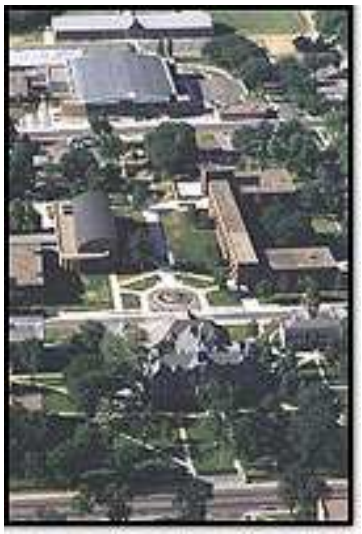
Electron Collisions: Experiment, Theory, and Applications

Klaus Bartschat

Drake University, Des Moines, Iowa 50311, USA

Allis-Prize Talk, GEC 2017



OVERVIEW:

Acknowledgements

I. Motivation: The Need for Electron Collision Data

II. Examples of Experimental Progress

III. Examples of Theoretical/Computational Progress

IV. Examples of Applications

V. Conclusions, Outlook, and Related Topics

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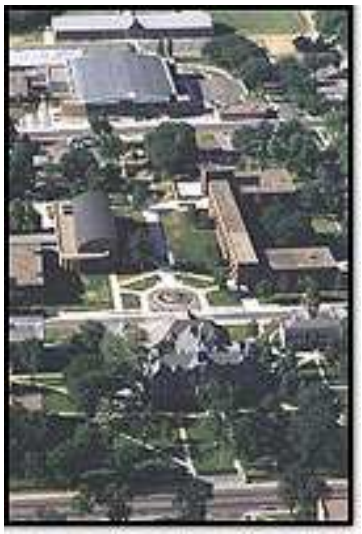

DISCLAIMER:
This talk is a (hopefully coherent) story. It is NOT a Review!
I apologize in advance if your favorite experiment, theory, or application is not mentioned :-(

III. Examples of Theoretical/Computational Progress
IV. Examples of Applications
V. Conclusions, Outlook, and Related Topics

Acknowledgements:
Why I am here today ...

Will Allis
Without his pioneering work,
there would be no Will Allis Prize.

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2016 Allis Prize Selection Committee:
James Lawler (Chair), Gregory Hebner, David Graves, James Colgan, Morty Khakoo

Acknowledgements:

My parents and Joachim Keßler (my Diploma supervisor)

I used to be an experimentalist, but I was much better seeing the light with the eyes of a theorist than installing and using a photo-multiplier.

But there is more ...

Friedrich Hanne

let me work in his lab anyway.
[(No) UHV and a GaAs crystal
sealed my conversion to theory.]

And more ...

Karl Blum

co-supervised my Diploma and PhD theses.
[He also showed me that a *real theorist* can do with just 0, +/- 1, and i. Everything else can be renormalized or be called $<T_{KQ}^{+}>$.]

And more ...

Phil Burke (Allis Prize winner in 2012)
taught me about computers and especially the R-matrix method. According to a colleague, there was nothing to worry about in Belfast, because **"Phil knows EVERYTHING!"**

Don Madison
brought me to Des Moines and
is ultimately responsible for my
position at Drake University.
Don also dragged me along to my first Gaseous Electronics Conference.

And more...

John Giuliani
came to one of my GEC posters and said:
“Why don’t you do something useful?”

And more...

Oleg Zatsarinny
has been a close collaborator at Drake University since 2003.
Oleg produced a lot of high-quality data with his B-spline R-matrix code.

And more...

There are many more colleagues/friends who have played a significant role in my scientific career – experimentalists, theorists, data producers, and data users. I can't name you all, but

Thank You!

And it certainly wouldn't have been possible without financial support from:
German Research Council, British Council, NATO,
Drake University, Research Corporation, and the
United States National Science Foundation

GEC 2016 Bochum

69th ANNUAL GASEOUS ELECTRONICS CONFERENCE

October 10th–14th, 2016
Ruhr-Universität Bochum

▸ www.gec2016.de

PROF. DR. KLAUS BARTSCHAT
DRAKE UNIVERSITY
WILL ALLIS PRIZE 2016

Klaus,
get well soon!

Many Thanks also for the Good Wishes!

Nor would it have been possible without ....

Teresa Erika Nick

Thanks for listening so far.
The rest of the talk is on physics.

Some (but not all) points of this talk are summarized here.

PERSPECTIVE

Electron collisions with atoms, ions, molecules, and surfaces: Fundamental science empowering advances in technology

Klaus Bartschat[a,1] and Mark J. Kushner[b]

Edited by David A. Weitz, Harvard University, Cambridge, MA, and approved May 16, 2016 (received for review April 16, 2016)

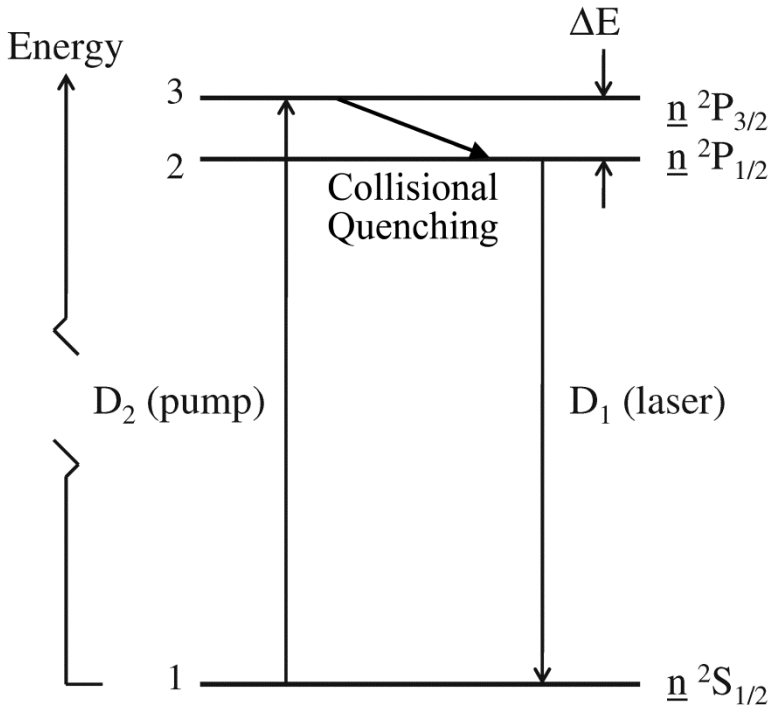
Electron collisions with atoms, ions, molecules, and surfaces are critically important to the understanding and modeling of low-temperature plasmas (LTPs), and so in the development of technologies based on LTPs. Recent progress in obtaining experimental benchmark data and the development of highly sophisticated computational methods is highlighted. With the cesium-based diode-pumped alkali laser and remote plasma etching of Si_3N_4 as examples, we demonstrate how accurate and comprehensive datasets for electron collisions enable complex modeling of plasma-using technologies that empower our high-technology–based society.

electron scattering | close coupling | ab initio | plasmas | kinetic modeling

Motivation: The Need for Electron Collision Data

DIODE-PUMPED ALKALI LASERS (DPALs)

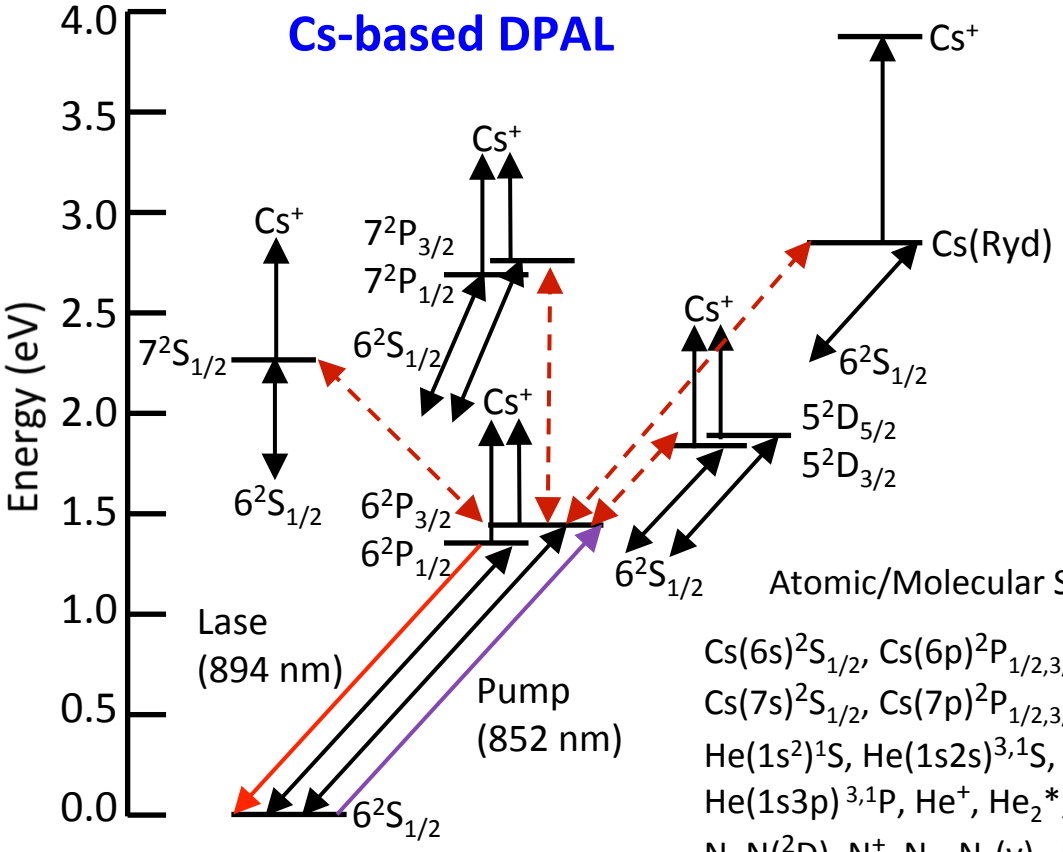
- **DPAL is a class of optically pumped lasers that leverage inexpensive semiconductor diode lasers to pump alkali vapor.**
- **Poor optical quality, wide bandwidth of diode laser (DL) is converted into high optical quality, narrow bandwidth from alkali laser.**



- **DL pumps the $D_2(^2S_{1/2} \rightarrow {}^2P_{3/2})$**
- **Collisional quenching: $^2P_{3/2} \rightarrow {}^2P_{1/2}$**
- **Lasing on $D_1(^2P_{1/2} \rightarrow {}^2S_{1/2})$**
- **Requires inversion of ground state.**
- **Collisional quenching agent N_2**

(slide adapted from a presentation by M. J. Kushner, University of Michigan, Institute for Plasma Science & Engineering.)

Mark Kushner (Allis Prize 2010)

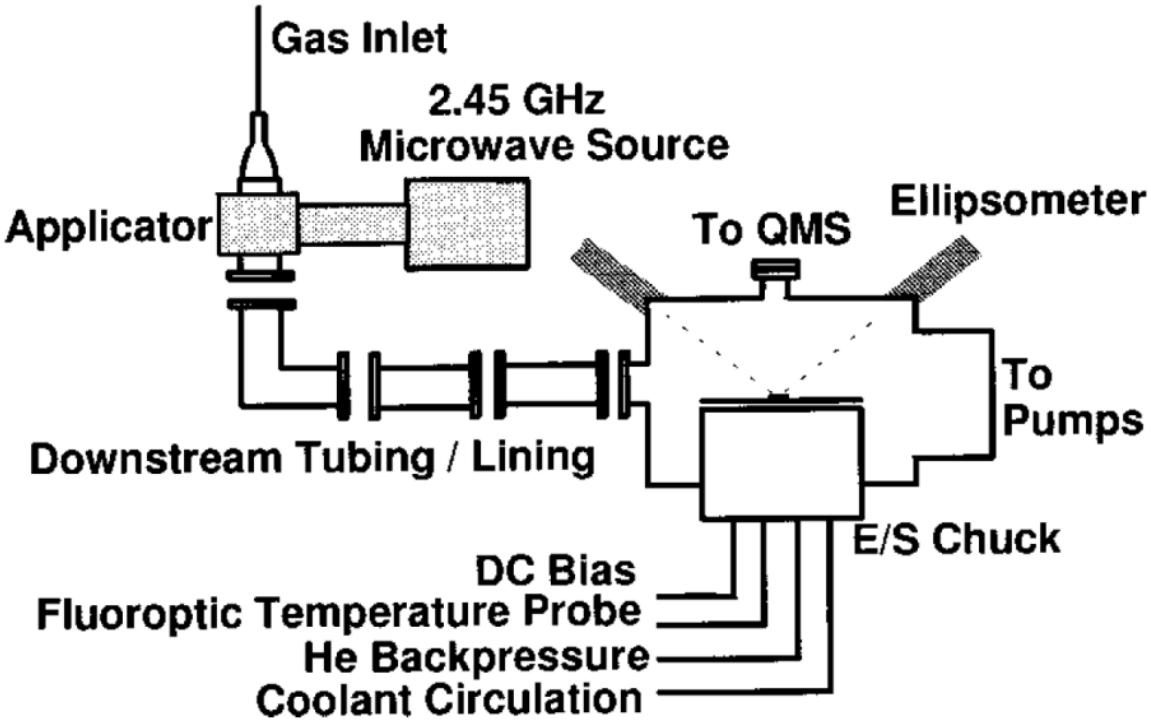


Atomic/Molecular Species in the Model

$Cs(6s)^2S_{1/2}$, $Cs(6p)^2P_{1/2,3/2}$, $Cs(5d)^2D_{5/2,3/2}$,
$Cs(7s)^2S_{1/2}$, $Cs(7p)^2P_{1/2,3/2}$, Cs(Ryd), Cs^+, Cs_2, Cs_2^+
$He(1s^2)^1S$, $He(1s2s)^{3,1}S$, $He(1s2p)^{3,1}P$, $He(1s3s)^{3,1}S$,
$He(1s3p)^{3,1}P$, He^+, He_2*, He_2^+
N, $N(^2D)$, N^+, N_2, $N_2(v)$, $N_2(A)$, $N_2(B,C)$, N_2^+,N_4^+

REMOTE PLASMA SOURCES

- Remote plasma sources (RPS) for microelectronics fabrication
- Separate plasma production, transport and processing regions.

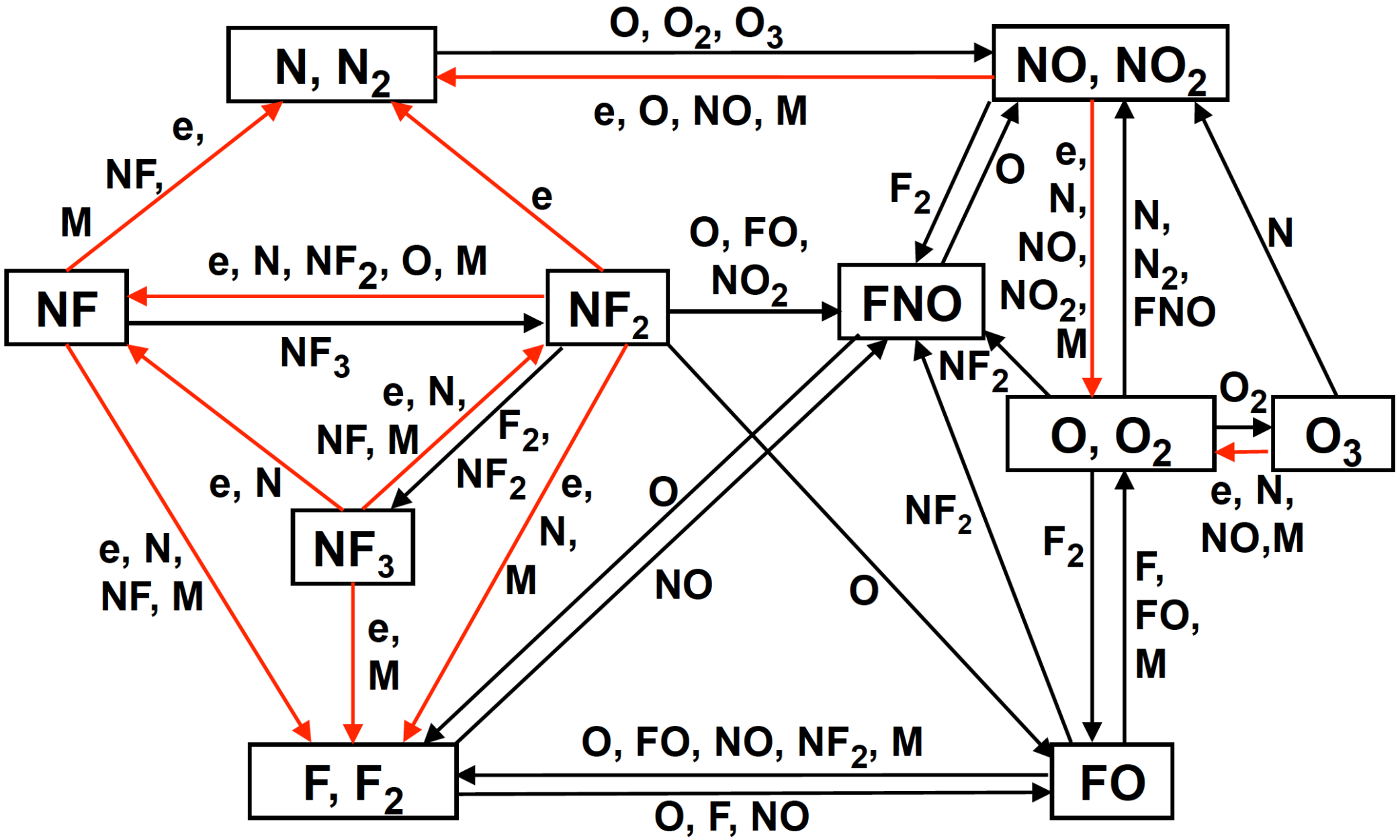


- Schematic of RPS.[1]

- Produce dominantly neutral fluxes of radicals for etching, cleaning, surface passivation.
- Decrease damage by charging and energetic ion bombardment.
- Example: NF_3/O_2 RPS for Si_3N_4 etching.

(slide adapted from a presentation by M. J. Kushner, University of Michigan, Institute for Plasma Science & Engineering.)

WOW! Modelers need a lot of data ...



Production and Assessment of Atomic Data

- Data for electron collisions with atoms and ions are needed for **modeling processes** in
  - **laboratory plasmas**, such as discharges in lighting and lasers
  - **astrophysical plasmas**
  - **planetary atmospheres**
- The data are obtained through
  - **experiments**
    - valuable but expensive (**$$$**) benchmarks (often differential in energy, angle, spin, ...)
    - often problematic when **absolute (cross section) normalization** is required
  - **calculations** (Opacity Project, Iron Project, ...)
    - relatively cheap
    - almost any transition of interest is possible
    - often restricted to particular energy ranges:
      - high (→ Born-type methods)
      - low (→ close-coupling-type methods)
    - cross sections may peak at "intermediate energies" (→ **???**)
  - **good (or bad ?) guesses**
- **Sometimes the results are (obviously) wrong or (more often) inconsistent !**

Basic Question: WHO IS RIGHT ? (And WHY ???)

For *complete* data sets, theory is often the "only game in town"!

Let's start with experiment: Total Cross Sections

PHYSICAL REVIEW A VOLUME 19, NUMBER 2 FEBRUARY 1979

Absolute total cross sections for electron-mercury scattering

K. Jost and B. Ohnemus
Physikalisches Institut, Westfälische Wilhelms Universität, Münster, Germany
(Received 25 April 1978)

The total cross section for e^--Hg scattering has been measured in the energy range between 0.1 and 500 eV. Absolute data taken at a few energies by means of a static target were used to normalize the relative cross sections, which were measured in the whole energy range by scattering from an atomic beam. This technique was used to help meet the high-angular-resolution requirements. The cross sections obtained are considerably larger than those obtained in most of the other measurements performed around 1930. Satisfactory agreement is found, however, with semiempirical cross sections (mainly based on recent measurements) and with a recent theoretical calculation. The most pronounced structure is a cross section maximum at 0.4 eV, which probably can be ascribed to a $(6s\,^2 6p_{1/2})^2P_{1/2}$ shape resonance.

