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

Greg Ver Steeg, Seamus Riordan, and Klaus Bartschat

Drake University

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OVERVIEW:

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II. **Extraction of Excitation and Ionization Cross Sections**

III. **Results for Excitation and Ionization**

IV. **Visualization**

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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

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

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

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

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

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

Extension to Energy-Differential Ionization

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

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

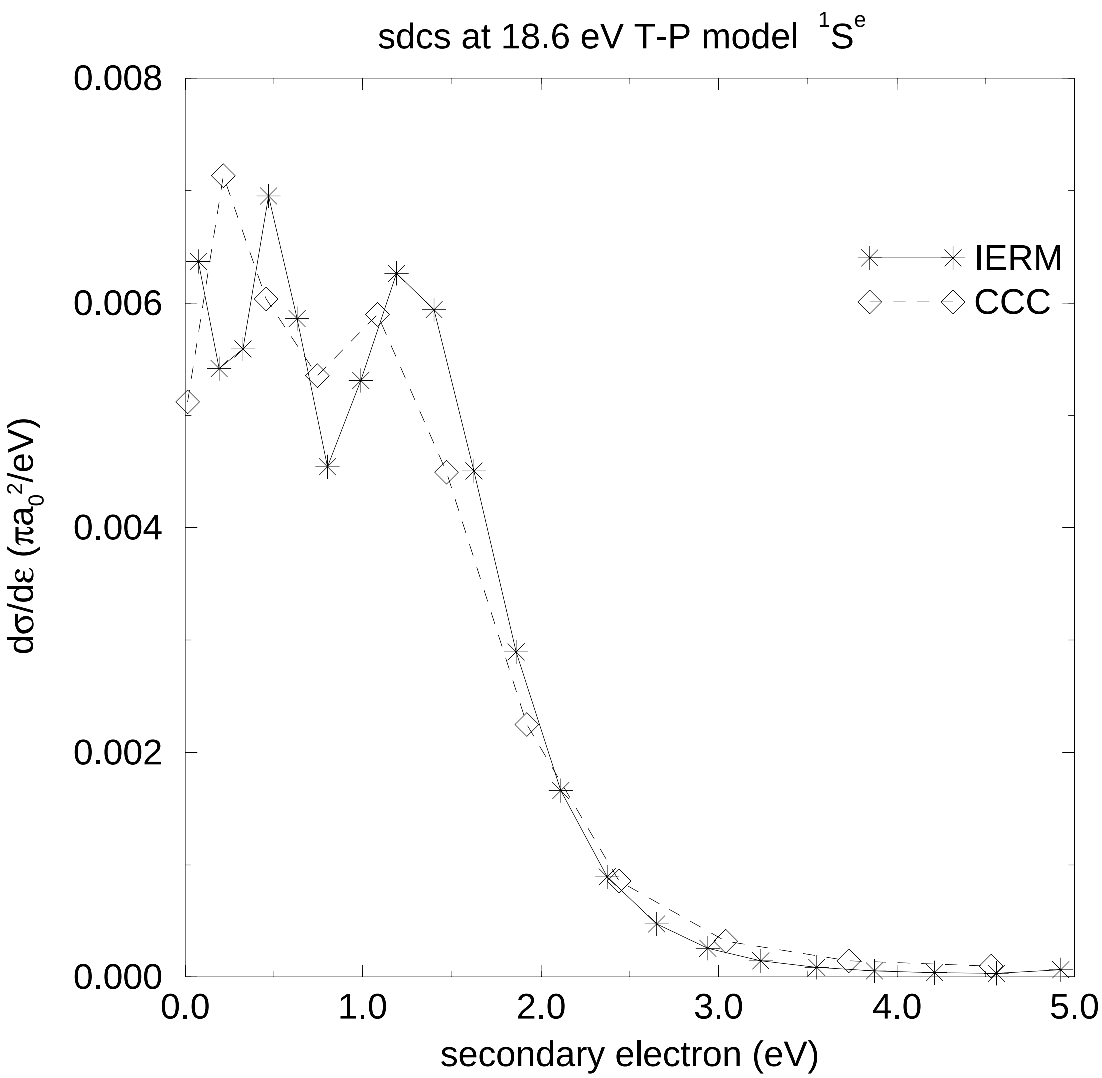
$$\bar{\sigma}_{ks} \equiv \lim_{t\to\infty}\frac{\pi}{4k_0^2}\, 2\cdot\int_0^\infty dr_2|F_{ks}(r_2,t)|^2.$$

- If $\lim_{r\to\infty} P_{ks}(r_1) = k^{-1/2}\times\sin(kr\ldots)$, 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.

