Electron Collisions with Atoms, Ions, and Molecules: Experiment, Theory, and Applications

Klaus Bartschat

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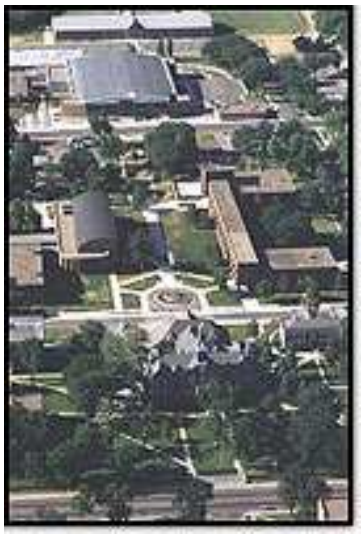
ICPEAC 2019; July 25, 2019



OVERVIEW:

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.

Friedrich Hanne

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

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 $\langle T_{KQ}^{+} \rangle$.]

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.

John Giuliani

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

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.

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

Our family – you might have seen them at several ICPEACs.

Teresa (11 ICPEACs) sends her regards; Nick (4) was one of the "1995 ICPEAC Babies"; another one of those babies will give a progress report on Tuesday! Erika (4) was at the last two in Toledo and Cairns.

Teresa Erika Nick

And now the sad part:

Phil Burke (18.10.1932 – 3.6.2019)

ICPEAC International Chair 1975 (Seattle)

Phil taught me about computers and especially the R-matrix method. When I came to Belfast as PhD student in 1982, Stan Scott told me at the first coffee break:

"There is nothing to worry about in Belfast, because ….

Phil knows EVERYTHING!"

The essential 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]

Plasma Physics and Electron Collisions Save the World!

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

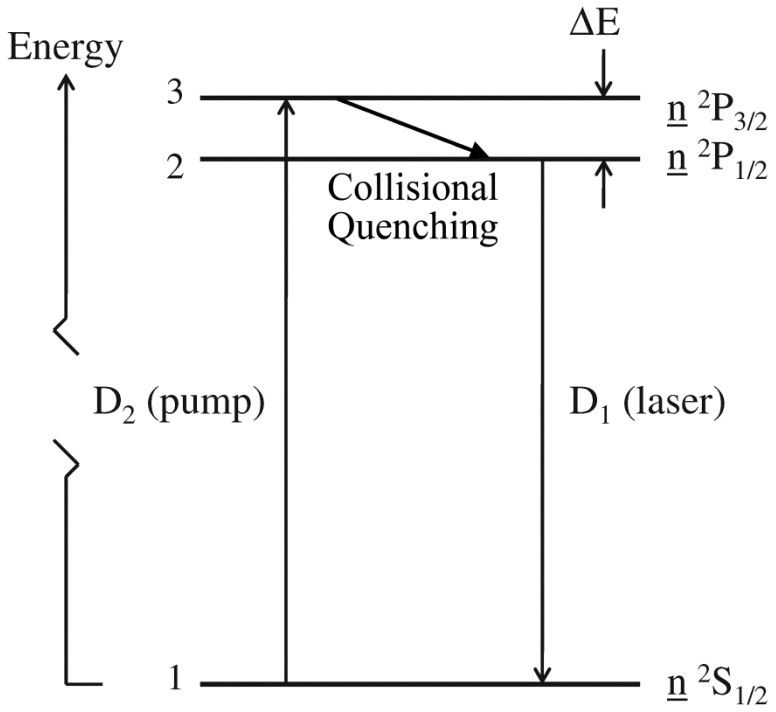
Electron collisions with atoms, ions, molecules, and surfaces are critically important to the understanding and modeling of low-temperature plasmas (LTPs), and so in the development of technologies based on LTPs. Recent progress in obtaining experimental benchmark data and the development of highly sophisticated 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