Nevertheless, there are surprisingly few measurements of the total cross section,[3-6] and moreover these are not very recent. These old data are now considered to be rather unreliable.[7]

Transmission Setup: $I = I_0 \exp(-nlQ)$

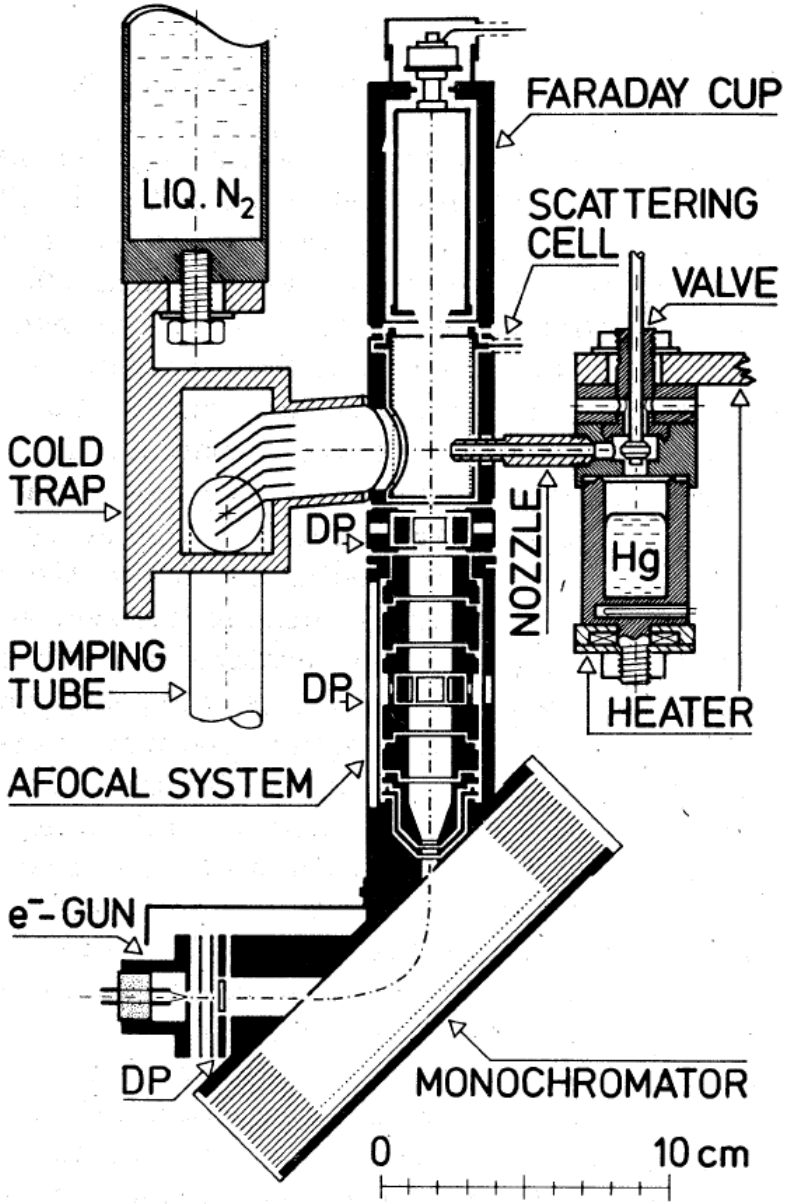


FIG. 1. Electron optical arrangement for low energie (0.1–70 eV) with atomic beam target. Deflector plates are denoted by DP.

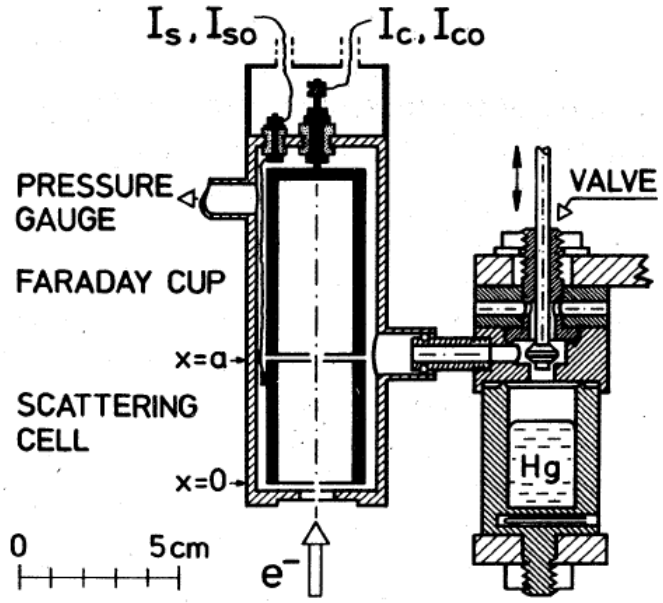


FIG. 3. Target cell for absolute measurements. This arrangement is used together with the electron optics of Fig. 1.

$$I = I_0 \exp(-nlQ)\,, \tag{1}$$

where

$$Q = (nl)^{-1} \ln(I_0/I) \sim \ln(I_0/I) \tag{2}$$

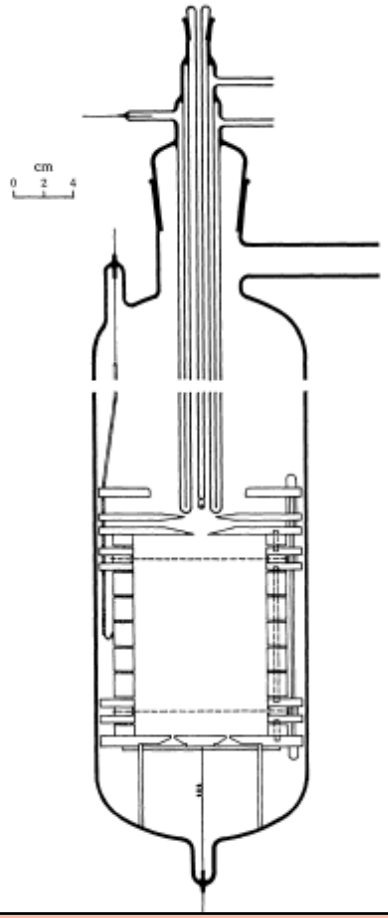
is the total cross section. An absolute measurement of Q requires knowledge of n and l, whereas the relative shape of the cross-section curve versus energy E can be obtained even in an inhomogeneous target such as an atomic beam, if care is taken to keep the product of mean path length l and mean target density n constant during the measurement. In order to check the constancy

Swarm Experiments (Phelps, Crompton, ...)

THE MOMENTUM TRANSFER CROSS SECTION FOR ELECTRONS IN HELIUM

By R. W. Crompton,* M. T. Elford,* and R. L. Jory*†

Measurements of the drift velocity, the ratio of diffusion coefficient to mobility, and the "magnetic drift velocity" for electrons in helium have been made at 293°K in the range $1{\cdot}8\times10^{-19} < E/N < 3\times10^{-17}$ V cm². From an analysis of the drift velocity data, an energy-dependent momentum transfer cross section has been derived for which an error of less than ±2% is claimed over the central portion of the energy range. The cross section agrees with the theoretical cross section of ...



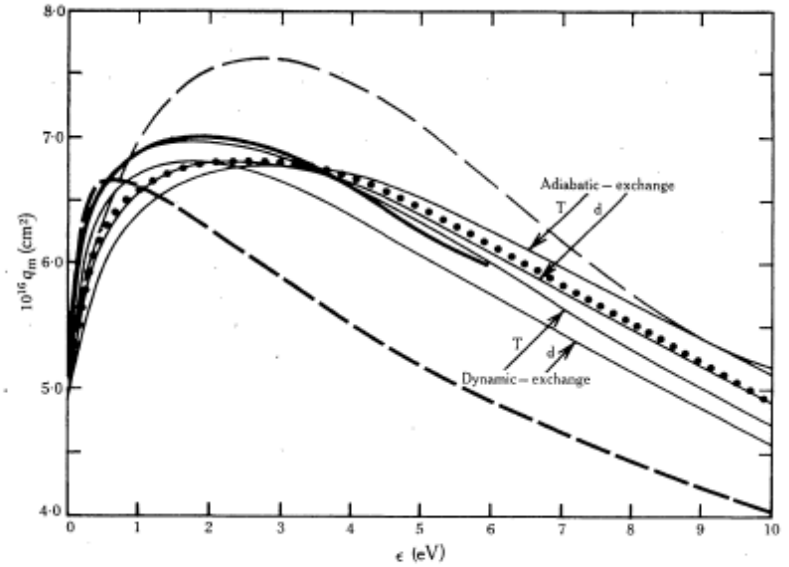


Fig. 7.—A comparison between theoretical and experimental momentum transfer cross sections. —— Crompton, Elford, and Jory; — — Frost and Phelps; — — Bauer and Browne; ——— La Bahn and Callaway; ••• Williamson and McDowell.

Since the first extensive calculations of the total scattering cross section by Morse and Allis (1933)...

Will Allis did calculations for this in 1933!

Art Phelps was the first Allis Prize recipient (1990)

Swarm Experiments and Their Interpretation

- **Pioneered by "GEC Giants" such as Art Phelps and Bob Crompton.**
- **General Idea (thanks to Leanne Pitchford for enlightening me):**
  - Pull electrons through a gas and measure macroscopic parameters such as:
    - transition times ($\rightarrow$ **drift velocity, mobility**)
    - radial or axial spreading ($\rightarrow$ **diffusion coefficients**)
    - current growth ($\rightarrow$ **ionization rates**)
  - In "equilibrium conditions", these parameters depend on the **"reduced electric field"** $\boldsymbol{E/N}$, the **gas (composition)**, and the **relevant cross sections**. In low-energy elastic scattering, the **momentum transfer cross section** dominates.
- **Absolute** (momentum transfer) **cross sections** are determined **indirectly** as follows:

  indirect measurement

  (1) Assume an initial set of cross sections.
  (2) Calculate the macroscopic parameters.
  (3) Assume that any deviations are due to errors in the assumed cross sections.
  (4) Adjust the cross section(s) until things fit.
  (5) Hope for:
    - convergence of the procedure;
    - uniqueness of the results in multi-parameter fits.

Other Techniques (Incomplete List)

- **Optical Emission**:
  - **State-Selective**
  - **Relative**
  - **Cascade Effects**

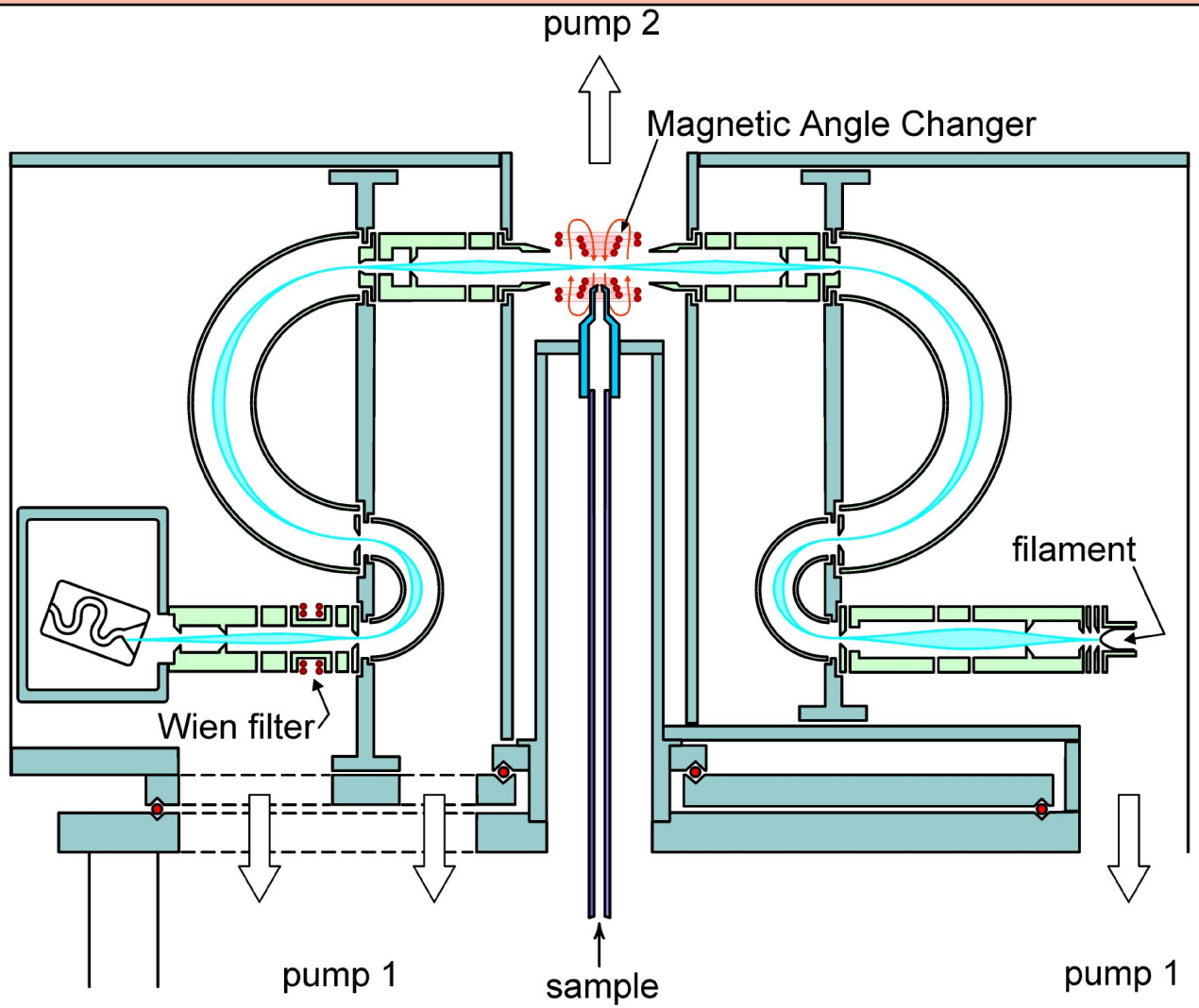
Recall: This talk is NOT a review!

- **Time-of-Flight Setups (Metastables)**
- **Storage Rings (e-Ion Collisions)**
- **Integrate Angle-Differential Cross Sections from Crossed-Beam Setups**
  - **State-Selective** (measure energy loss/gain)
  - **Often Relative** – **Absolute Normalization Attempts** include
    - **Mixed-Flow Technique with a Reference Gas**
    - **Generalized Oscillator Strength**
    - **Help from Theory** (**Yes, we are good for something!**)

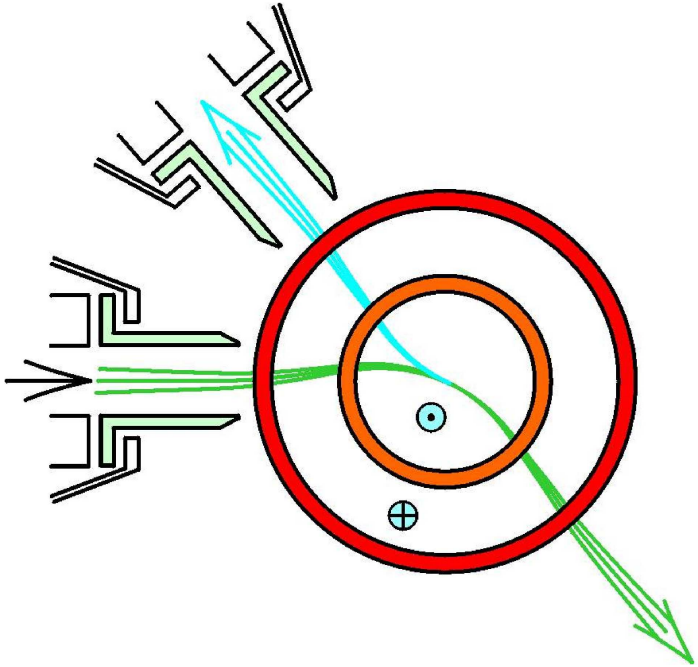
Angle-Differential Cross Sections

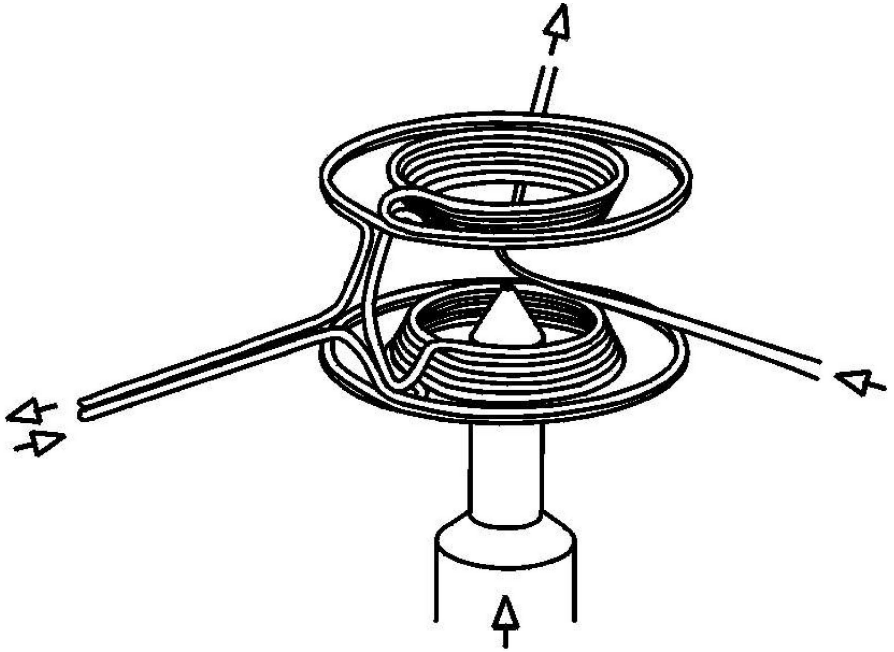
Michael Allan's high-resolution spectrometer to measure:

- **specific angles**
- **specific transitions (energy selection)**



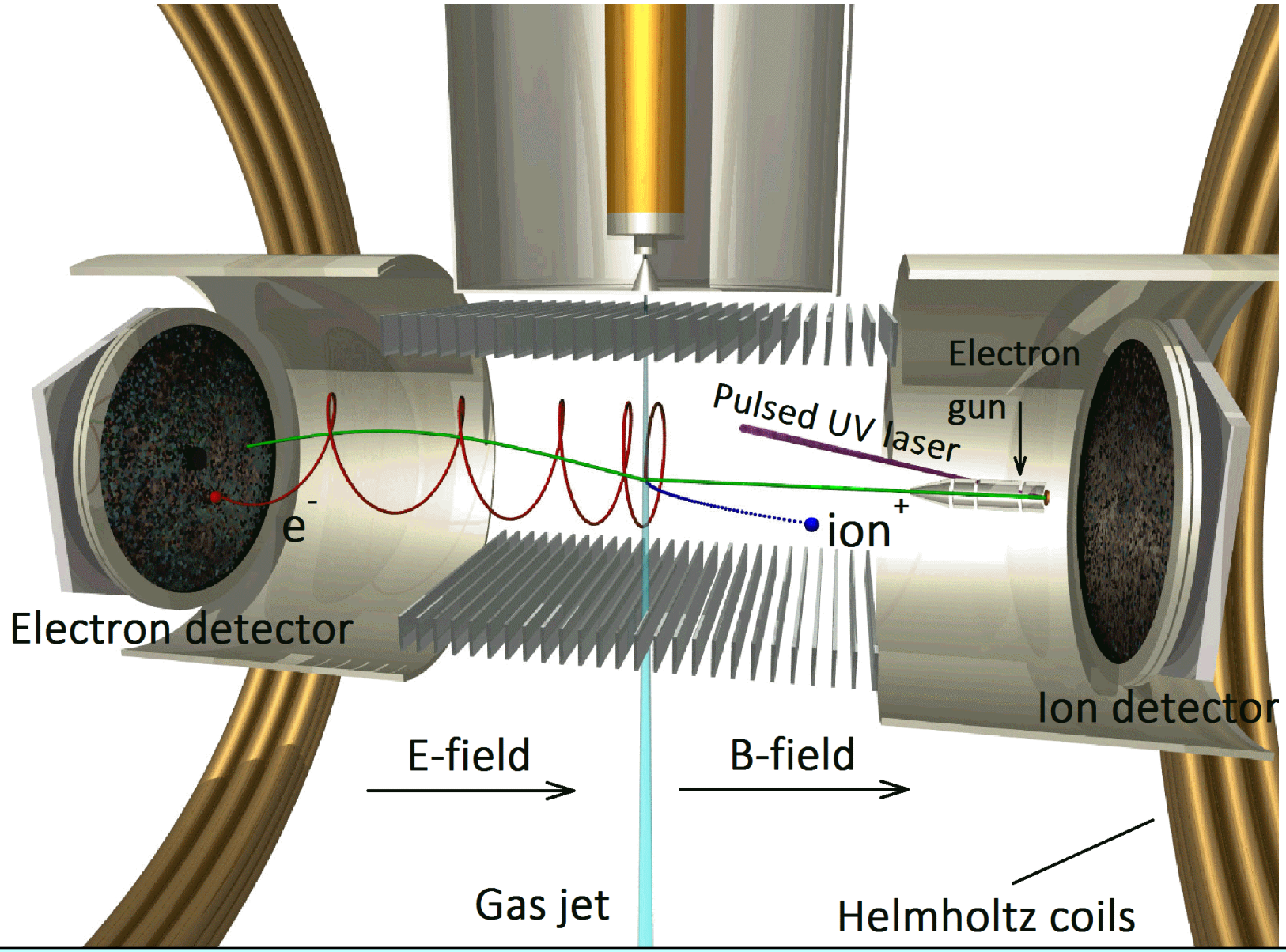
The "Magnetic Angle Changer" (MAC), developed by Reid and Channing, makes it possible to measure the full angular range, including 180º.