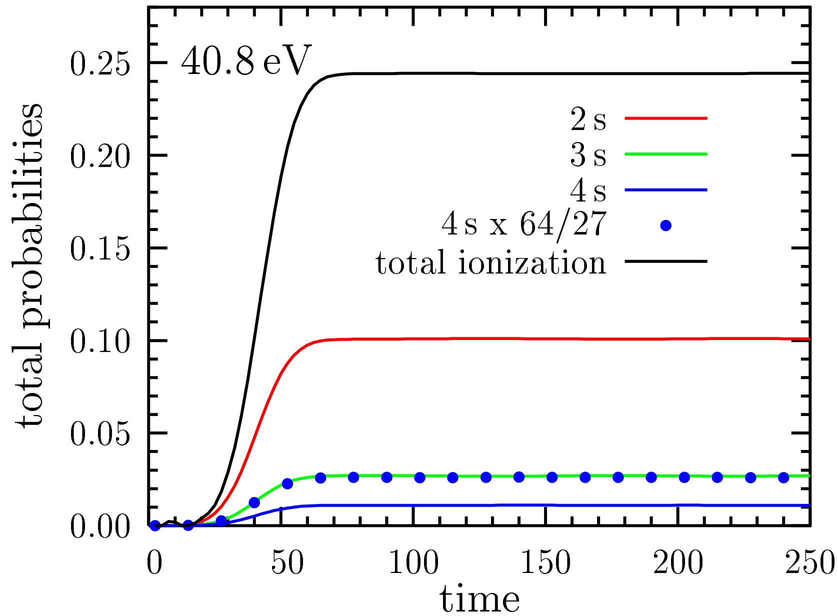
  [A similar idea was suggested by Colgan, Pindzola, and Robicheaux.]

