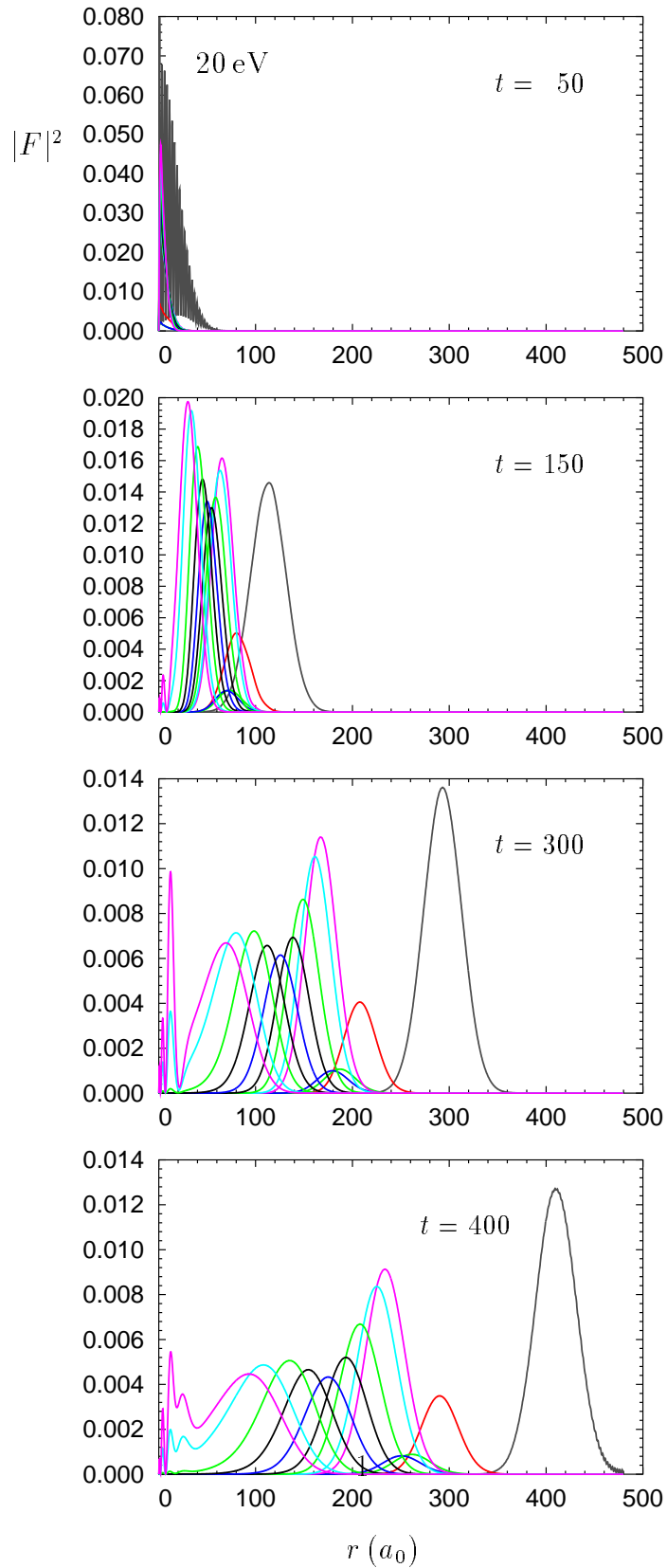
Excitation and Ionization Probabilities at 20 eV



- Note the symmetry in the ionization probabilities around $E/2$!
($\epsilon = E/40$.)