The Reaction Microscope

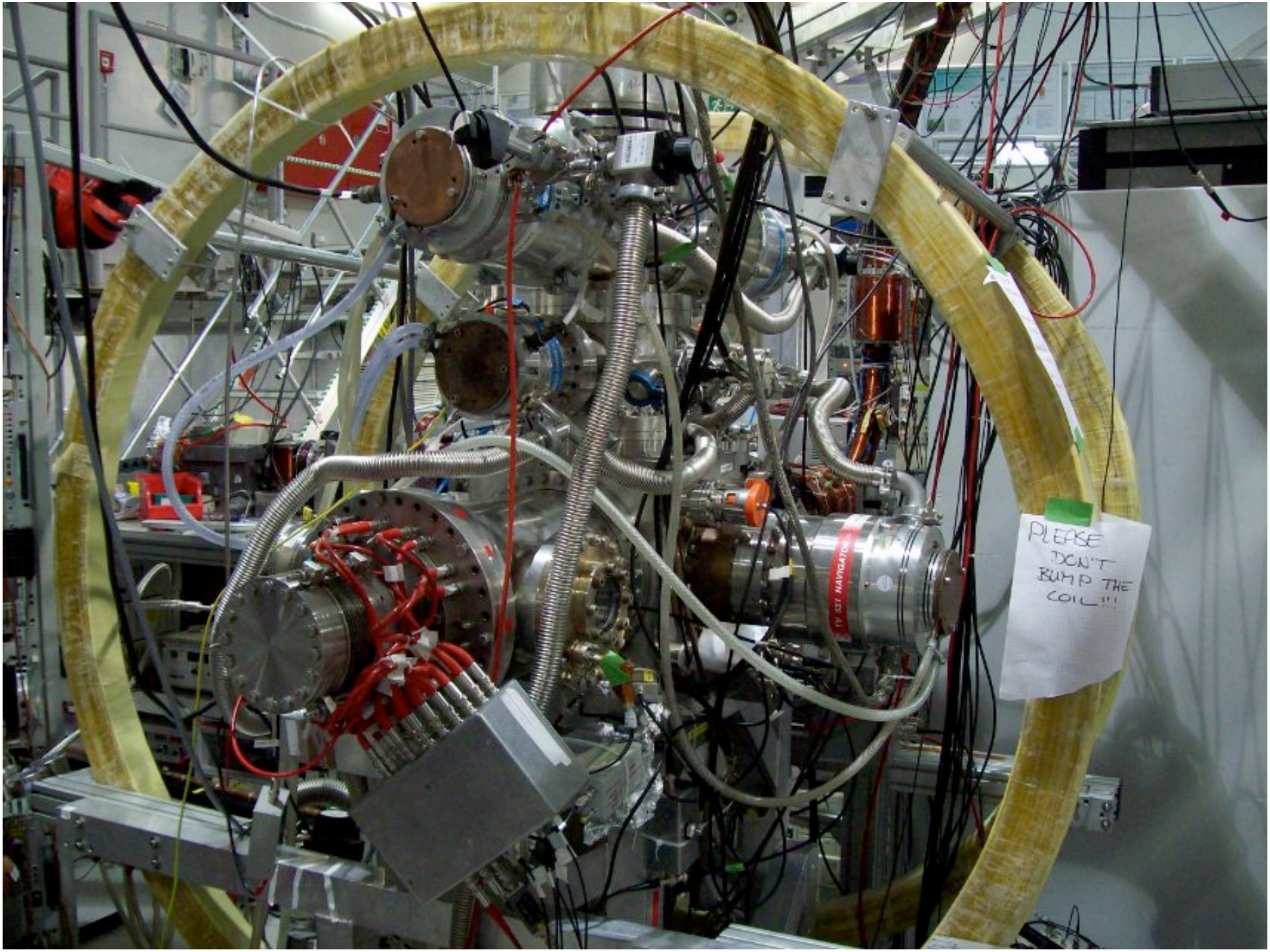
Ullrich, Moshammer, Dorn, *et al.*, Rep. Prog. Phys. 66 (2003) 1463



Used in A. Dorn's group for (e,2e) and even (e,2eγ)

They can get the full 3D-picture in a single shot!

This is how it really looks like!



Move on to Computational Methods

Choice of Computational Approaches

- **Which one is right for YOU?**
  - **Perturbative (Born-type) or Non-Perturbative (close-coupling, time-dependent, ...)?**
  - **Semi-empirical or fully ab initio?**
  - **How much input from experiment?**
  - **Do you trust that input?**
  - **Predictive power? (input $\leftrightarrow$ output)**
- **The answer depends on many aspects, such as:**
  - **How many transitions do you need?** (elastic, momentum transfer, excitation, ionization, ... how much lumping?)
  - **How complex is the target** (H, He, Ar, W, H_2, H_2O, radical, DNA, ...)?
  - **Do the calculation yourself or beg/pay somebody to do it for you?**
  - **What accuracy can you live with?**
  - **Are you interested in numbers or "correct" numbers?**
  - **Which numbers do really matter?**

Classification of Numerical Approaches

- **Special Purpose (elastic/total)**: OMP (pot. scatt.); Polarized Orbital
- **Born-type methods**
  - PWBA, DWBA, FOMBT, PWBA2, DWBA2, ...
  - fast, easy to implement, flexible target description, test physical assumptions
  - two states at a time, no channel coupling, problems for low energies and optically forbidden transitions, results depend on the choice of potentials, unitarization

Recall: This talk is NOT a review!

- **(Time-Independent) Close-coupling-type methods**
  - CCn, CCO, CCC, RMn, IERM, RMPS, DARC, BSR, ...
  - Standard method of treating low-energy scattering; based upon the expansion

$$\Psi_E^{LS\pi}(\mathbf{r}_1,\ldots,\mathbf{r}_{N+1}) = \mathcal{A}\sum_i \Phi_i^{LS\pi}(\mathbf{r}_1,\ldots,\mathbf{r}_N,\hat{\mathbf{r}})\,\frac{1}{r}\,F_{E,i}(r)$$

  - simultaneous results for transitions between **all states** in the expansion; sophisticated, publicly available codes exist; results are **internally consistent**
  - expansion must be cut off (→ **CCC, RMPS, IERM**)
  - **usually, a single set of mutually orthogonal one-electron orbitals is used for all states in the expansion** (→ **BSR with non-orthogonal orbitals**)
- **Time-dependent and other direct methods**
  - TDCC, ECS
  - solve the Schrödinger equation directly on a grid
  - very expensive, only possible for (quasi) one- and two-electron systems.

Inclusion of Target Continuum (Ionization)

- imaginary absorption potential (OMP)
- final continuum state in DWBA
- directly on the grid and projection to continuum states (TDCC, ECS)
- **add square-integrable pseudo-states to the CC expansion (CCC, RMPS, ...)**

Inclusion of Relativistic Effects

- **Re-coupling** of non-relativistic results (problematic near threshold)
- Perturbative (**Breit-Pauli**) approach; matrix elements calculated between **non-relativistic wavefunctions**
- **Dirac-based approach**

Time-Independent Close-Coupling

- Standard method of treating low-energy scattering
- Based upon an expansion of the total wavefunction as

$\mathbf{H\,\Psi = E\,\Psi}$

$$\Psi_E^{LS\pi}(\mathbf{r}_1,\ldots,\mathbf{r}_{N+1}) = \mathcal{A}\sum\!\!\!\!\!\!\int_i \Phi_i^{LS\pi}(\mathbf{r}_1,\ldots,\mathbf{r}_N,\hat{\mathbf{r}})\,\frac{1}{r}\,F_{E,i}(r)$$

- Target states Φ_i diagonalize the N-electron target Hamiltonian according to

$$\langle \Phi_{i'} \mid H_T^N \mid \Phi_i \rangle = E_i\,\delta_{i'i}$$

- The unknown radial wavefunctions $F_{E,i}$ are determined from the solution of a system of coupled integro-differential equations given by

$$\left[\frac{d^2}{dr^2} - \frac{\ell_i(\ell_i+1)}{r^2} + k^2\right] F_{E,i}(r) = 2\sum\!\!\!\!\!\!\int_j V_{ij}(r)\,F_{E,j}(r) + 2\sum\!\!\!\!\!\!\int_j W_{ij}\,F_{E,j}(r)$$

with the direct coupling potentials

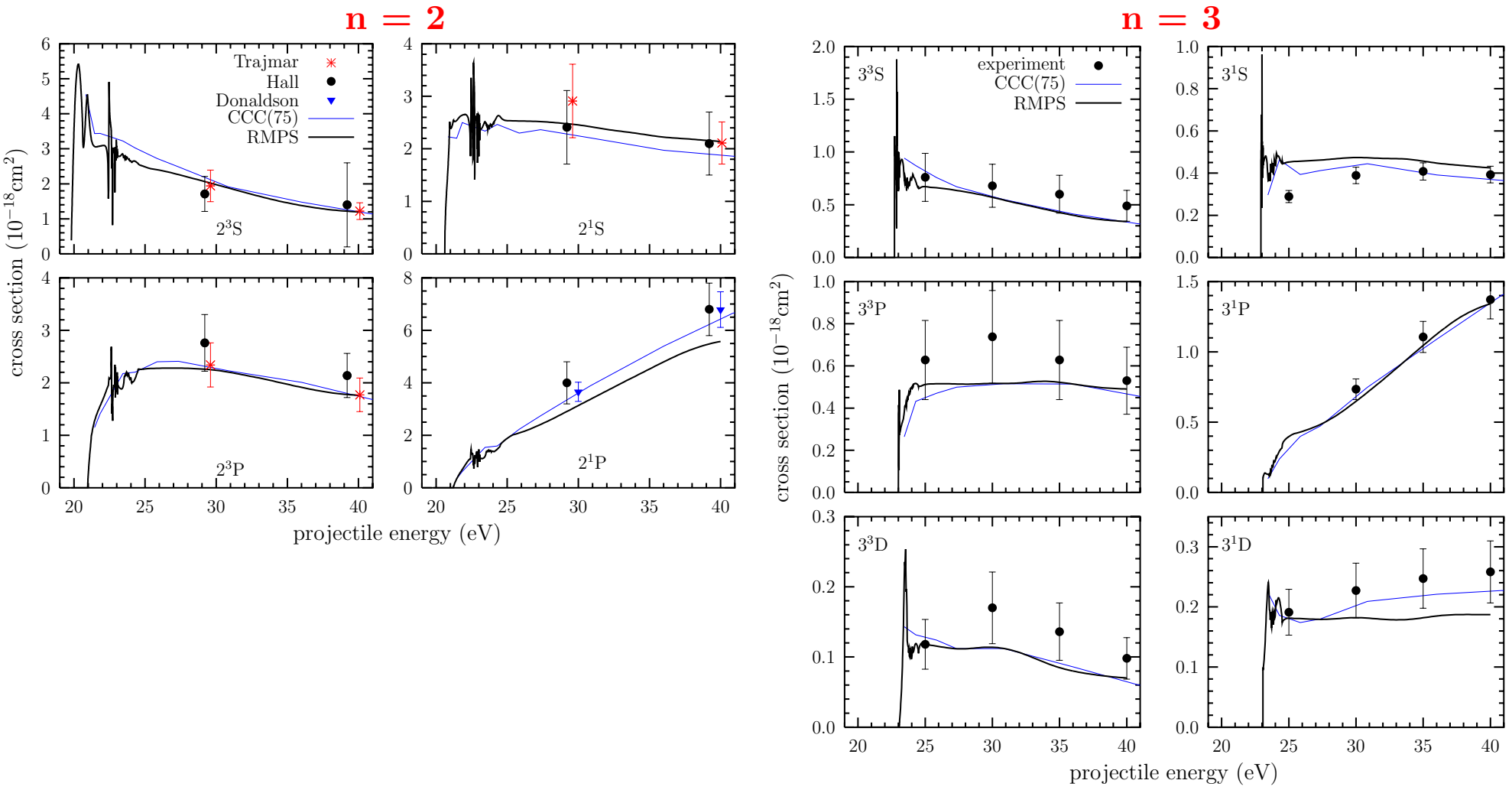
$$V_{ij}(r) = -\frac{Z}{r}\,\delta_{ij} + \sum_{k=1}^{N}\langle \Phi_i \mid \frac{1}{|\mathbf{r}_k - \mathbf{r}|} \mid \Phi_j \rangle$$

and the exchange terms

$$W_{ij}F_{E,j}(r) = \sum_{k=1}^{N}\langle \Phi_i \mid \frac{1}{|\mathbf{r}_k - \mathbf{r}|} \mid (\mathcal{A}-1)\,\Phi_j F_{E,j}\rangle$$

Close-coupling can yield *complete* data sets, and the results are *internally consistent* (unitary theory that conserves total flux)!

Total Cross Sections for Electron-Impact Excitation of Helium
K. Bartschat, J. Phys. B 31 (1998) L469

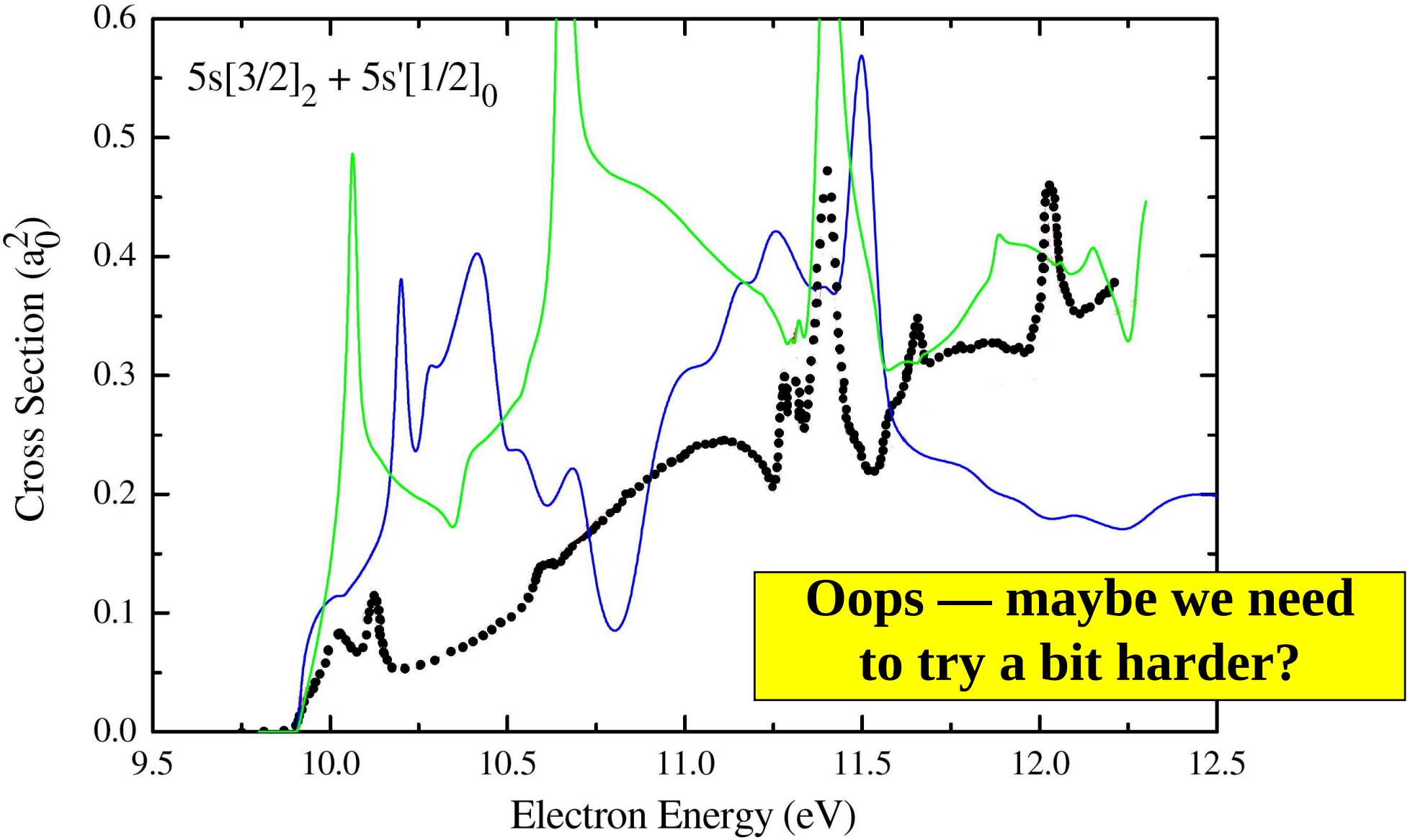


In 1998, de Heer recommends 0.5 x (CCC+RMPS) for uncertainty of 10% — independent of experiment!

Metastable Excitation Function in Kr

Experiment: Buckman *et al* (1983), multiplied by 0.67

Theories: 31-state Breit-Pauli R-matrix (Zeman & Bartschat 1998)
51-state Breit-Pauli R-matrix (Bartschat & Grum-Grzhimailo 2000)



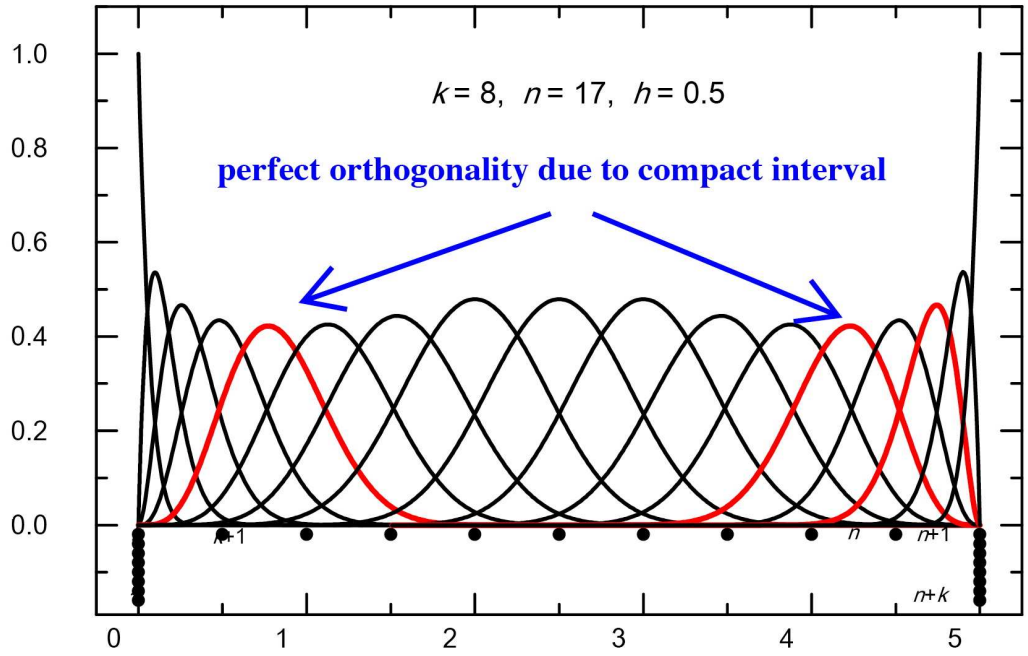
Oops — maybe we need to try a bit harder?

We have a great program now :):):)

General B-Spline R-Matrix (Close-Coupling) Programs (D)BSR

- **Key Ideas:**
  - Use *B*-**splines as universal basis** set to represent the continuum orbitals
  - Allow **non-orthogonal orbital sets** for bound and continuum radial functions

not just the numerical basis!



O. Zatsarinny, CPC 174 (2006) 273

- **Consequences:**
  - **Much improved target description possible with small CI expansions**
  - **Consistent description of the *N*-electron target and (*N*+1)-electron collision problems**
  - No "Buttle correction" since *B*-spline basis is effectively complete
- **Complications:**
  - Setting up the Hamiltonian matrix can be very complicated and lengthy
  - Generalized eigenvalue problem needs to be solved
  - Matrix size typically **100,000 or more** due to size of *B*-spline basis
  - Rescue: Excellent numerical properties of *B*-splines; use of (SCA)LAPACK *et al.*

record: 400,000 to do 50-100 times; 0.5 - 1.0 MSU (1 MSU = $50,000 in NSF Accounting)

We also have to solve the problem outside the box for each energy (from 100's to 100,000's).