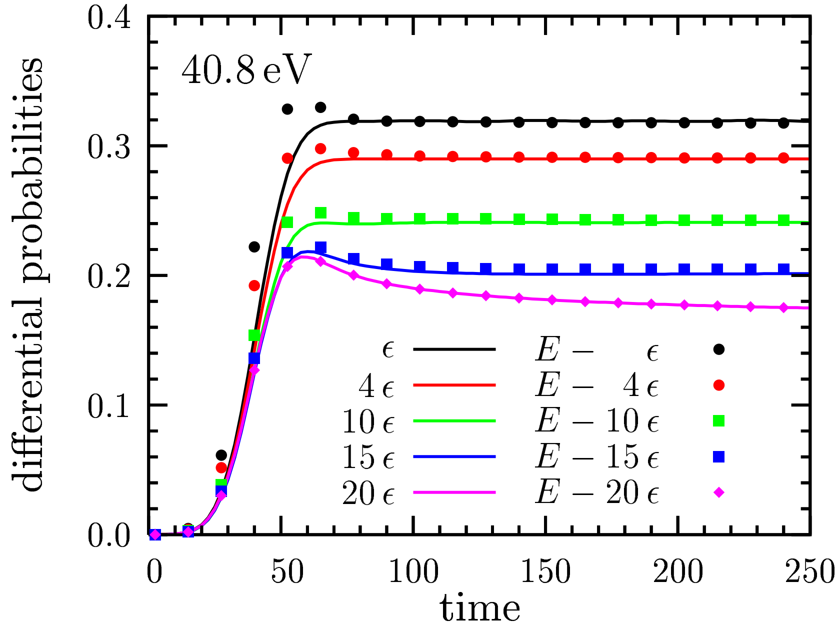
Goals of the Project

- 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

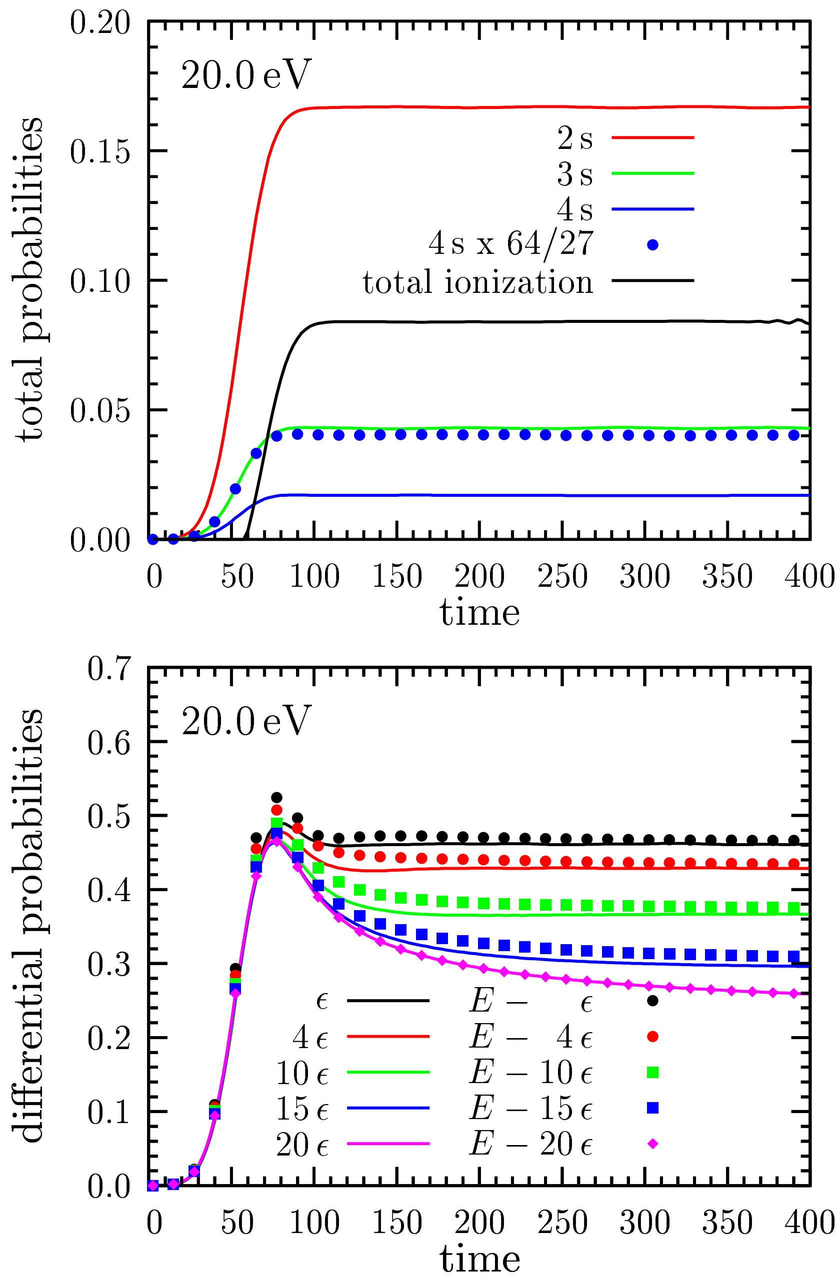




- **Note the symmetry in the ionization probabilities around $E/2$!**

  ($\epsilon = E/40.$)