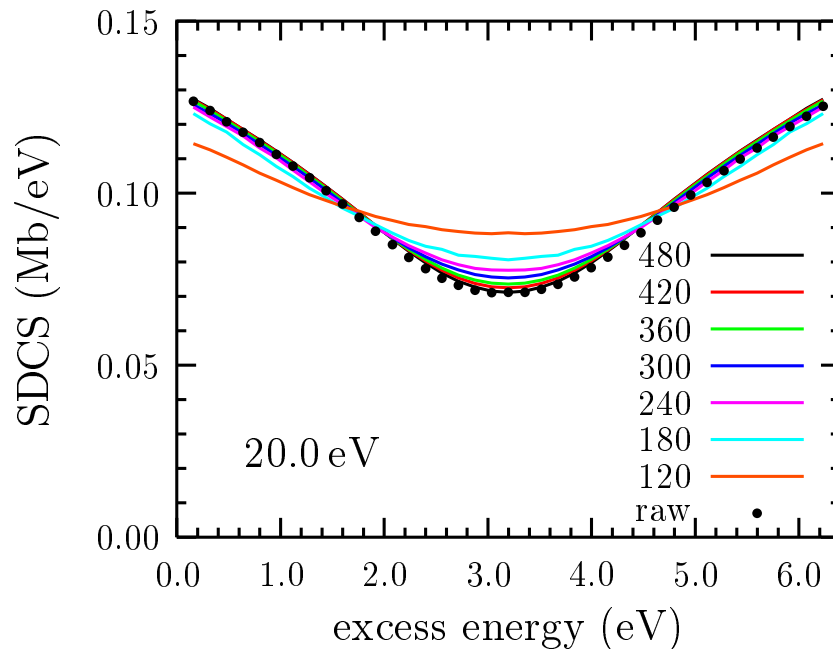
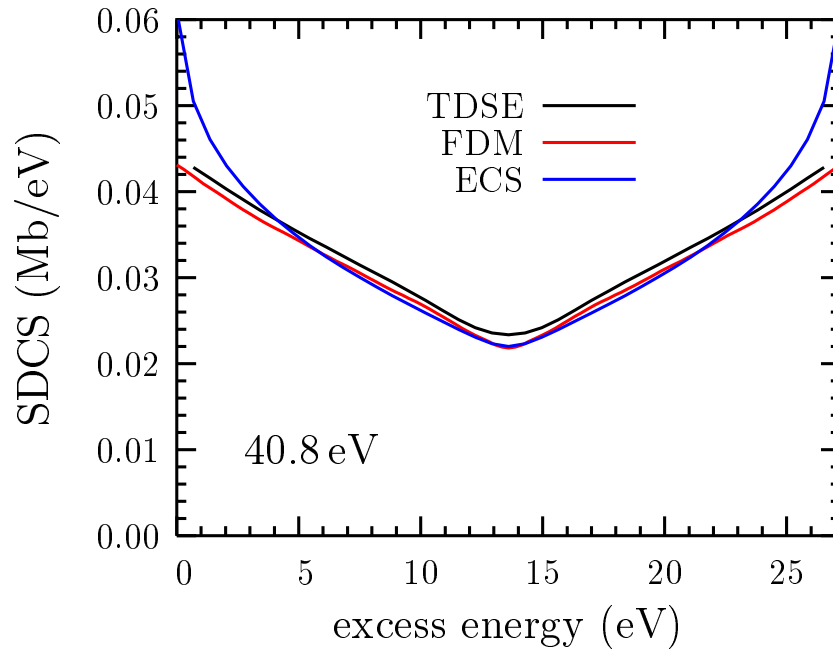
Visualization of $|F_{ks}(r_2, t)|^2$

(Note the integral under the curve and the speed of $|F_{ks}(r_2, t)|^2$.)