List of early calculations with the BSR code (rapidly growing)

***hν* + Li**	Zatsarinny O and Froese Fischer C *J. Phys. B* **33** 313 (2000)
***hν* + He**	Zatsarinny O, Gorczyca T W and Froese Fischer C *J. Phys. B.* **35** 4161 (2002)
***hν* + C**	Gibson N D *et al.* Phys. Rev. A **67**, 030703 (2003)
***hν* + B**	Zatsarinny O and Gorczyca T W Abstracts of XXII ICPEAC (2003)
***hν* + O**	Zatsarinny O and Bartschat K *Phys. Rev. A* **73** 022714 (2006)
***hν* + Ca**	Zatsarinny O *et al. Phys. Rev. A* **74** 052708 (2006)
e + He	Stepanovic *et al. J. Phys. B* **39** 1547 (2006)
	Lange M *et al. J. Phys. B* **39** 4179 (2006)
e + C	Zatsarinny O, Bartschat K, Bandurina L and Gedeon V *Phys. Rev. A* **71** 042702 (2005)
e + O	Zatsarinny O and Tayal S S *J. Phys. B* **34** 1299 (2001)
	Zatsarinny O and Tayal S S *J. Phys. B* **35** 241 (2002)
	Zatsarinny O and Tayal S S As. J. S. S. **148** 575 (2003)
e + Ne	Zatsarinny O and Bartschat K *J. Phys. B* **37** 2173 (2004)
	Bömmels J *et al.* Phys. Rev. A **71**, 012704 (2005)
	Allan M *et al. J. Phys. B* **39** L139 (2006)
e + Mg	Bartschat K, Zatsarinny O, Bray I, Fursa D V and Stelbovics A T *J. Phys. B* **37** 2617 (2004)
e + S	Zatsarinny O and Tayal S S *J. Phys. B* **34** 3383 (2001)
	Zatsarinny O and Tayal S S *J. Phys. B* **35** 2493 (2002)
e + Ar	Zatsarinny O and Bartschat K *J. Phys. B* **37** 4693 (2004)
e + K (inner-shell)	Borovik A A *et al. Phys. Rev. A,* **73** 062701 (2006)
e + Zn	Zatsarinny O and Bartschat K *Phys. Rev. A* **71** 022716 (2005)
e + Fe^+	Zatsarinny O and Bartschat K *Phys. Rev. A* **72** 020702(R) (2005)
e + Kr	Zatsarinny O and Bartschat K *J. Phys. B* **40** F43 (2007)
e + Xe	Allan M, Zatsarinny O and Bartschat K *Phys. Rev. A* 030701(R) (2006)
Rydberg series in C	Zatsarinny O and Froese Fischer C *J. Phys. B* **35** 4669 (2002)
osc. strengths in Ar	Zatsarinny O and Bartschat K *J. Phys. B: At. Mol. Opt. Phys.* **39** 2145 (2006)
osc. strengths in S	Zatsarinny O and Bartschat K *J. Phys. B: At. Mol. Opt. Phys.* **39** 2861 (2006)
osc. strengths in Xe	Dasgupta A *et al. Phys. Rev. A* **74** 012509 (2006)

at least 100 more since 2006

Topical Review: J. Phys. B 46 (2013) 112001

Our Apparatus — Supercomputers

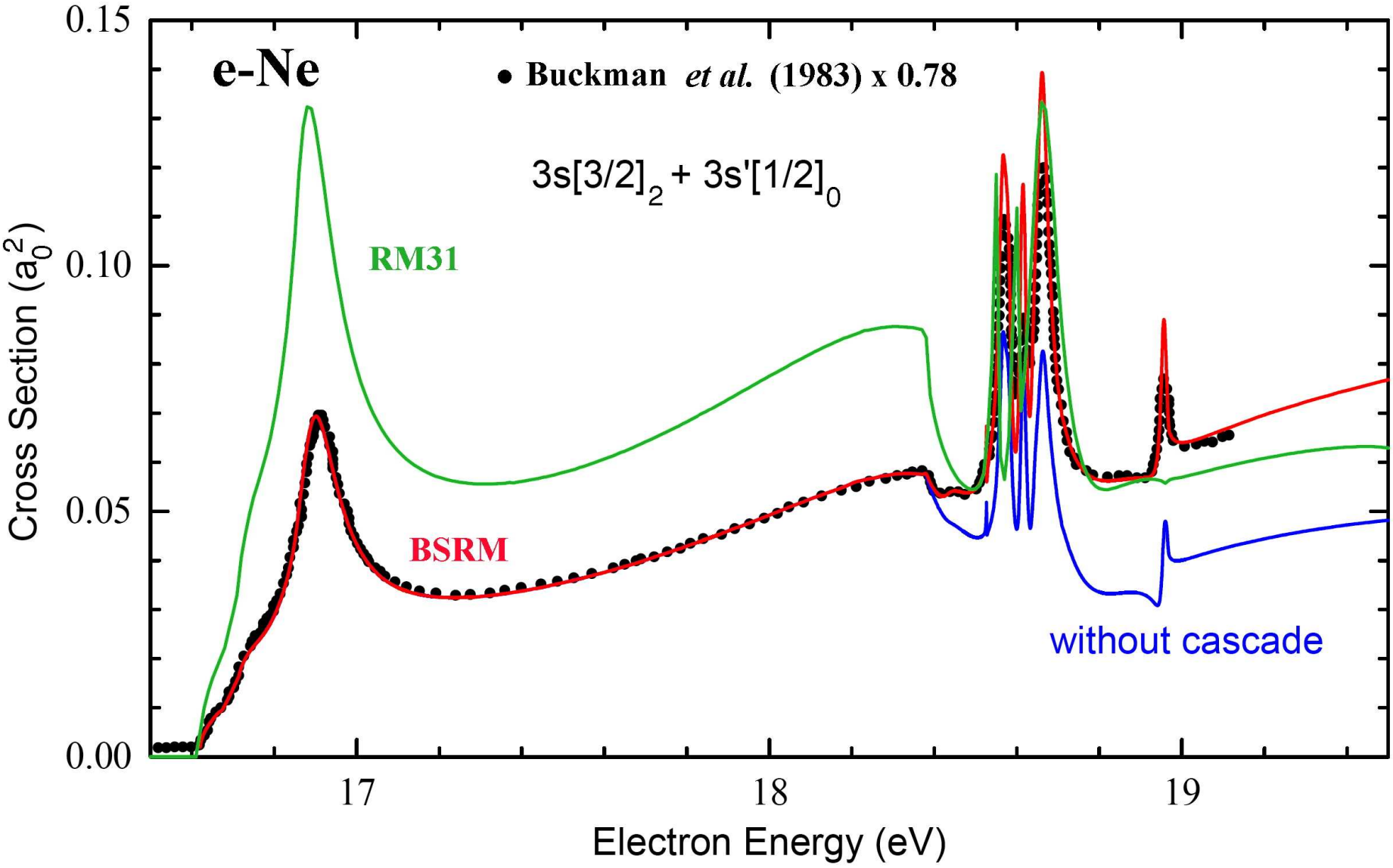
Kraken (NICS)

TACC TEXAS ADVANCED COMPUTING CENTER
Powering Discoveries That Change The World

Move on to Collisions ...

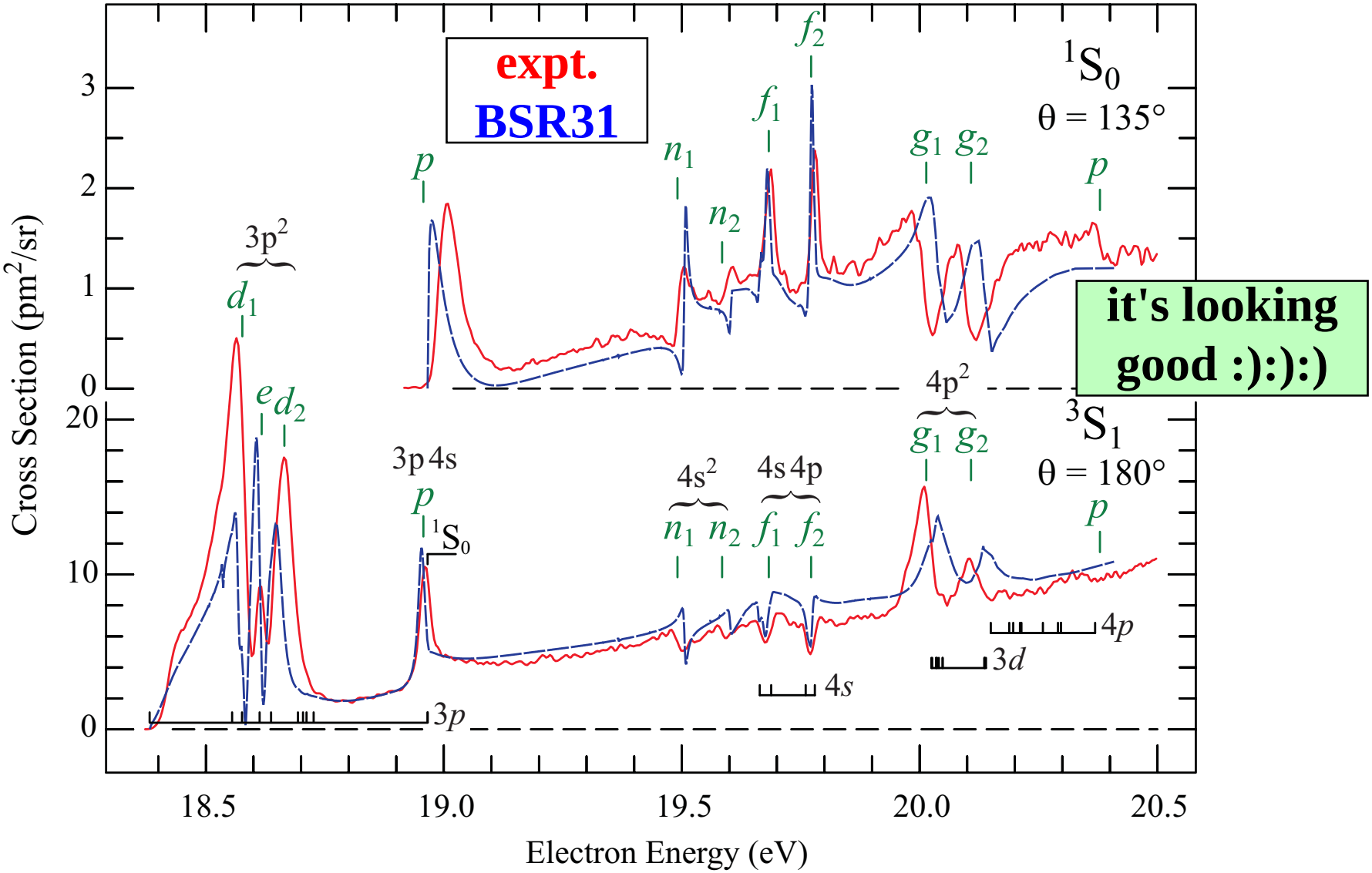
Metastable yield in e-Ne collisions

- Using our semi-relativistic *B*-spline *R*-matrix (BSR) method [Zatsarinny and Bartschat, J. Phys. B 37, 2173 (2004)], we achieved unprecendented agreement with experiment for angle-integrated cross sections in e−Ne collisions.



Resonances in the excitation of the Ne ($2p^5 3p$) states

Allan, Franz, Hotop, Zatsarinny, Bartschat (2009), J. Phys. B 42, 044009



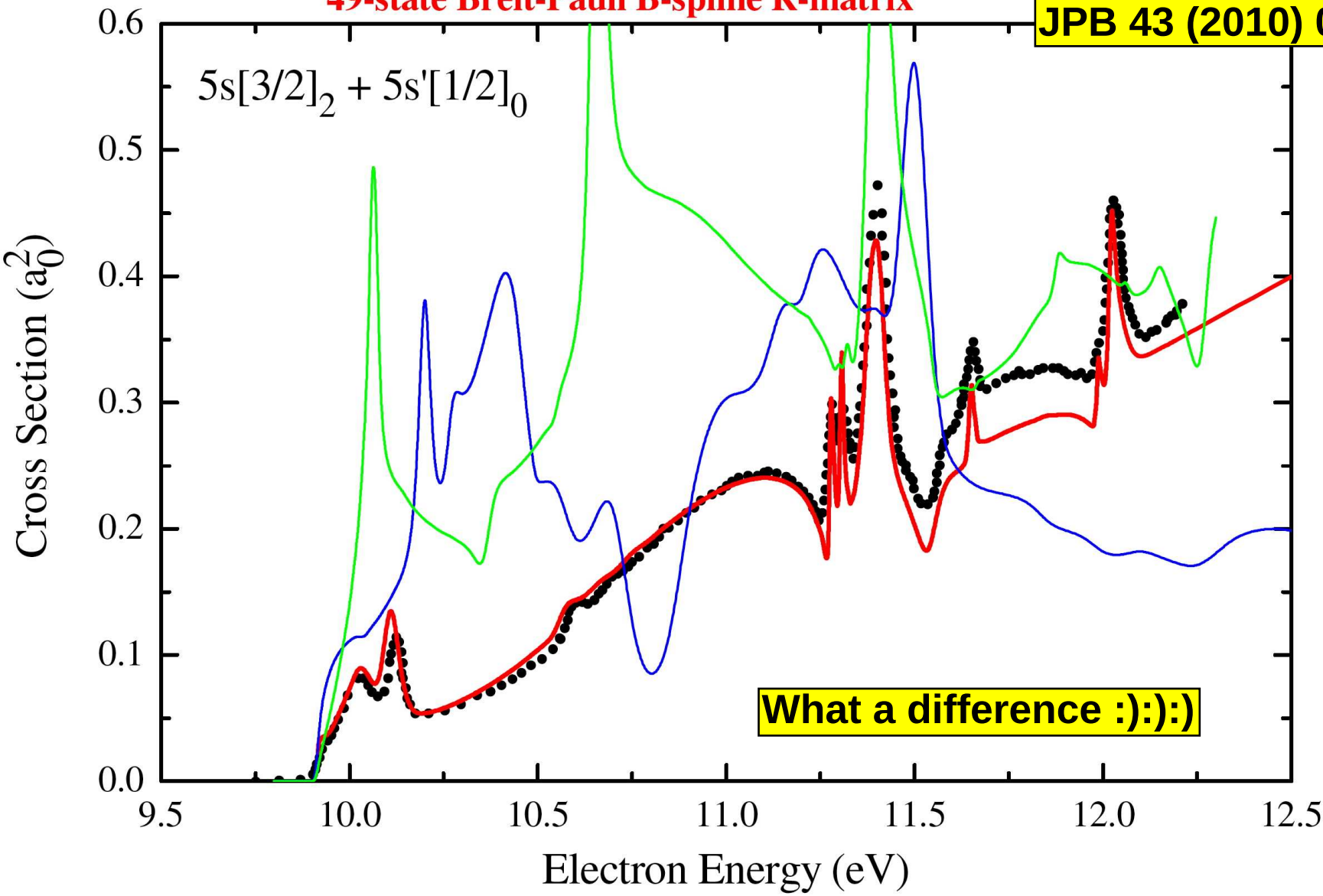
it's looking good :):):)

Expanded view of the resonant features in selected cross sections for the excitation of the 3p states. Experiment is shown by the more ragged red line, theory by the smooth blue line. The present experimental energies, labels (using the notation of Buckman *et al*. (1983), and configurations of the resonances are given above the spectra. Threshold energies are indicated below the lower spectrum.

Metastable Excitation Function in Kr

Experiment: Buckman *et al* (1983), multiplied by 0.67

Theories: 31-state Breit-Pauli R-matrix (Zeman & Bartschat 1998)
51-state Breit-Pauli R-matrix (Bartschat & Grum-Grzhimailo 2000)
49-state Breit-Pauli B-spline R-matrix

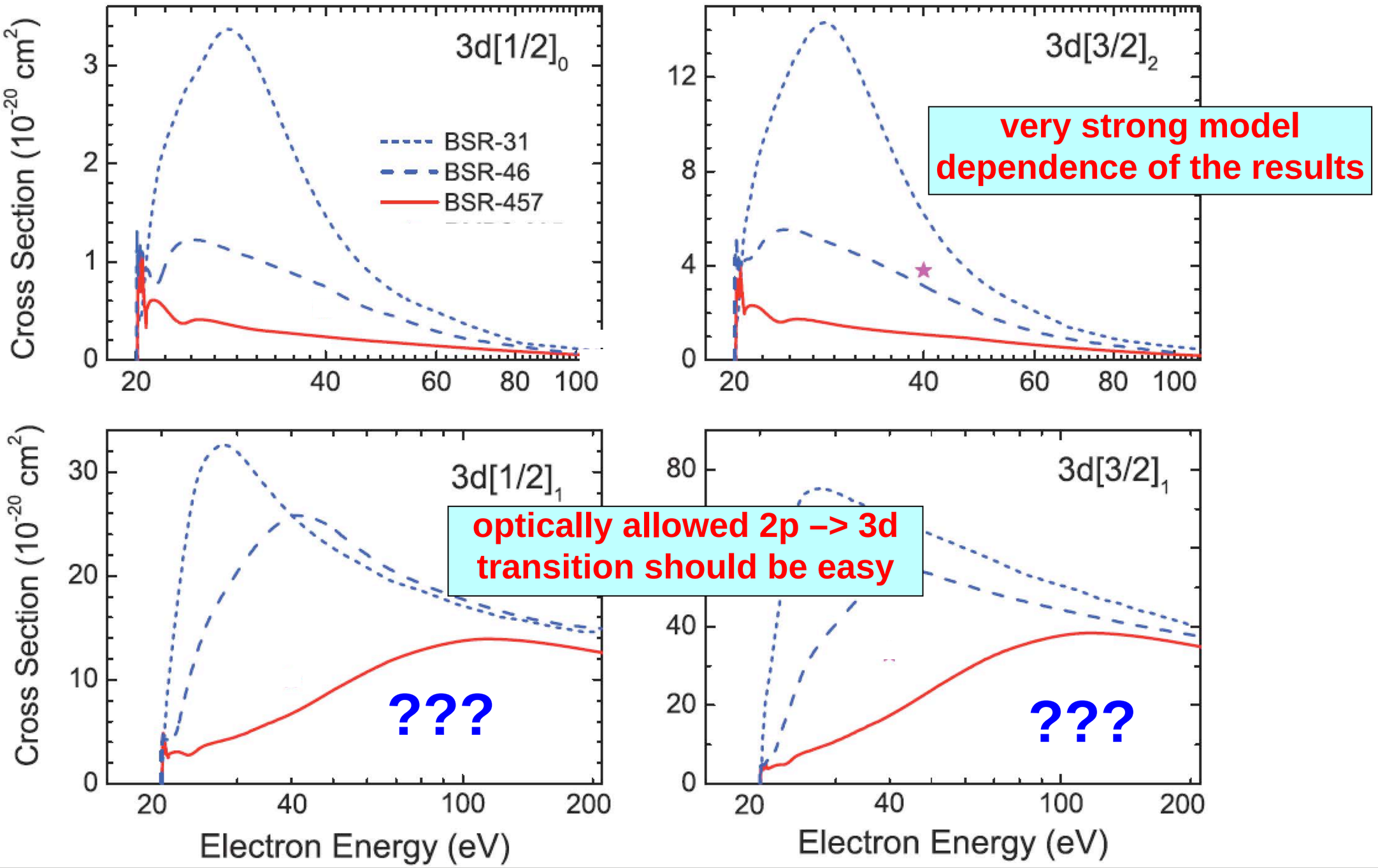


PHYSICAL REVIEW A **86**, 022717 (2012)

Electron-impact excitation of neon at intermediate energies

Oleg Zatsarinny and Klaus Bartschat

BIG SURPRISE (discovered through a GEC collaboration):
This is not what I learned in "Introduction to Atomic Collision Theory".



Collisions at "intermediate energies":
Coupling to the continuum can be very, very important.

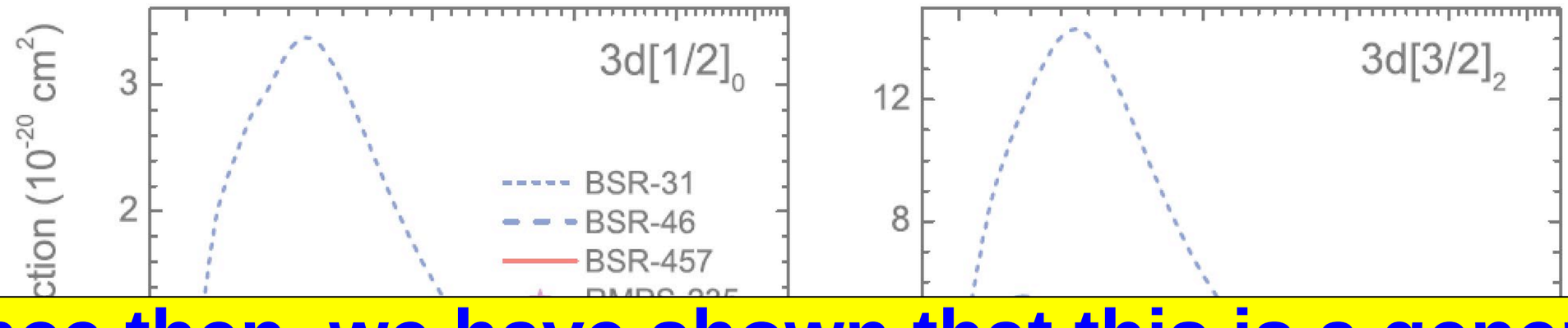
PHYSICAL REVIEW A **86**, 022717 (2012)

Electron-impact excitation of neon at intermediate energies

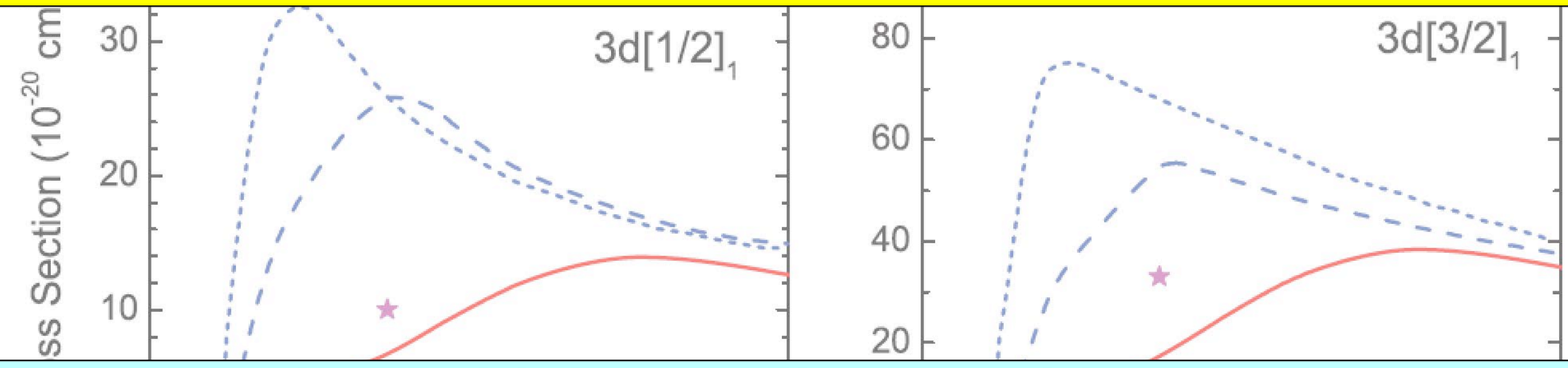
Oleg Zatsarinny and Klaus Bartschat

Department of Physics and Astronomy, Drake University, Des Moines, Iowa 50311, USA

(Received 18 July 2012; published 30 August 2012)



Since then, we have shown that this is a general problem in electron collisions with outer p-shell targets (e.g., C, N, F, Cl, Ar).