Excitation and Ionization Probabilities at 20 eV

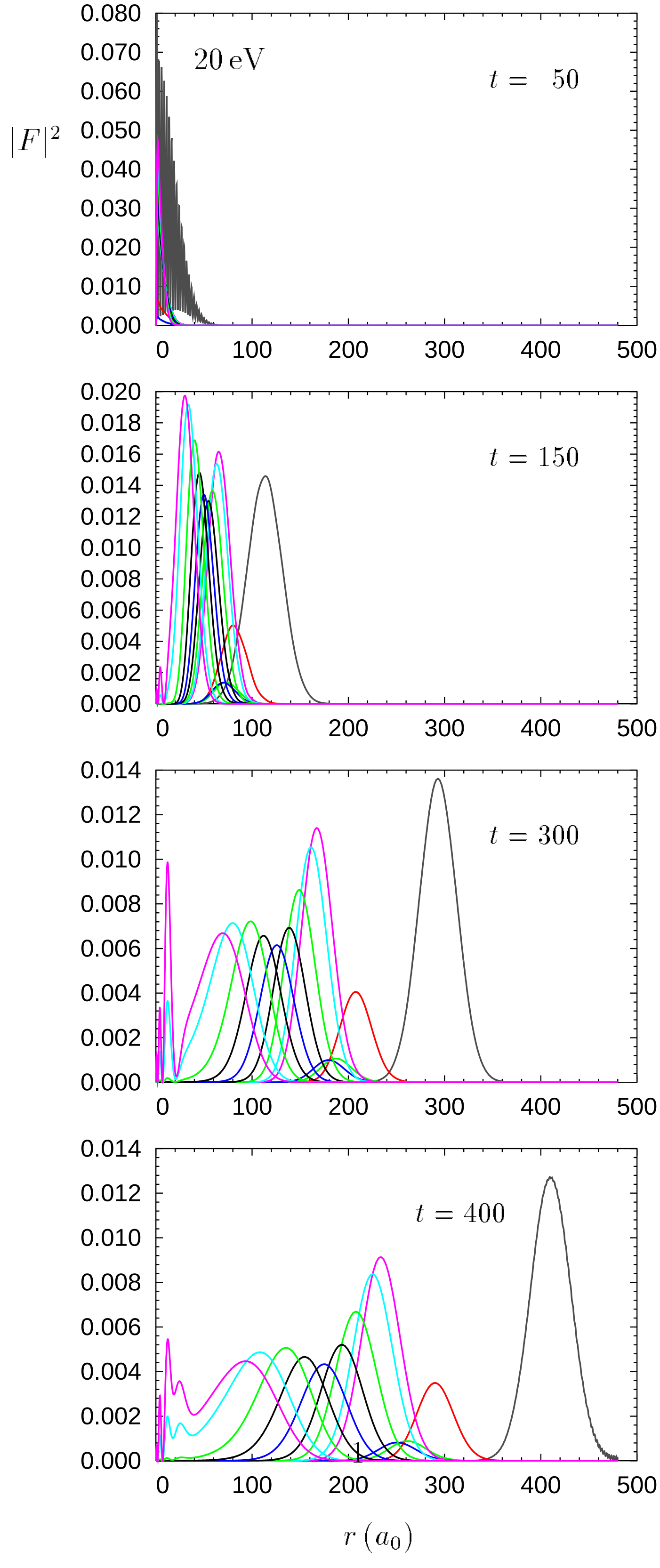


- **Note the symmetry in the ionization probabilities around $E/2$!**

  ($\epsilon = E/40$.)