Convergence of the Results

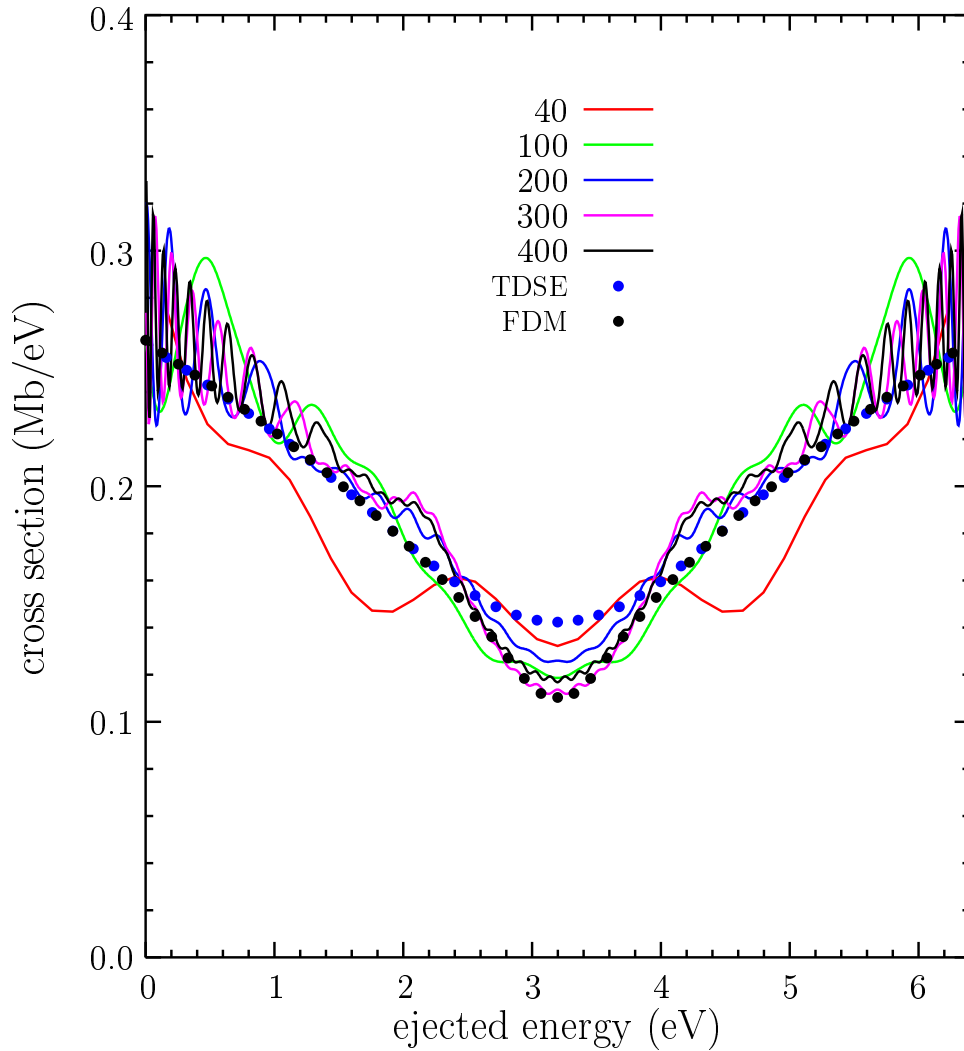
- **FDM**: Finite Difference Method (Jones & Stelbovics)
- **ECS**: Exterior Complex Scaling (Baertschy et al.)



- **A large radial mesh and long propagation times are needed for small excess energies and nearly symmetric energy sharing.**

Comparison with a T-matrix method

K. Bartschat *et al.* (2002), Physical Review A 66, in press



- The **finite mesh size** and the **energy width** of the package **cause problems for nearly symmetric energy sharing**.
- The **symmetrized T-matrix method** with IERM wavefunctions does **better for nearly symmetric energy sharing** but shows **unphysical oscillations in the asymmetric case**.

Conclusions and Outlook

- In contrast to standard pseudo-state methods (CCC, RMPS, IERM), the wavefunction obtained by integrating the time-dependent Schrödinger equation “knows” about the correct energy sharing between the two outgoing electrons.
- Consequently, **no explicitly symmetrized recipe is required** to extract the energy-differential ionization cross section.
- In fact, the **numerical accuracy can be checked** by comparing the numerical results against the symmetry required by the underlying physical problem.
- We obtained **very satisfactory agreement with other benchmark results** — higher accuracy can be achieved by increasing the computational resources.
- The **code has recently been parallelized** and will be extended to treat the full e–H problem.
- A **movie** has been created to **enhance the visualization**.