Convergence and sensitivity studies provide a systematic way to assign some uncertainty to theoretical predictions, which is becoming an increasingly "hot" topic. (PRA editorial 2011, IAEA/ITAMP workshop 2014, IAEA 2016, ...)

Ionization in the Close-Coupling Formalism

- **Recall: We are interested in the ionization process**

$$e_0(\boldsymbol{k}_0, \mu_0) + A(L_0, M_0; S_0, M_{S_0}) \rightarrow e_1(\boldsymbol{k}_1, \mu_1) + e_2(\boldsymbol{k}_2, \mu_2) + A^+(L_f, M_f; S_f, M_{S_f})$$

- **We need the ionization amplitude**

$$f(L_0, M_0, S_0; \boldsymbol{k}_0 \rightarrow L_f, M_f, S_f; \boldsymbol{k}_1, \boldsymbol{k}_2)$$

- **We employ the *B*-spline *R*-matrix method of Zatsarinny (CPC 174 (2006) 273) with a large number of pseudo-states:**
  - **These pseudo-states simulate the effect of the continuum.**
  - **The scattering amplitudes for excitation of these pseudo-states are used to form the ionization amplitude:**

This detour and direct projection is the essential idea – we'll see if it works.

$$f(L_0, M_0, S_0; \boldsymbol{k}_0 \rightarrow L_f, M_f, S_f; \boldsymbol{k}_1, \boldsymbol{k}_2) = \sum_p \langle \Psi_f^{\boldsymbol{k}_2 -} | \Phi(L_p S_p) \rangle \; f(L_0, M_0, S_0; \boldsymbol{k}_0 \rightarrow L_p, M_p, S_p; \boldsymbol{k}_{1p}).$$

for full disclosure ...

Ionization amplitudes in electron-hydrogen collisions

I. Bray, C. J. Guilfoile, A. S. Kadyrov, D. V. Fursa, and A. T. Stelbovics
ARC Centre for Antimatter-Matter Studies, Curtin University, GPO Box U1987, Perth, WA 6845, Australia
(Received 3 June 2014; published 15 August 2014)

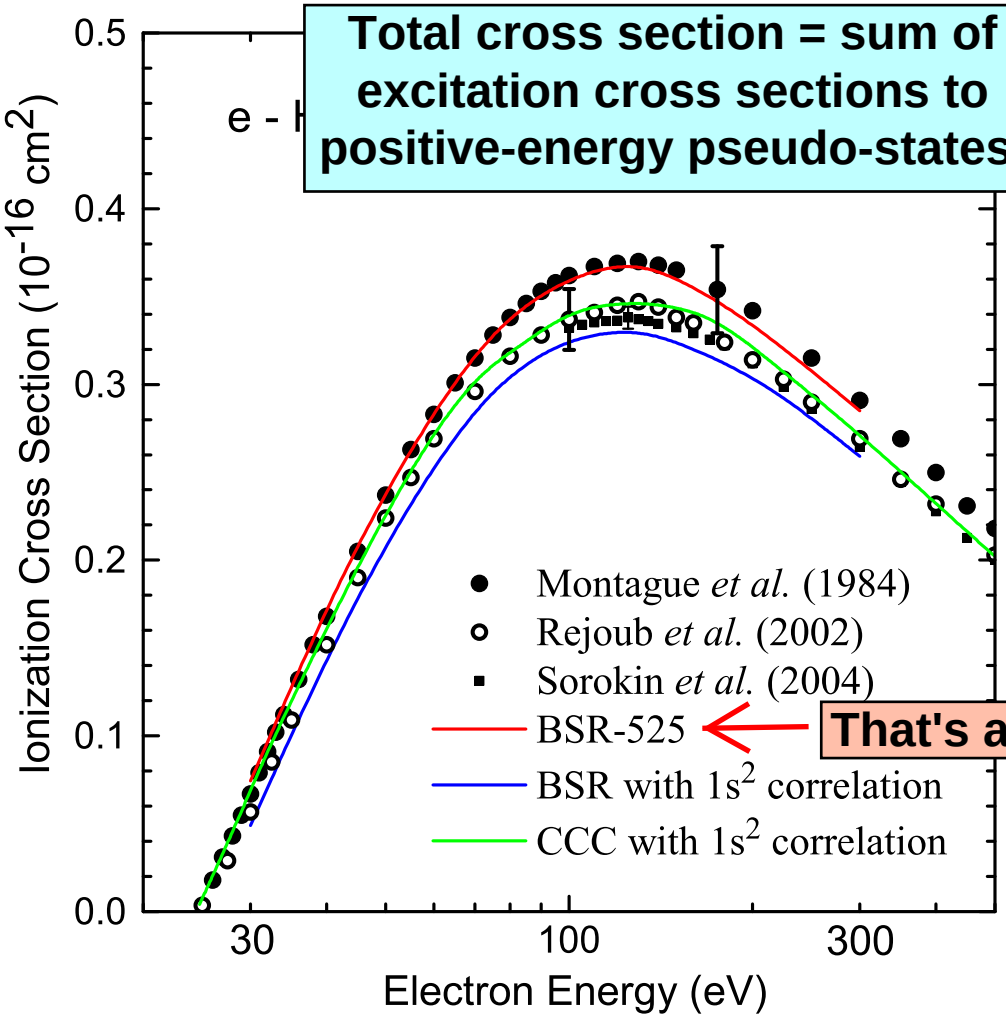
Recently Zatsarinny and Bartschat [Phys. Rev. Lett. **107**, 023203 (2011)] have given an ansatz for extracting ionization amplitudes from close-coupling calculations of electron-impact ionization of atoms. They applied it with extraordinary success to a fully differential cross section of electron-helium single ionization leaving the residual ion in an $n = 2$ state. By considering electron-impact ionization of atomic hydrogen we explain the origin of the ansatz and show that it forms an effective interpolation scheme for determining the amplitudes, so long as the pseudostate energy distribution is sufficiently dense.

In the Conclusions, it is stated:
[W]e believe the ansatz presented by Zatsarinny and Bartschat [13] is in effect a useful interpolation procedure for generating ionization amplitudes at any secondary energy, but it has no formal origin ...

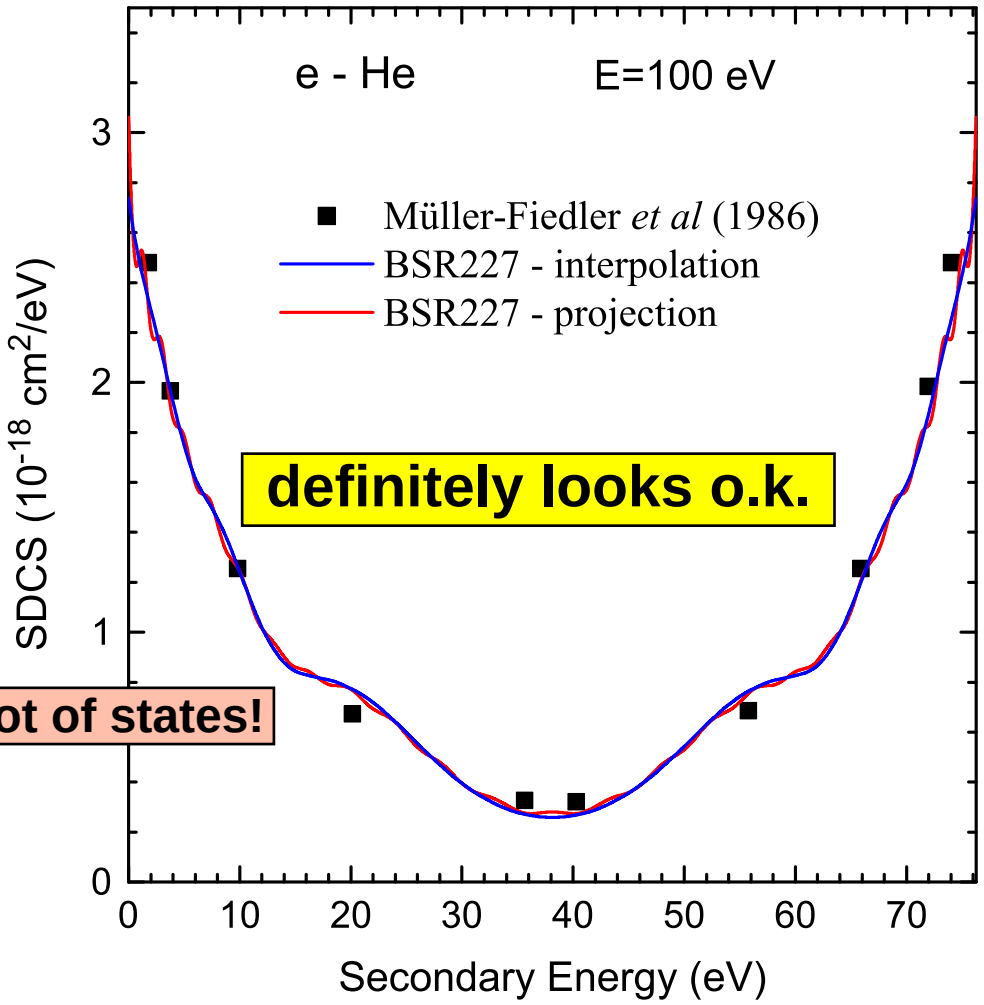
Some Checks: Ionization without Excitation (compare to CCC and TDCC)

Total and Single-Differential Cross Section

Total cross section = sum of excitation cross sections to positive-energy pseudo-states.



That's a lot of states!



definitely looks o.k.

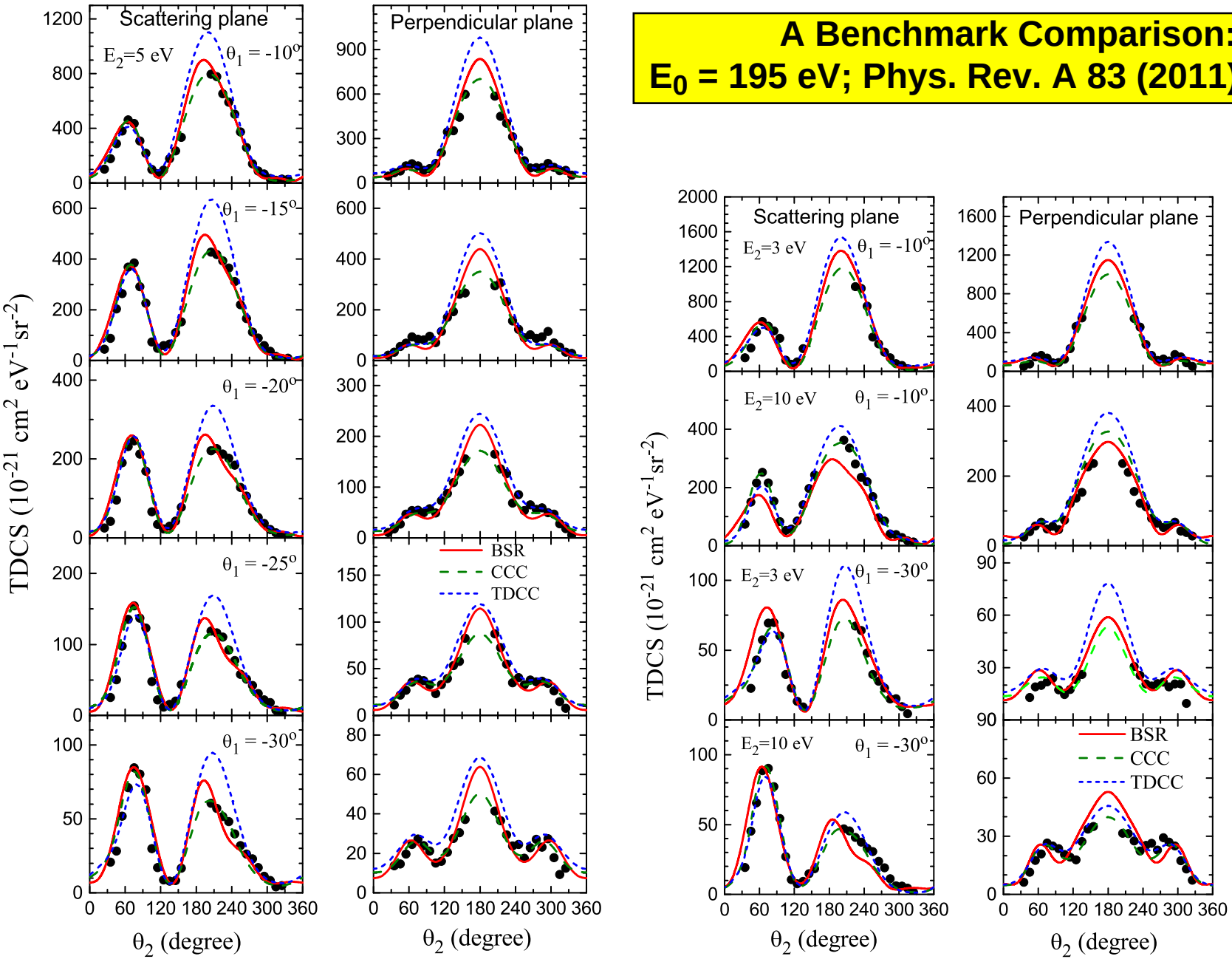
- **Including correlation in the ground state reduces the theoretical result.**
- **Interpolation yields smoother result, but direct projection is acceptable.**
- **DIRECT PROJECTION is NECESSARY for MULTI-CHANNEL cases!**

So far, so good ... Let's go for more detail!

Triple-Differential Cross Section for Direct Ionization

experiment: Ren et al. (2011)

A Benchmark Comparison:
E_0 = 195 eV; Phys. Rev. A 83 (2011) 052711

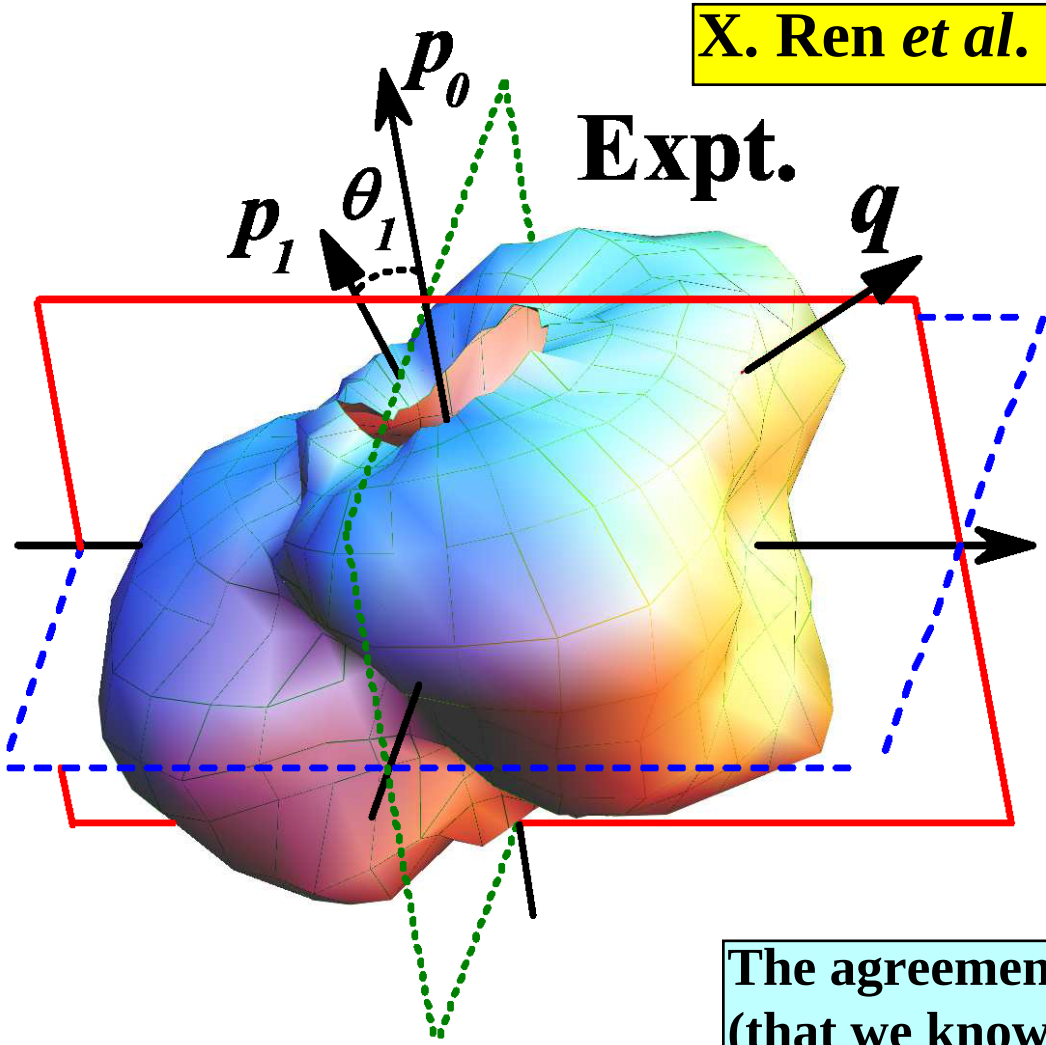


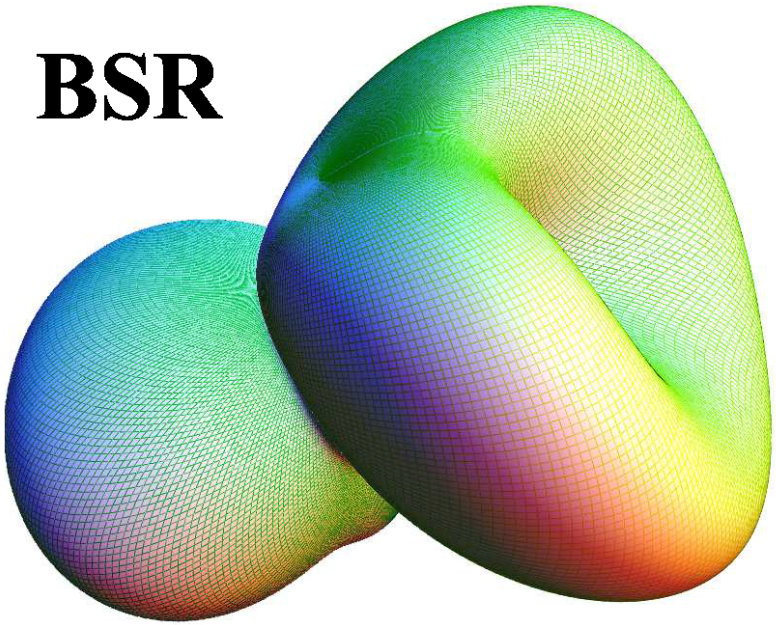
(e,2e) on Ar is a very l .. o .... n ..... g story. It includes the discovery of an error in the processing of the raw experimental data, which was found by the confidence gained in BSR predictions ...

The latest: (e,2e) on Ar ($3p^6$)

E_0 = 66 eV; E_1 = 47 eV; E_2 = 3 eV; $\theta_1 = 15^o$

X. Ren *et al*. (Phys. Rev. A 93 (2016) 062704)





The agreement is not perfect, but no other theory (that we know of) gets anywhere near experiment.