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

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



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

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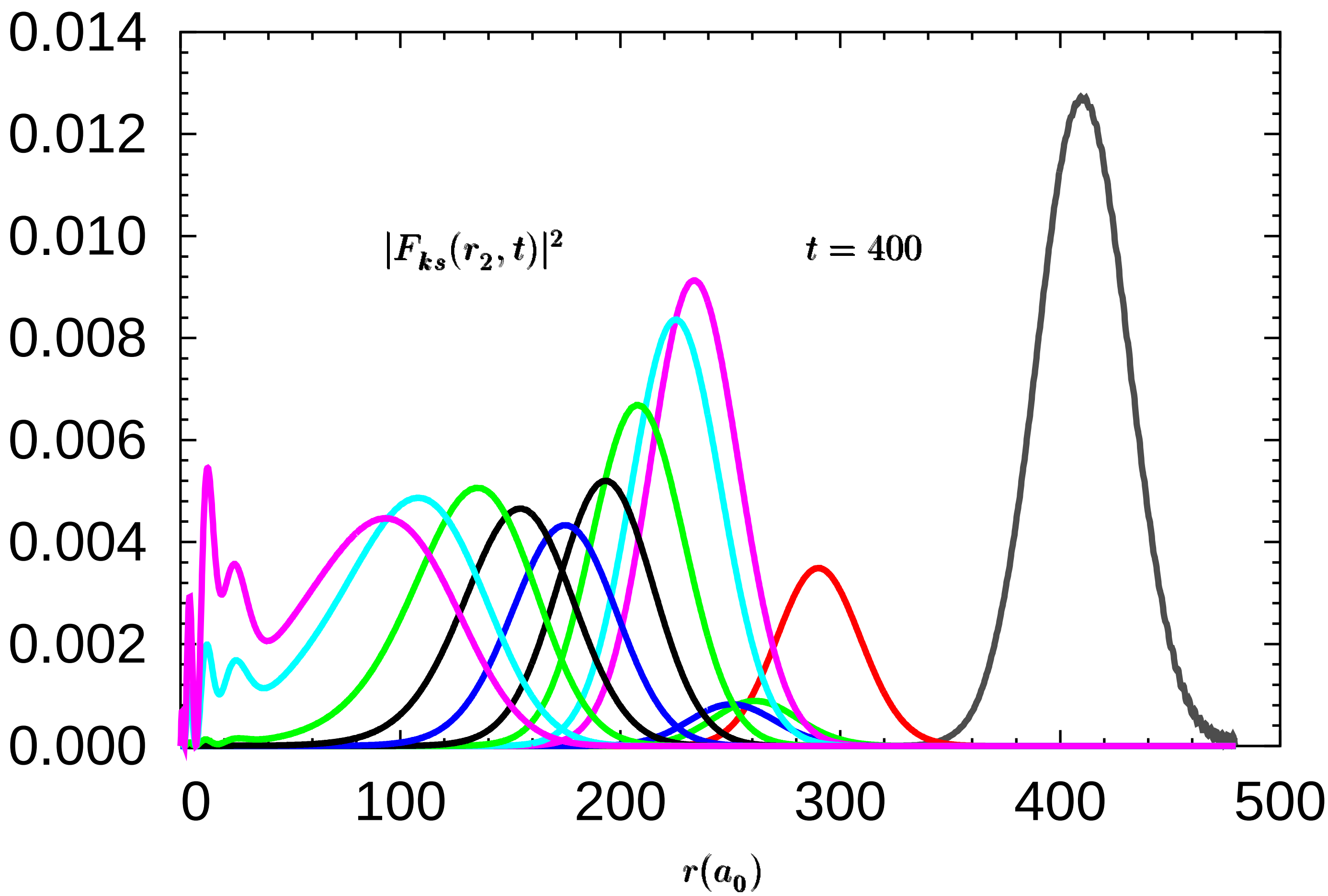
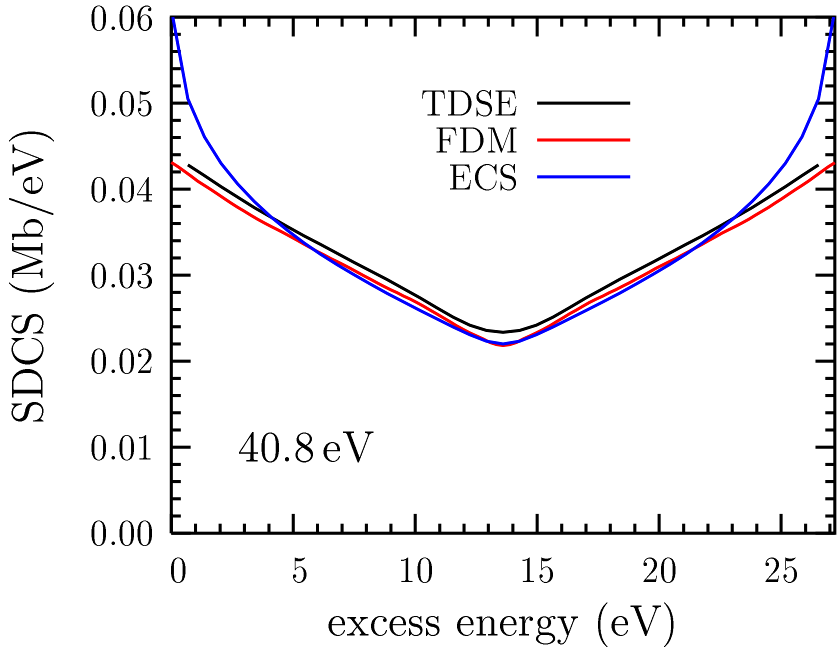
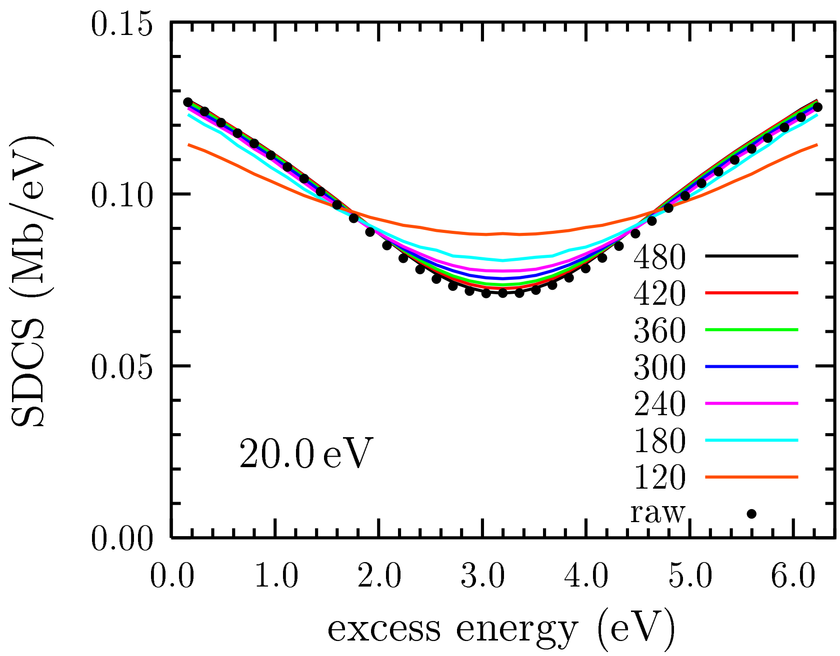