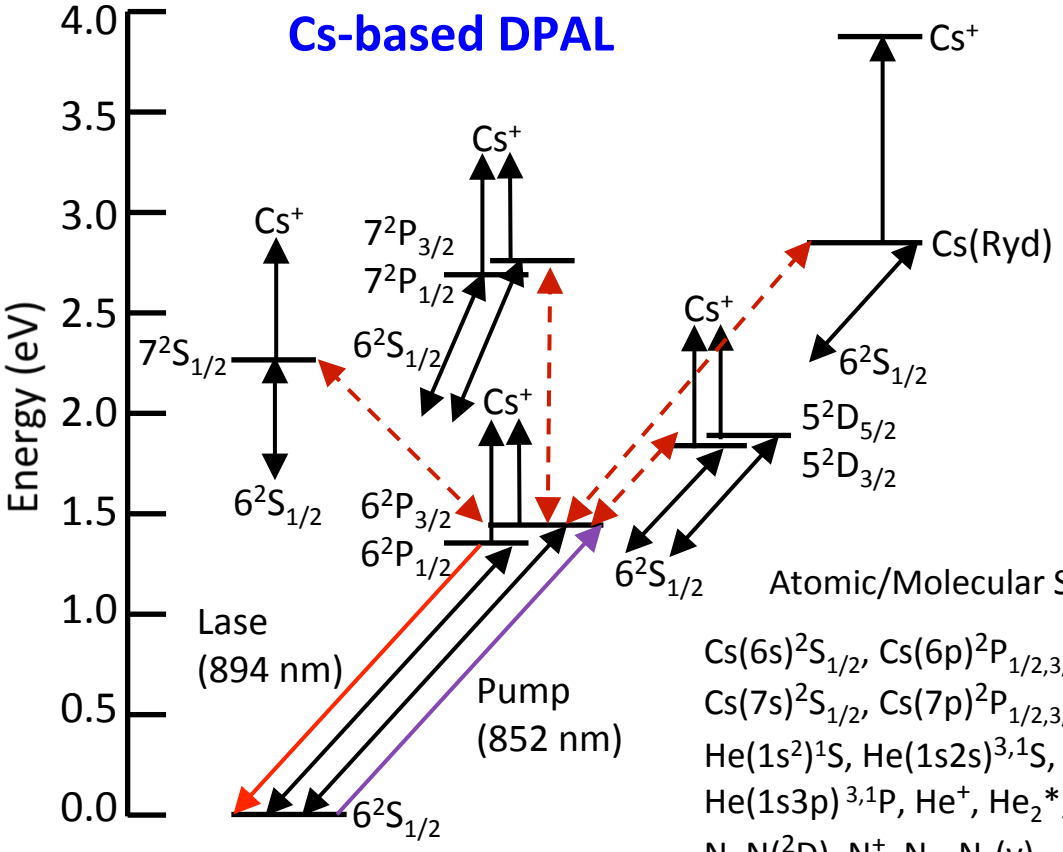
DIODE-PUMPED ALKALI LASERS (DPALs)

- **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.)