No More Spectators:

Ionization with Excitation of Helium

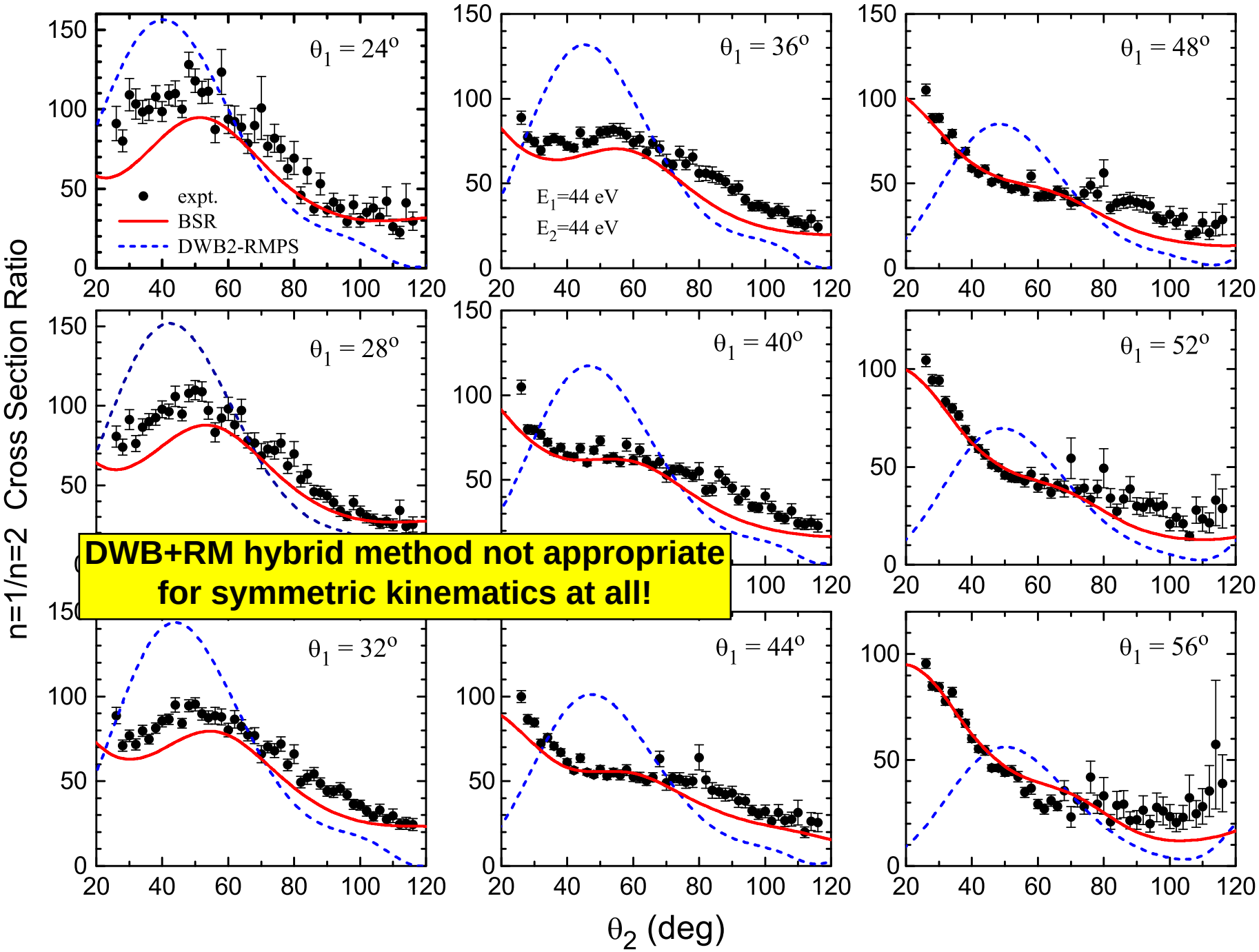
All Three Electrons Change Their Quantum State

(Movie by Allison Harris, Illinois State University)

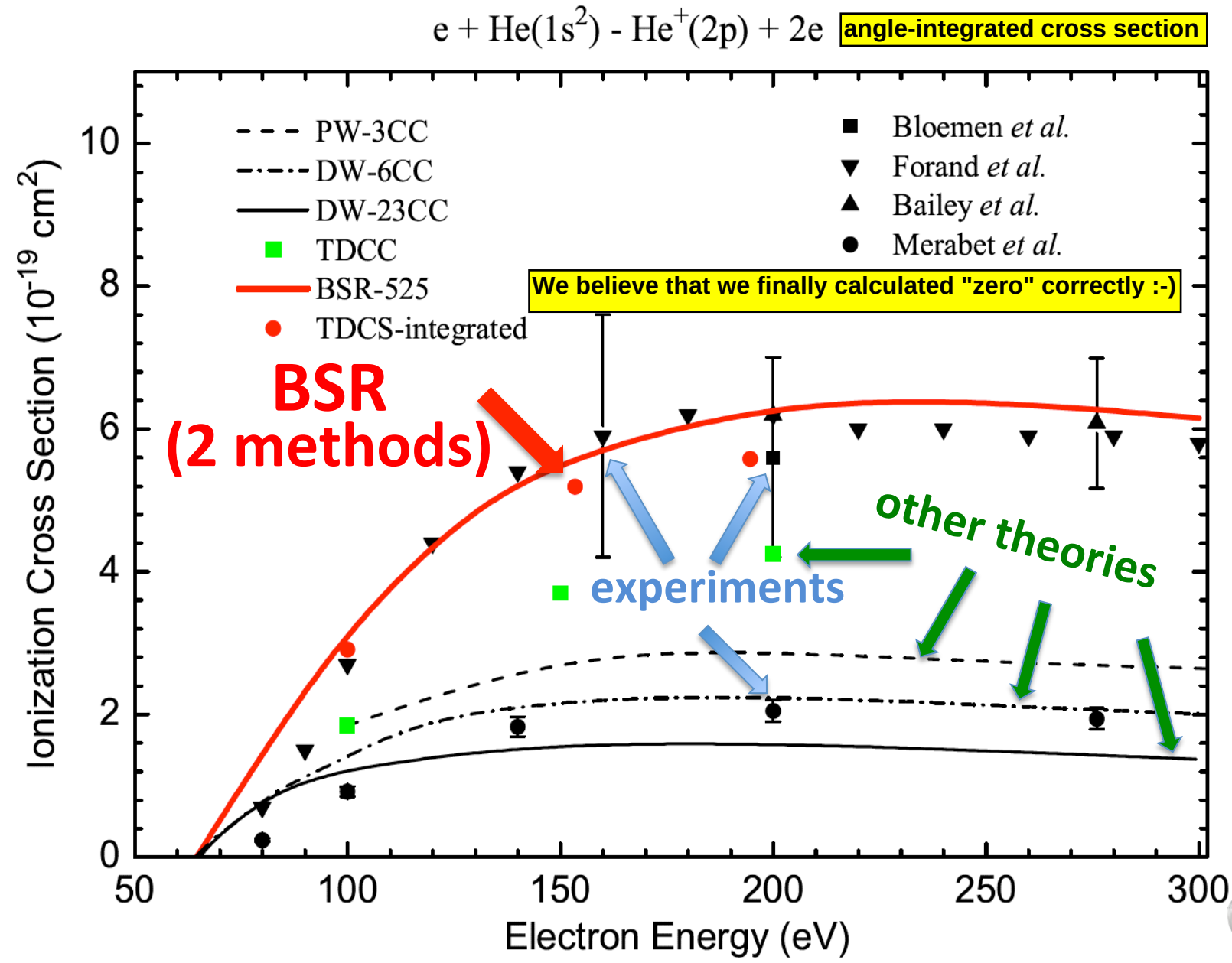
BSRMPS works great: PRL 107 (2011) 023203

Triple-Differential Cross Section Ratio

experiment: Bellm, Lower, Weigold; measured directly



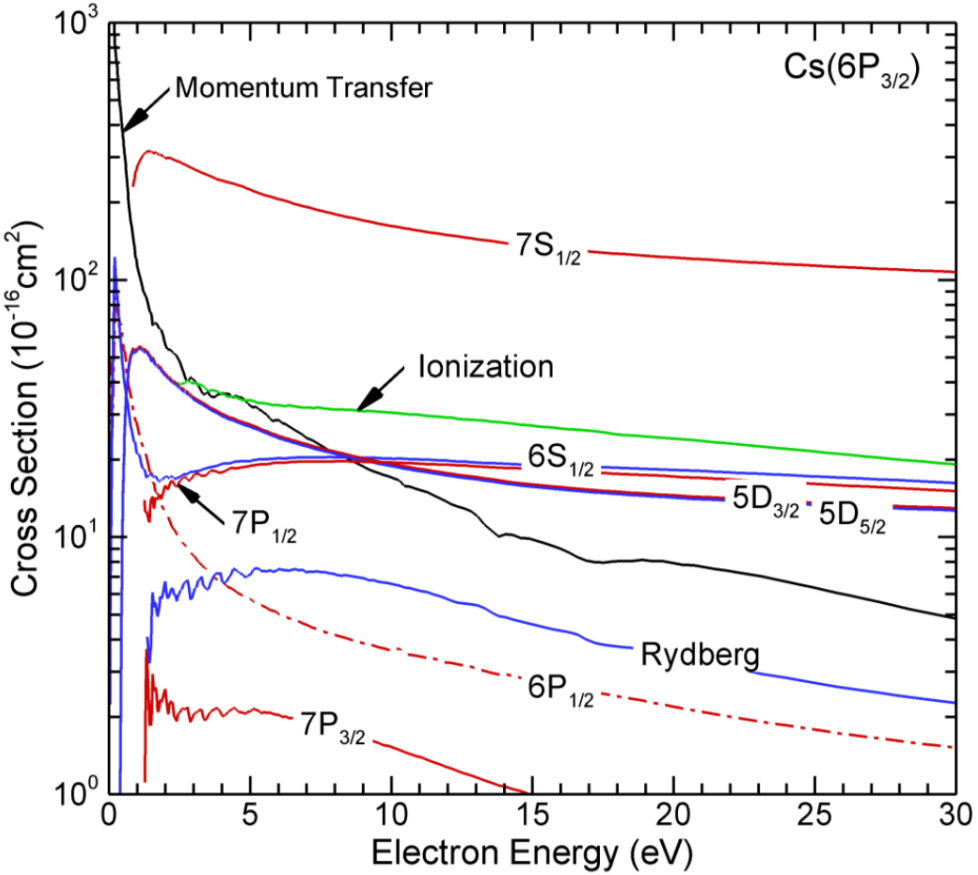
DWB+RM hybrid method not appropriate for symmetric kinematics at all!


e + He(1s²) - He⁺(2p) + 2e
angle-integrated cross section
PW-3CC
DW-6CC
DW-23CC
TDCC
BSR-525
TDCS-integrated
Bloemen et al.
Forand et al.
Bailey et al.
Merabet et al.
We believe that we finally calculated "zero" correctly :-)
BSR
(2 methods)
other theories
experiments
Ionization Cross Section (10⁻¹⁹ cm²)
Electron Energy (eV)
0
2
4
6
8
10
50
100
150
200
250
300

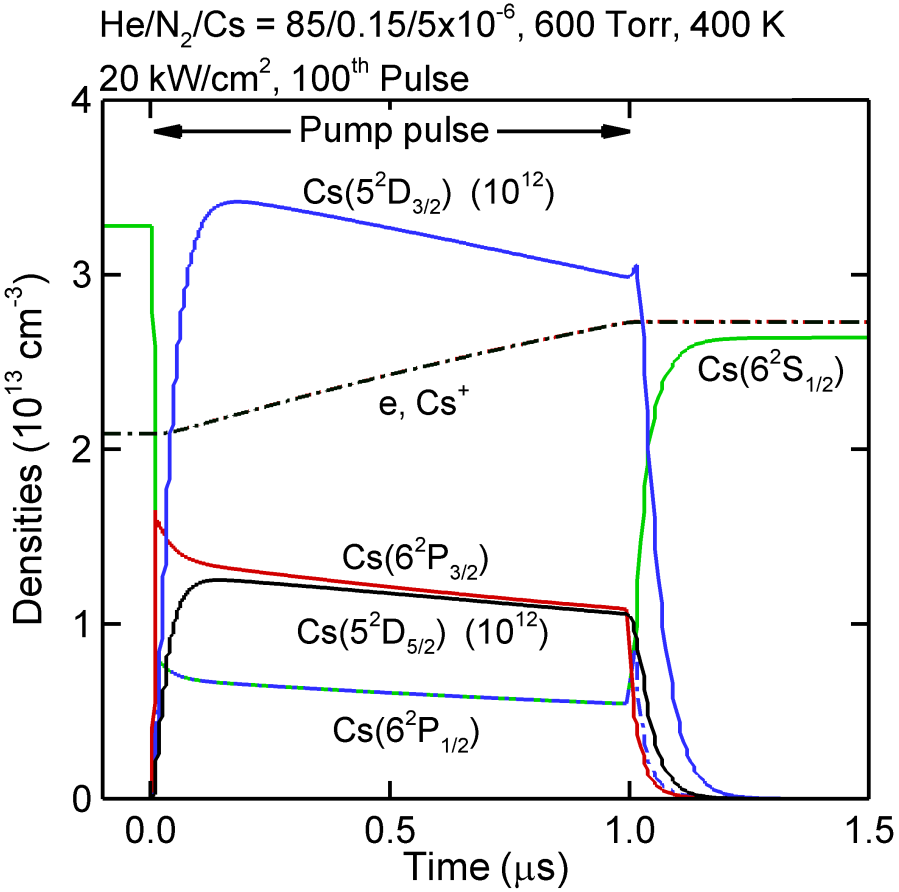
Closing the Loop:
Collision Input —> Modeling Output —> System Information

Modeling a Cs-based DPAL

Input: DBSR cross sections



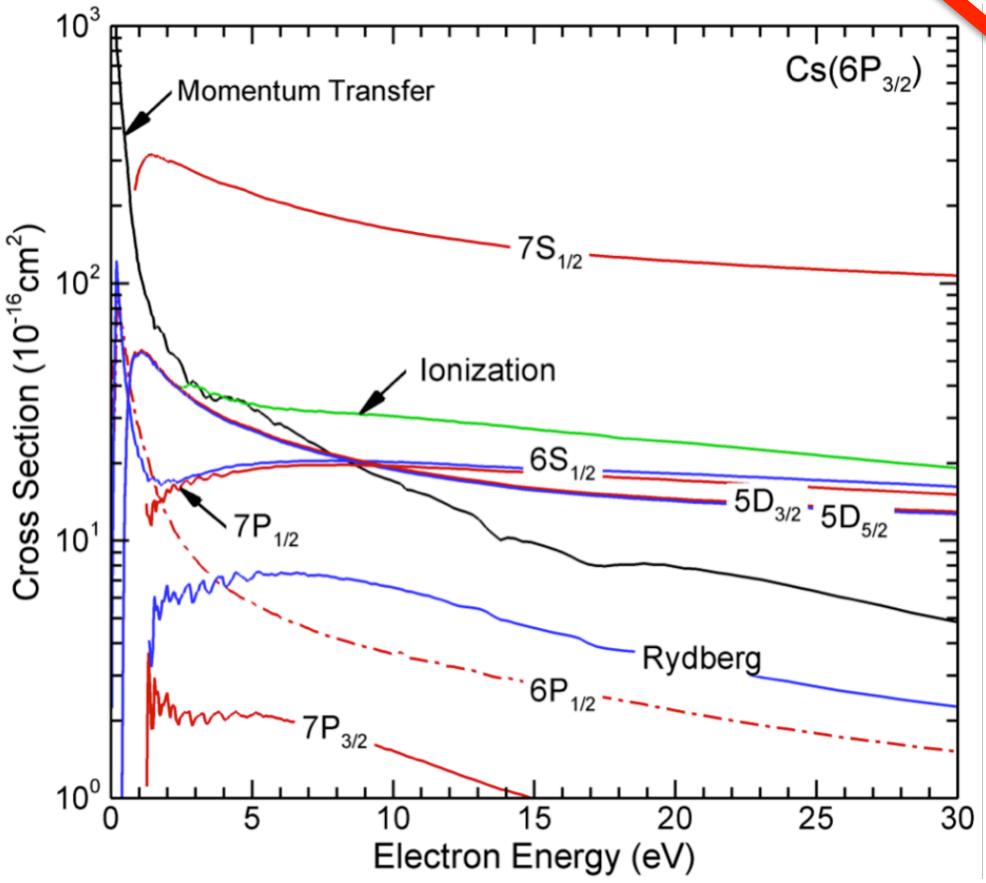
Output (M. J. Kushner's group): Densities of various species



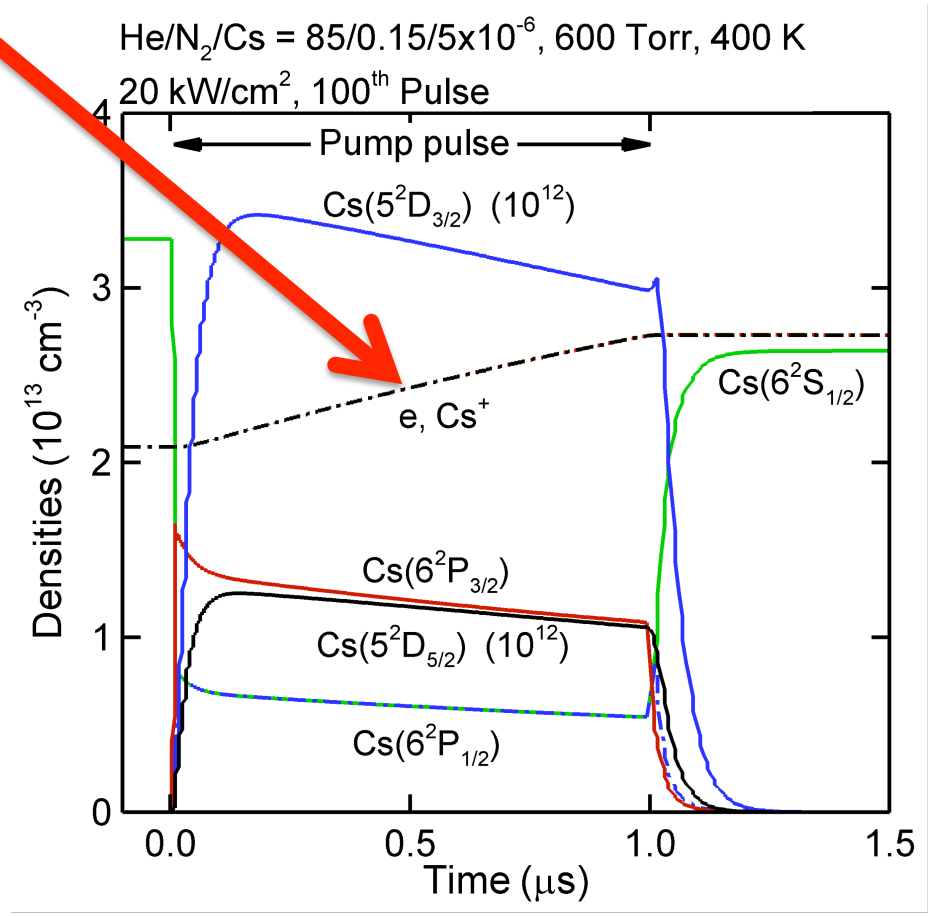
Modeling a Cs-based DPAL

Information: There is significant plasma formation after a number of shots. This reduces the length of the pump pulse due to depletion of the neutral levels.