Convergence of the Results

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

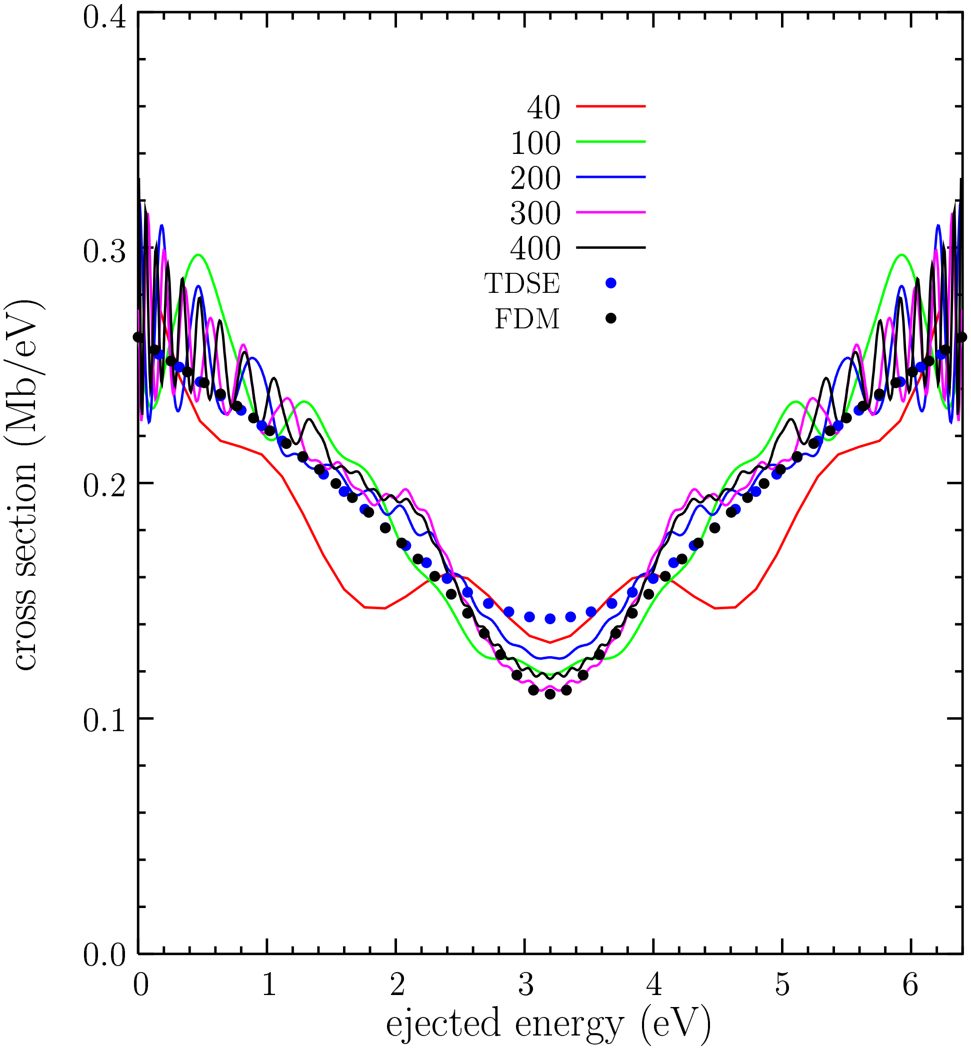




- **A large radial mesh and long propagation times are needed for small excess energies and nearly symmetric energy sharing.**

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.