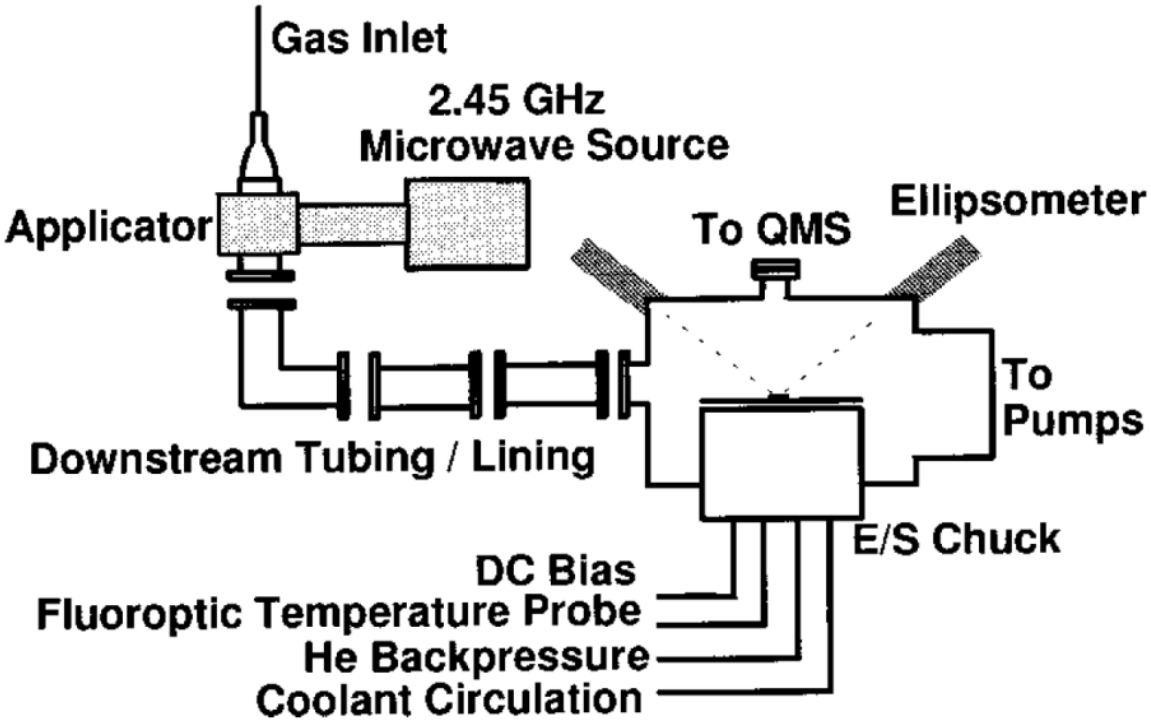


Atomic/Molecular Species in the Model

$Cs(6s)^2S_{1/2}$, $Cs(6p)^2P_{1/2,3/2}$, $Cs(5d)^2D_{5/2,3/2}$,
$Cs(7s)^2S_{1/2}$, $Cs(7p)^2P_{1/2,3/2}$, 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.