Input: DBSR cross sections

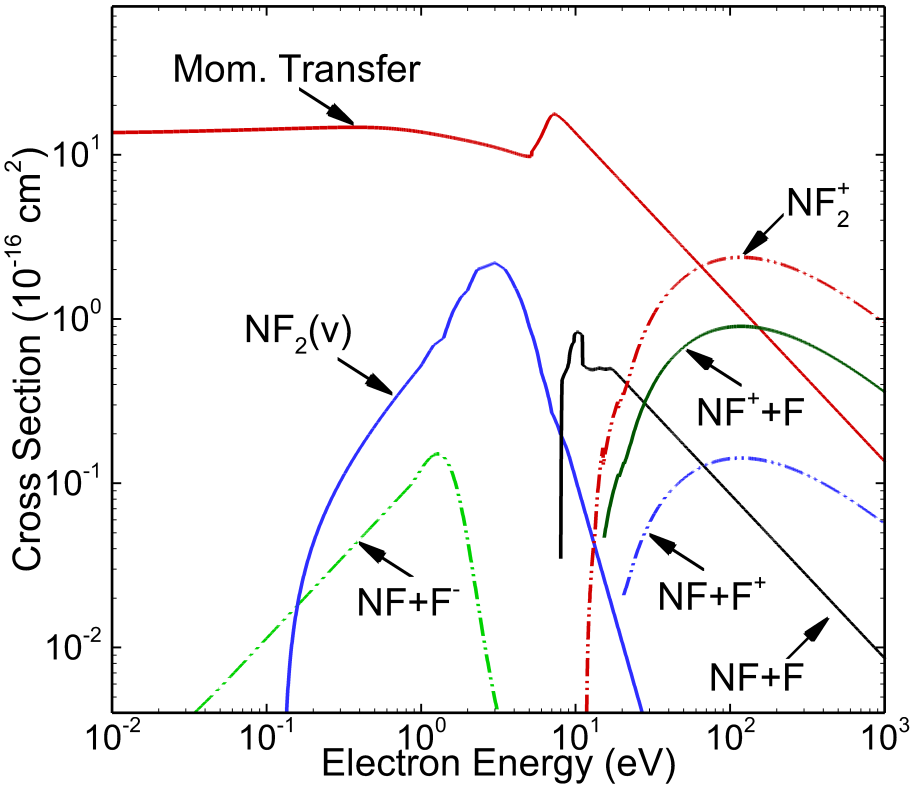


Output (M. J. Kushner's group): Densities of various species

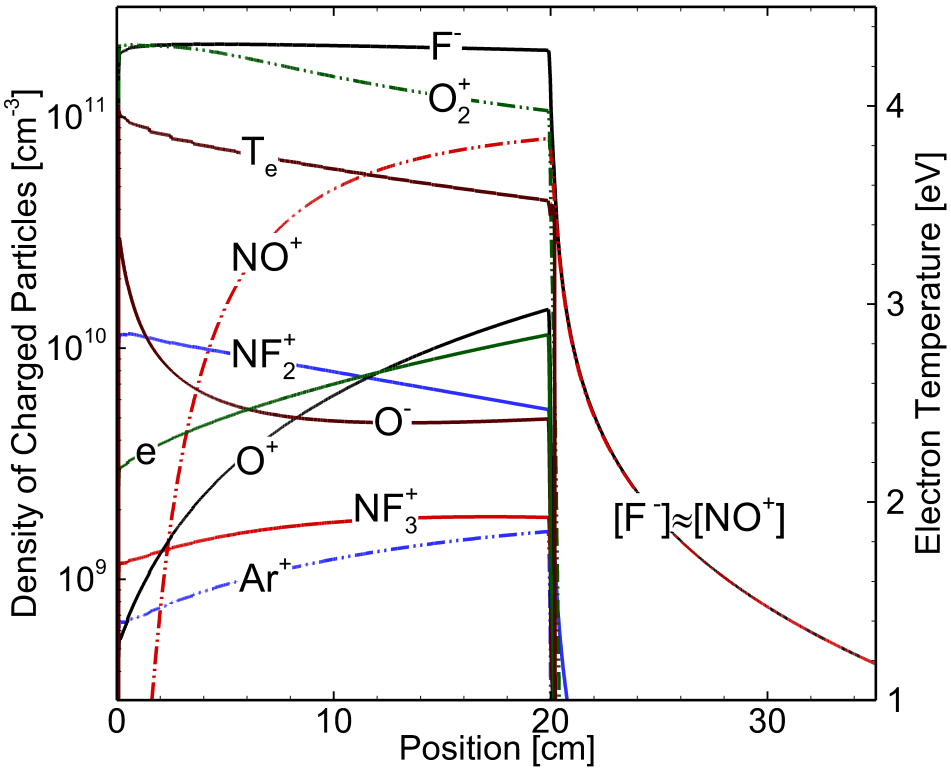


Remote plasma etching using an $Ar/NF_3/O_2$ mixture

Input from J. Tennyson's group:
Many cross sections, including those for e-NF_2 (not available from experiment)



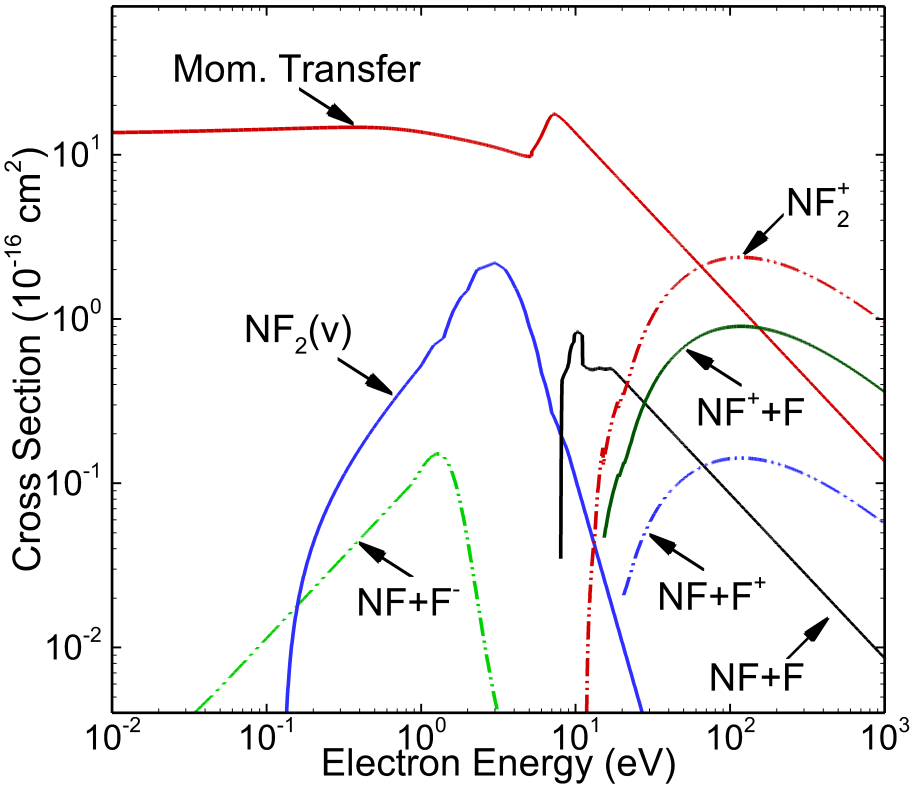
Output (M. J. Kushner's group):
Densities of various species



Remote plasma etching using an $Ar/NF_3/O_2$ mixture

Information: These results are being used to choose the most effective feedstock gases.Then optimize their mixture and other plasma parameters.

Input from J. Tennyson's group:
Many cross sections, including those for e-NF_2 (not available from experiment)



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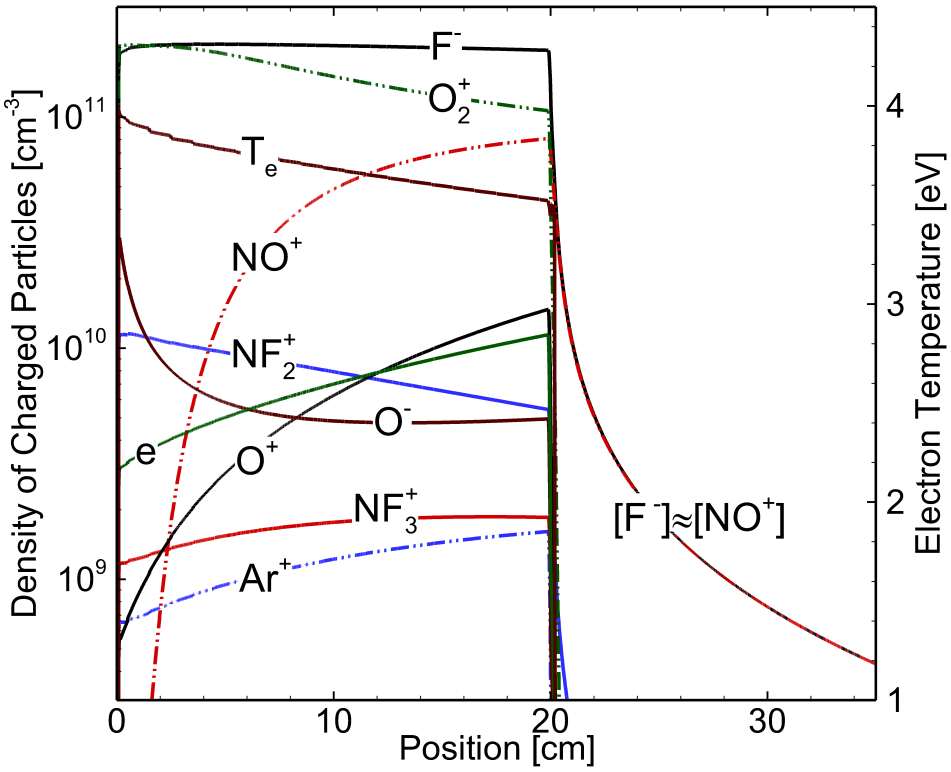
Densities of various species



Conclusions and Outlook

- **Despite the field's maturity, significant innovations are constantly being made to study electron collisions with atoms and molecules – and they are needed!**
- **There exist many fruitful collaborations between experimentalists, theorists, and users outside of AMO who need (and use) these data.**
- **Experimental benchmark data remain very important to test and push theory!**
- **With such benchmark data and comparisons between predictions from highly sophisticated methods in hand, we can finally estimate uncertainties of these predictions.**

IOP Publishing Journal of Physics D: Applied Physics

J. Phys. D: Appl. Phys. **49** (2016) 363002 (27pp) doi:10.1088/0022-3727/49/36/363002

Topical Review

Uncertainty estimates for theoretical atomic and molecular data

See also:
The Editors 2011 Phys. Rev. A 83 040001

H-K Chung[1], B J Braams[1], K Bartschat[2], A G Császár[3], G W F Drake[4], T Kirchner[5], V Kokoouline[6] and J Tennyson[7]

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[2] Department of Physics and Astronomy, Drake University, Des Moines, IA, 50311, USA
[3] MTA-ELTE Complex Chemical Systems Research Group, H-1118 Budapest, Pázmány sétány 1/A, Hungary
[4] Department of Physics, University of Windsor, Windsor, Ontario N9B 3P4, Canada
[5] Department of Physics and Astronomy, York University, Toronto, Ontario M3J 1P3, Canada
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Published 17 August 2016

Abstract

Sources of uncertainty are reviewed for calculated atomic and molecular data that are important for plasma modeling: atomic and molecular structures and cross sections for electron-atom, electron-molecule, and heavy particle collisions. We concentrate on model uncertainties due to approximations to the fundamental many-body quantum mechanical equations and we aim to provide guidelines to estimate uncertainties as a routine part of computations of data for structure and scattering.

Conclusions and Outlook

- **Despite the field's maturity, significant innovations are constantly being made to study electron collisions with atoms and molecules – and they are needed!**
- **There exist many fruitful collaborations between experimentalists, theorists, and users outside of AMO who need (and use) these data.**
- **Experimental benchmark data remain very important to test and push theory!**
- **With such benchmark data and comparisons between predictions from highly sophisticated methods in hand, we can finally estimate uncertainties of these predictions.**
- **Although we usually need supercomputers to get a reliable answer, there is room for interpretation of the physics. $\rightarrow$ Propensity in equal-energy sharing (e,2e).**

Propensity for distinguishing two free electrons with equal energies in electron-impact ionization of helium

Xueguang Ren,[1,2,*] Arne Senftleben,[2,3] Thomas Pflüger,[2] Klaus Bartschat,[4] Oleg Zatsarinny,[4] Jamal Berakdar,[5] James Colgan,[6] Michael S. Pindzola,[7] Igor Bray,[8] Dmitry V. Fursa,[8] and Alexander Dorn[2]

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[4]*Department of Physics and Astronomy, Drake University, Des Moines, Iowa 50311, USA*

[5]*Institut für Physik, Martin-Luther Universität Halle-Wittenberg, D-06099 Halle/Saale, Germany*

[6]*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

[7]*Department of Physics, Auburn University, Auburn, Alabama 36849, USA*

[8]*Curtin Institute for Computation and Department of Physics and Astronomy, Curtin University, GPO Box U1987, Perth WA6845, Australia*

(Received 27 August 2015; published 16 November 2015)

We report a combined experimental and theoretical study on the electron-impact ionization of helium at $E_0 = 70.6$ eV and equal energy sharing of the two outgoing electrons ($E_1 = E_2 = 23$ eV), where a double-peak or dip structure in the binary region of the triple differential cross section is observed. The experimental cross sections are compared with results from convergent close-coupling (CCC), *B*-spline *R*-matrix-with-pseudostates (BSR), and time-dependent close-coupling (TDCC) calculations, as well as predictions from the dynamic screening three-Coulomb (DS3C) theory. Excellent agreement is obtained between experiment and the nonperturbative CCC, BSR, and TDCC theories, and good agreement is also found for the DS3C model. The data are further analyzed regarding contributions in particular coupling schemes for the spins of either the two outgoing electrons or one of the outgoing electrons and the 1*s* electron remaining in the residual ion. While both coupling schemes can be used to explain the observed double-peak structure in the cross section, the second one allows for the isolation of the exchange contribution between the incident projectile and the target. For different observation angles of the two outgoing electrons, we interpret the results as a propensity for distinguishing these two electrons—one being more likely the incident projectile and the other one being more likely ejected from the target.

DOI: 10.1103/PhysRevA.92.052707 PACS number(s): 34.80.Dp

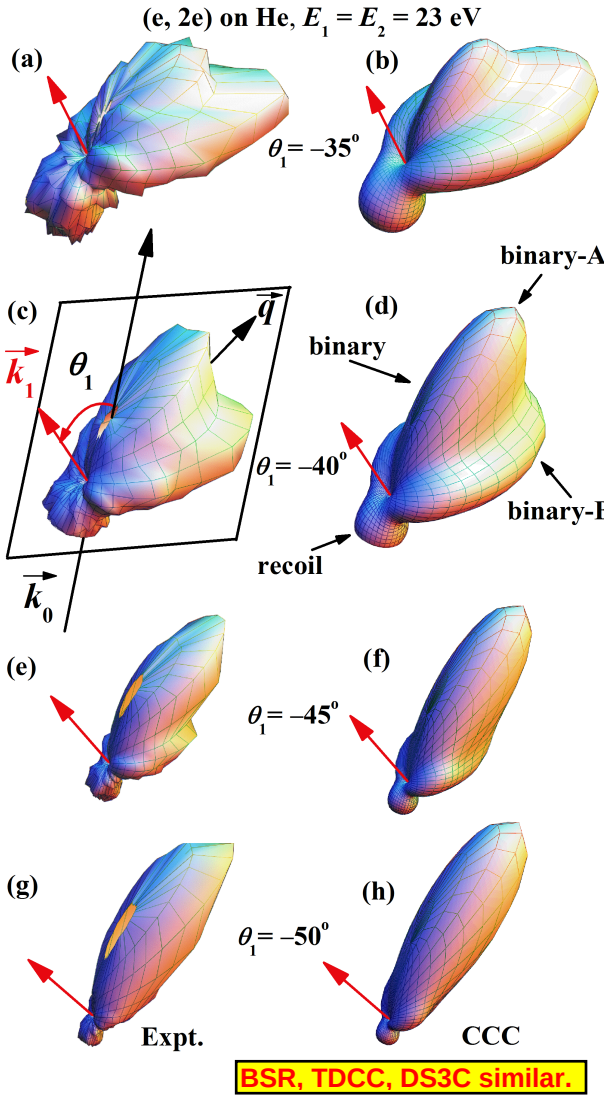
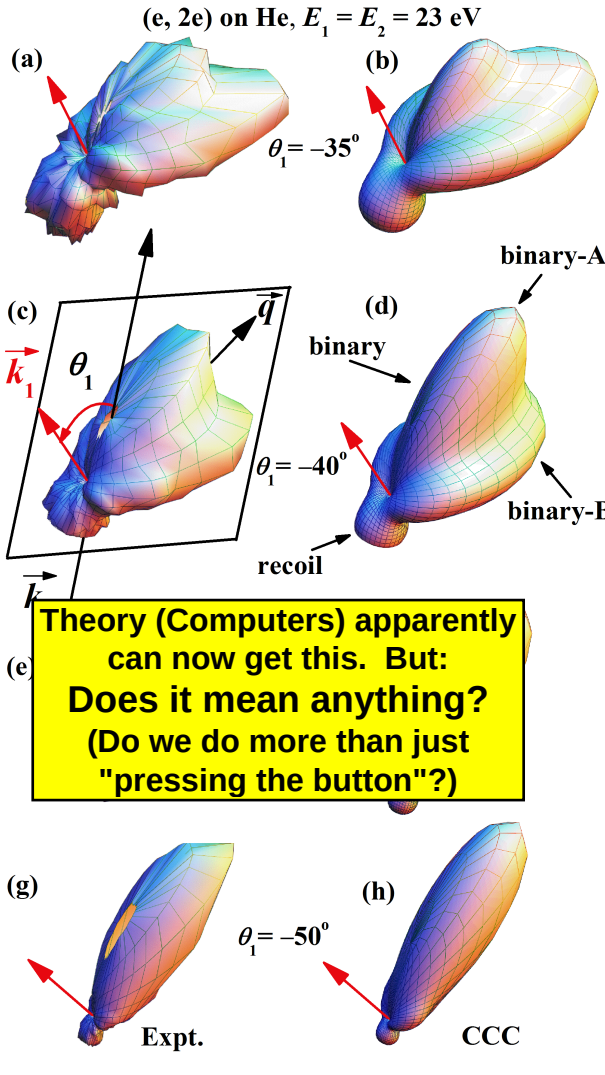


FIG. 2. (color online) Three-dimensional (3D) representation of the TDCS for $(e, 2e)$ on He at equal energy sharing ($E_1 = E_2 = 23$ eV) as a function of the emission angle θ_2 of one electron with the other electron's detection angle θ_1 being fixed to: (a) and (b) $\theta_1 = -35°$; (c) and (d) $\theta_1 = -40°$; (e) and (f) $\theta_1 = -45°$; (g) and (h) $\theta_1 = -50°$. Left column: experiment. Right column: CCC calculation.



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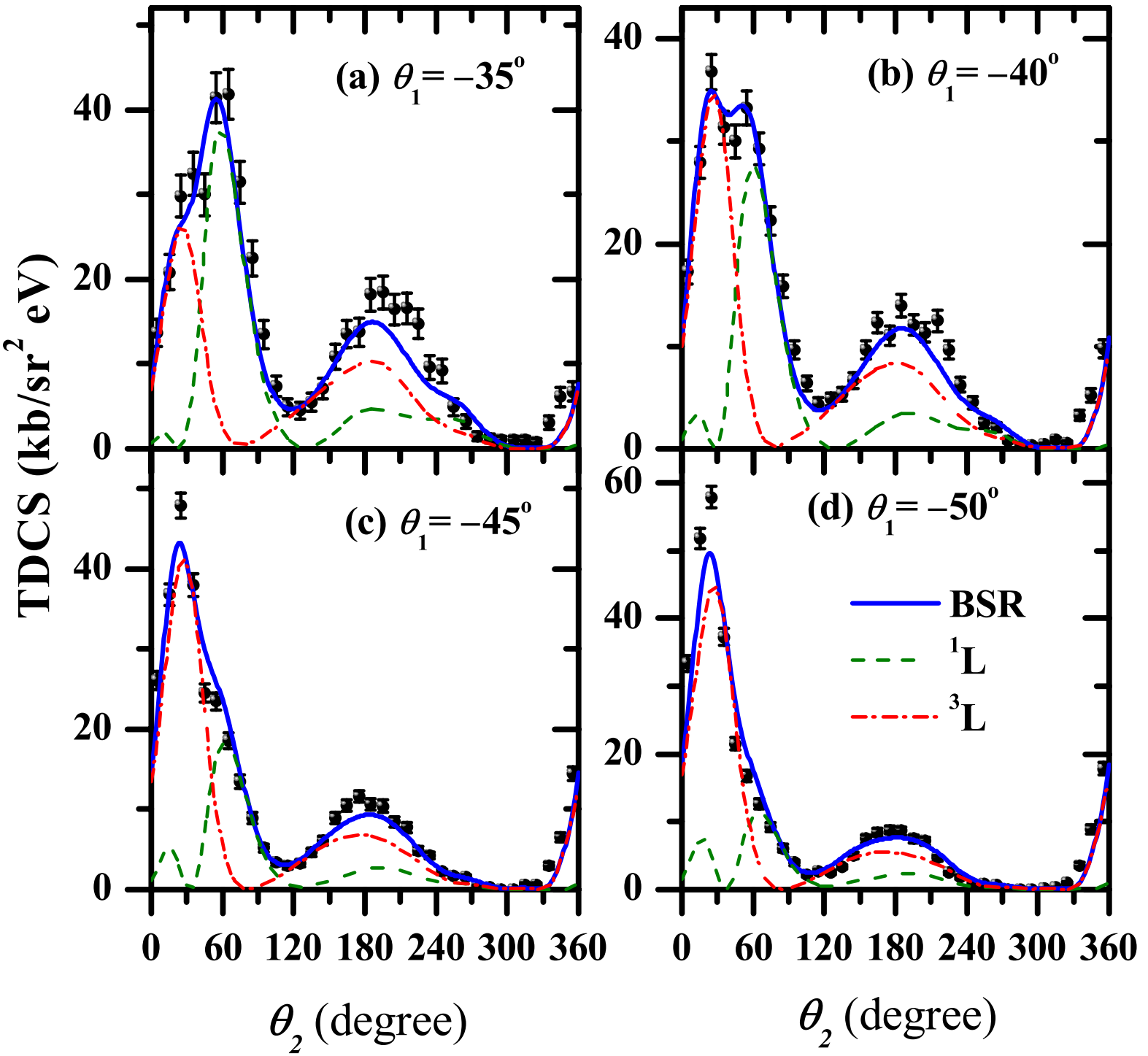

Physical Interpretation: Even though both outgoing electrons have the same energy, one can assign a propensity to which peak is made by the projectile!?!? If you do not believe this, please read the paper.

Conclusions and Outlook

- **Despite the field's maturity, significant innovations are constantly being made to study electron collisions with atoms and molecules – and they are needed!**
- **There exist many fruitful collaborations between experimentalists, theorists, and users outside of AMO who need (and use) these data.**
- **Experimental benchmark data remain very important to test and push theory!**
- **With such benchmark data and comparisons between predictions from highly sophisticated methods in hand, we can finally estimate uncertainties of these predictions.**
- **Although we usually need supercomputers to get a reliable answer, there is room for interpretation of the physics. → Propensity in equal-energy sharing (e,2e).**
- **Knowledge about electron collisions also helps to understand photon-induced processes, in weak-field, strong-field, steady-state, and time-dependent cases.**

I only have time to show a few title pages, where BSR results were used as input data for such problems.

Time delays for attosecond streaking in photoionization of neon

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We revisit the time-resolved photoemission in neon atoms as probed by attosecond streaking. We calculate streaking time shifts for the emission of $2p$ and $2s$ electrons and compare the relative delay as measured in a recent experiment by Schultze *et al*. [Science **328**, 1658 (2010)]. The B-spline R-matrix method is employed to calculate accurate Eisenbud-Wigner-Smith time delays from multielectron dipole transition matrix elements for photoionization. The additional lase[illegible] parate, time-dependent simulations of a full st[illegible]ion on the single-active-electron level. The re[illegible]nd $2p$ emission lie well below the experimental data. We identify the presence of unresolved shake-up satellites in the experiment as a potential source of error in the determination of streaking time shifts.

closing a potential loop-hole through accurate multi-electron dipole matrix elements

PHYSICAL REVIEW A **76**, 053411 (2007)

relevant for current experiments at FELs

General approach to few-cycle intense laser interactions with complex atoms

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A general *ab initio* and nonperturbative method to solve the time-dependent Schrödinger equation (TDSE) for the interaction of a strong attosecond laser pulse with a general atom, i.e., beyond the models of quasi-one-electron or quasi-two-electron targets, is described. The field-free Hamiltonian and the dipole matrices are generated using a flexible *B*-spline *R*-matrix method. This numerical implementation enables us to construct term-dependent, nonorthogonal sets of one-electron orbitals for the bound and continuum electrons. The solution of the TDSE is propagated in time using the Arnoldi-Lanczos method, which does not require the diagonalization of any large matrices. The method is illustrated by an application to the multiphoton excitation and ionization of Ne atoms. Good agreement with *R*-matrix Floquet calculations for the generalized cross sections for two-photon ionization is achieved.

IOP Publishing Journal of Physics B: Atomic, Molecular and Optical Physics

J. Phys. B: At. Mol. Opt. Phys. **42** (2009) 134015 (8pp) doi:10.1088/0953-4075/42/13/134015

A time-dependent *B*-spline *R*-matrix approach to double ionization of atoms by XUV laser pulses

double ionization is very interesting in fundamental AMO physics

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Abstract

We present an *ab initio* and non-perturbative time-dependent approach to the problem of double ionization of a general atom driven by intense XUV laser pulses. After using a highly flexible *B*-spline *R*-matrix method to generate field-free Hamiltonian and electric dipole matrices, the initial state is propagated in time using an efficient Arnoldi–Lanczos scheme. Test calculations for double ionization of He by a single laser pulse yield good agreement with benchmark results obtained with other methods. The method is then applied to two-colour pump–probe processes, for which momentum and energy distributions of the two outgoing electrons are presented.

(Some figures in this article are in colour only in the electronic version)

PHYSICAL REVIEW A **92**, 063427 (2015)

Numerical simulation of the double-to-single ionization ratio for the helium atom in strong laser fields

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We present calculations on the ratio between double and single ionization of helium by a strong laser pulse at a wavelength of 780 nm using the quantitative rescattering (QRS) model. According to this model, the yield for the doubly charged ion He^{2+} can be obtained by multiplying the returning electron wave packet (RWP) with the total cross sections (TCSs) for electron impact ionization and electron impact excitation of He^{+} in the singlet spin channel. The singlet constraint was imposed since the interaction of the helium atom with the laser and the re to ob on for high-energy photoelectrons. The laser field, which lowers the required energy for the electron to escape from the nucleus at the time of recollision, is also taken into account. The simulated results are in good agreement with the measured He^{2+}/He^{+} ratio over a broad range of laser intensities. The result demonstrates that the QRS approach based on the rescattering model is fully capable of quantitatively interpreting nonsequential double ionization processes.

These projects need e-He^{+} (next are Ne^{+} and Ar^{+}) collision data.

The very latest: Electron scattering for quantum state engineering

Entanglement and Bell Correlation in Electron-Exchange Collisions

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Elastic collisions between initially unpolarized electrons and hydrogenlike atoms are discussed, aiming to analyze the entanglement properties of the correlated final spin system. Explicit spin-dependent interactions are neglected and electron exchange only is taken into account. We show the final spin system to be completely characterized by a single spin correlation parameter depending on scattering angle and energy. Its numerical value identifies the final spins of the collision partners to be either in the separable, entangled, or Bell correlated regions. We emphasize explicit examples for the mixed spin system in order to illustrate the abstract concepts. The analysis of published experimental and numerical data reveals the possibility to create tunable pairs of collision partners with any desired degree of spin entanglement.

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Tunable entanglement resource in elastic electron-exchange collisions out of chaotic spin systems

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Elastic collisions between initially unpolarized electrons and hydrogenlike atoms are discussed aiming to analyze the entanglement properties of the correlated final spin system. Explicit spin-dependent interactions are neglected and electron exchange only is taken into account. We show the final spin system to be completely characterized by a single spin correlation parameter depending on scattering angle and energy. Its numerical value identifies the final spins of the collision partners to be either in the separable, entangled, or Bell correlated regions. The symmetry of the scattering process allows for the construction of explicit examples applying methods of classical communication and local operations for illustrating the concepts of nonlocality versus separability. It is shown that strong correlations can be produced violating Bell's inequalities significantly. Furthermore, the degree of entanglement can be continuously varied simply by changing either the scattering angle and/or energy. This allows for the generation of tunable spin pairs with any desired degree of entanglement. It is suggested to use such nonlocally entangled spin pairs as a resource for further experiments, for example in quantum information processes.

DOI: 10.1103/PhysRevA.94.032331

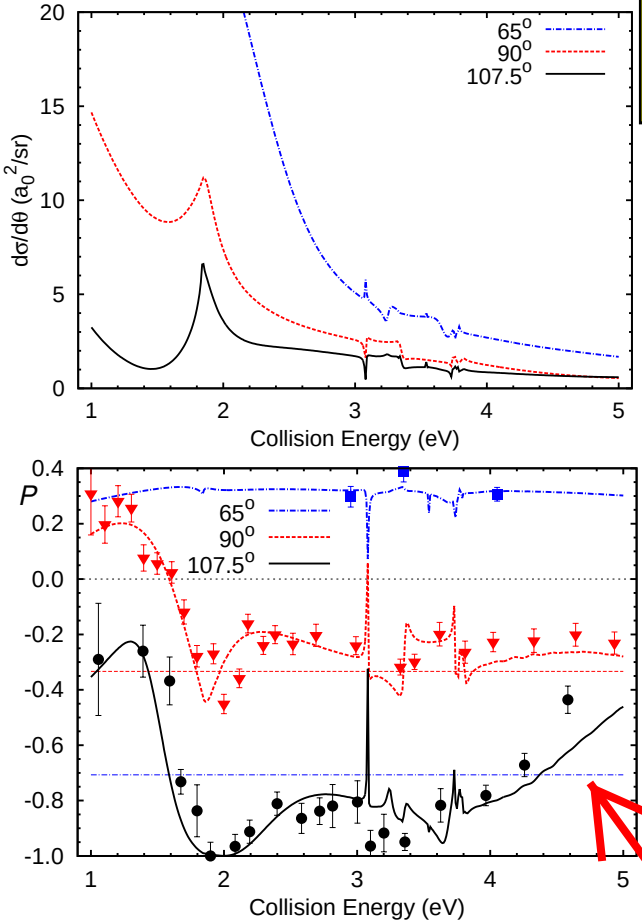


FIG. 1: Differential cross section (top) and spin correlation parameter P (bottom) for elastic electron scattering from Li atoms as a function of energy at scattering angles of $65°$, $90°$, and $107.5°$. The lines at $-1/3$ and $-1/\sqrt{2}$ in the panel for P mark the borders between separable and entangled as well as entangled and Bell-correlated regions, respectively. The experimental data for $P = -A_{\rm ex}$ are taken from Baum *et al.* [3].

5-state close-coupling for e-Li scattering is good enough here!

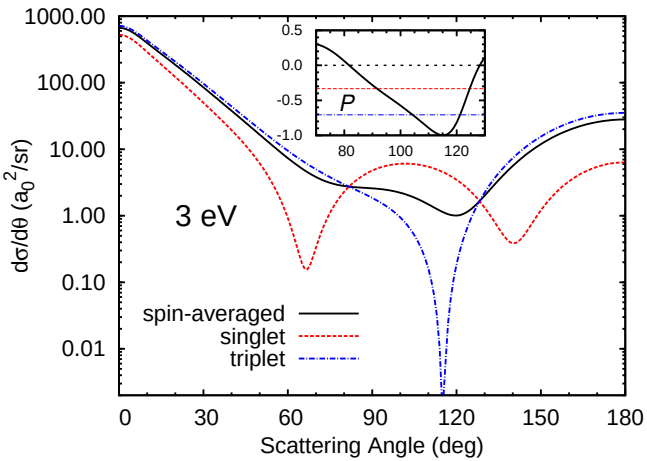
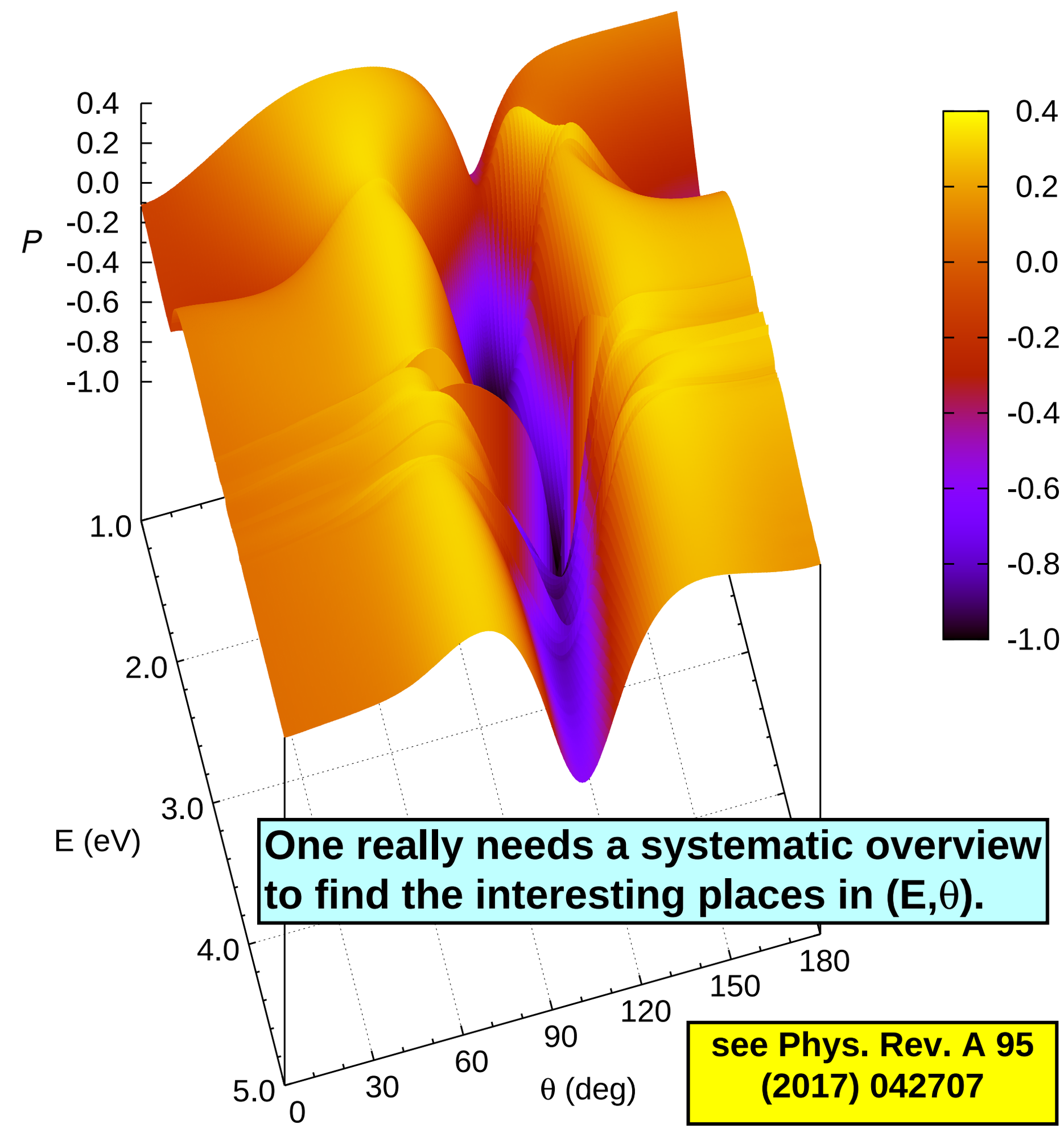
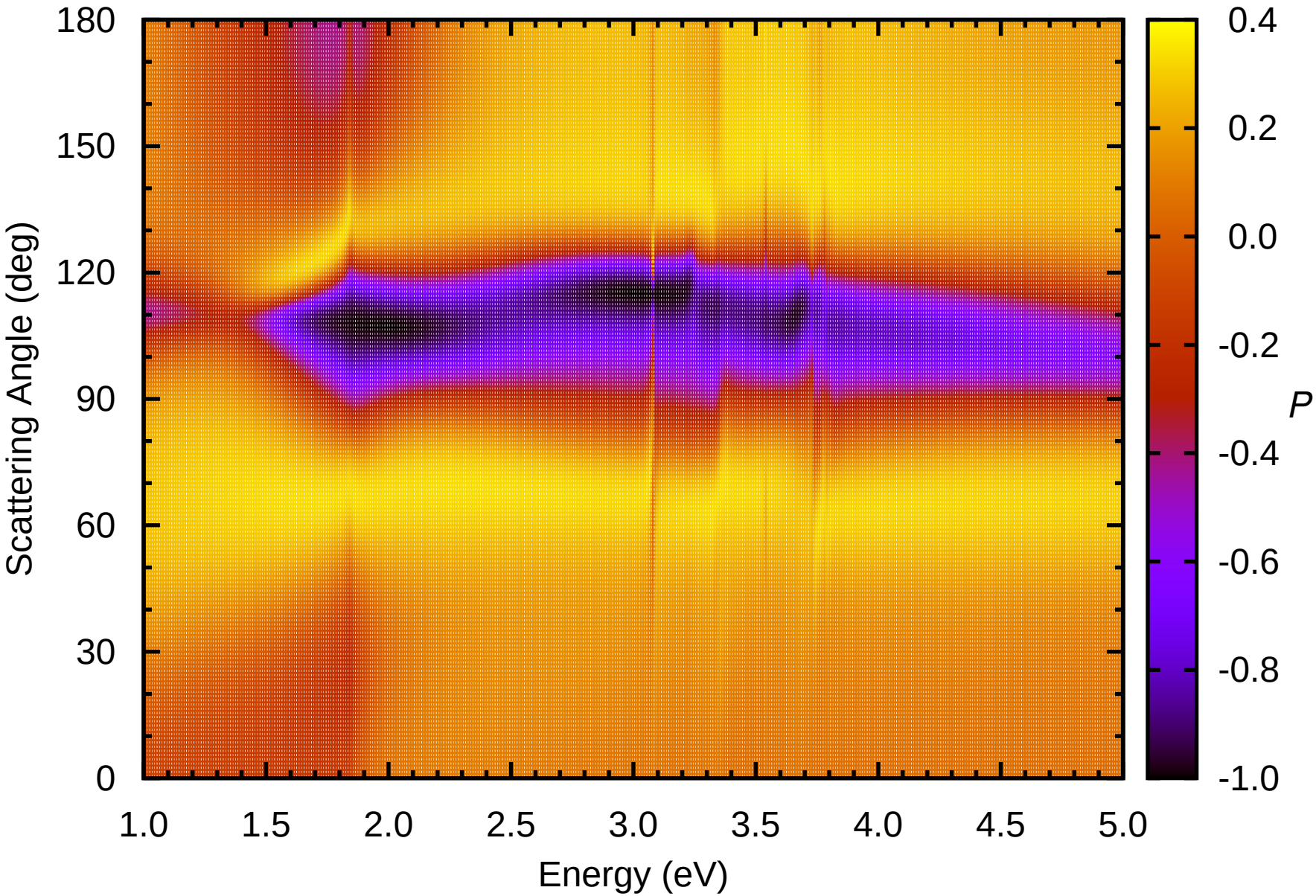


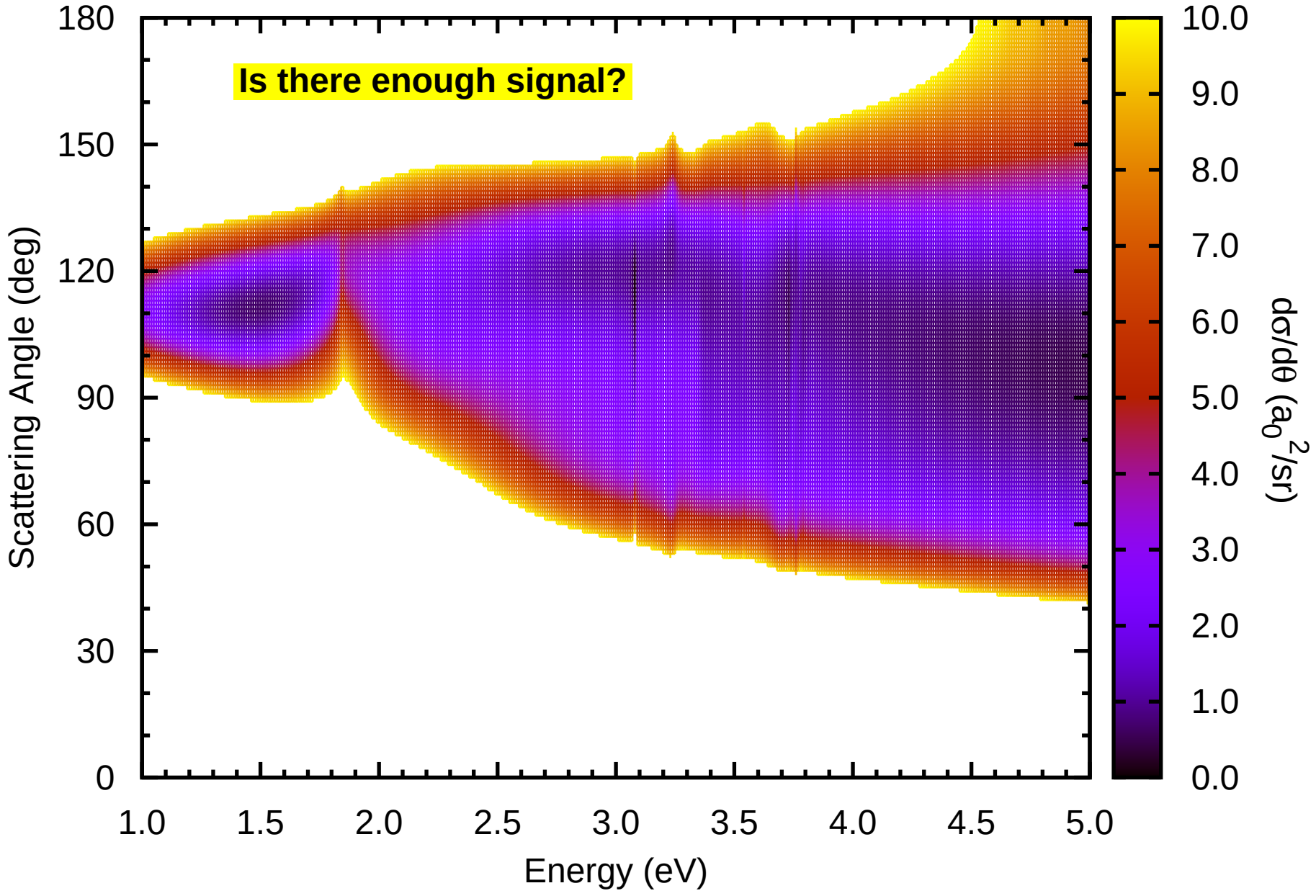
FIG. 2: Differential cross section as well as the individual contributions from the singlet and triplet total spin channels for elastic electron scattering from Li atoms at a collision energy of 3 eV. The insert shows the parameter P in the region $70° - 130°$. The lines at $-1/3$ and $-1/\sqrt{2}$ mark the borders between separable and entangled as well as entangled and Bell-correlated regions, respectively.

Experiment: Baum *et al.* Bielefeld (1986)

P < – 0.707... = Bell-entangled


P
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
E (eV)
1.0
2.0
3.0
4.0
5.0
θ (deg)
0
30
60
90
120
150
180
One really needs a systematic overview to find the interesting places in (E,θ).
see Phys. Rev. A 95 (2017) 042707


Scattering Angle (deg)
180
150
120
90
60
30
0
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
Energy (eV)
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
-1.0
P


Is there enough signal?
Scattering Angle (deg)
180
150
120
90
60
30
0
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
5.0
Energy (eV)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
dσ/dθ (a0 2/sr)

Conclusions and Outlook

- **Despite the field's maturity, significant innovations are constantly being made to study electron collisions with atoms and molecules – and they are needed!**
- **There exist many fruitful collaborations between experimentalists, theorists, and users outside of AMO who need (and use) these data.**
- **Experimental benchmark data remain very important to test and push theory!**
- **With such benchmark data and comparisons between predictions from highly sophisticated methods in hand, we can finally estimate uncertainties of these predictions.**
- **Although we usually need supercomputers to get a reliable answer, there is room for interpretation of the physics. → Propensity in equal-energy sharing (e,2e).**
- **Knowledge about electron collisions also helps to understand photon-induced processes, in weak-field, strong-field, steady-state, and time-dependent cases.**
- **And maybe the field is just about to be (re)discovered in quantum information ...**

Thank You for Your Attention!