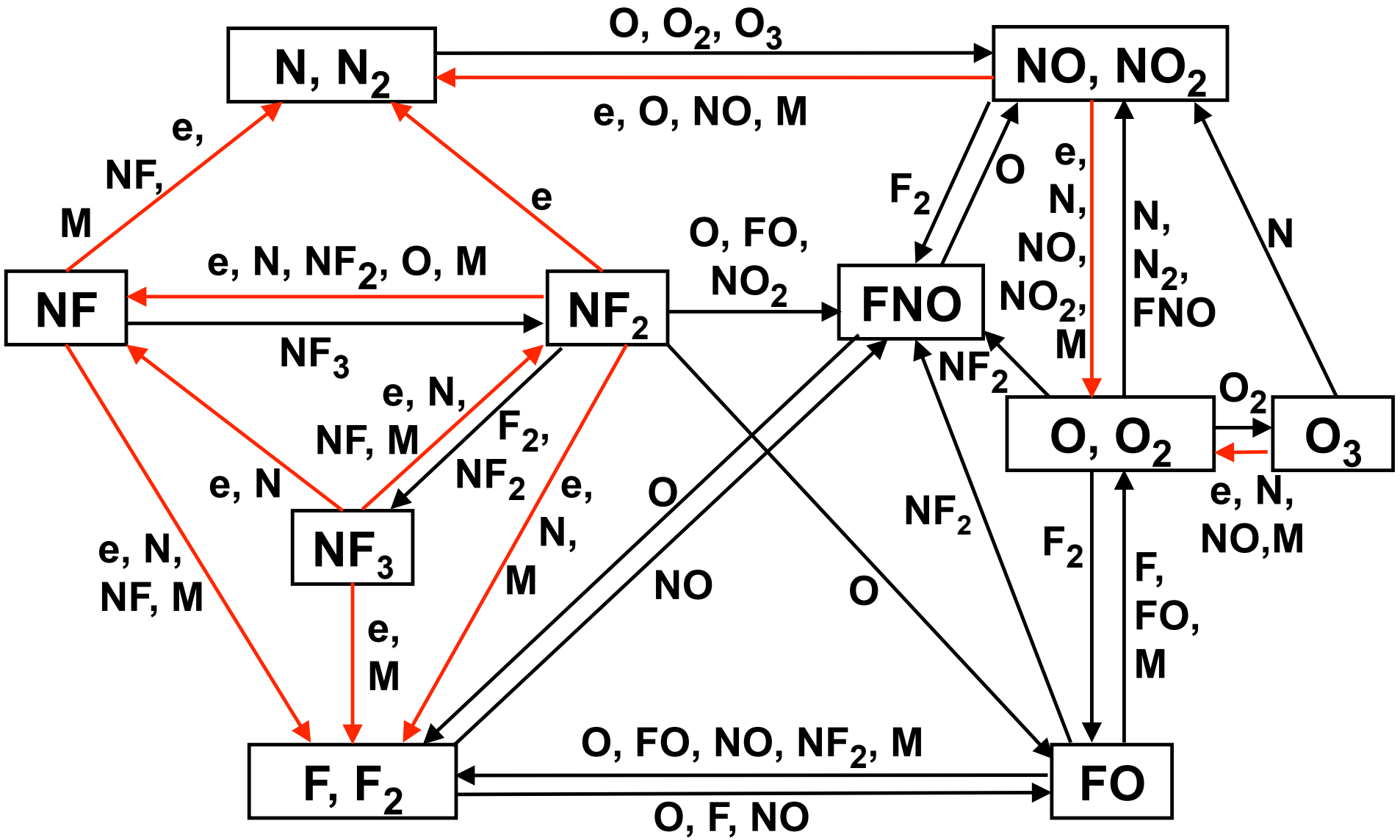


- Schematic of RPS.[1]

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

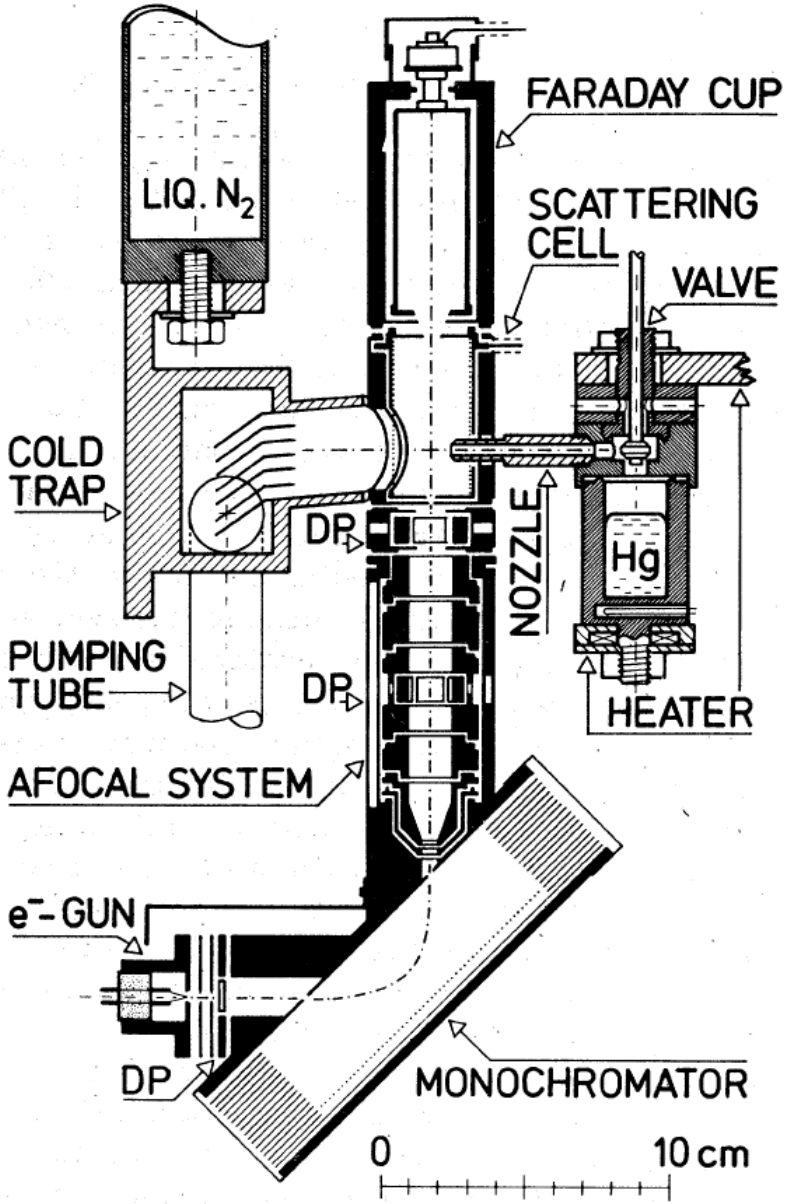


FIG. 1. Electron optical arrangement for low energie (0.1–70 eV) with atomic beam target. Deflector plates are denoted by DP.

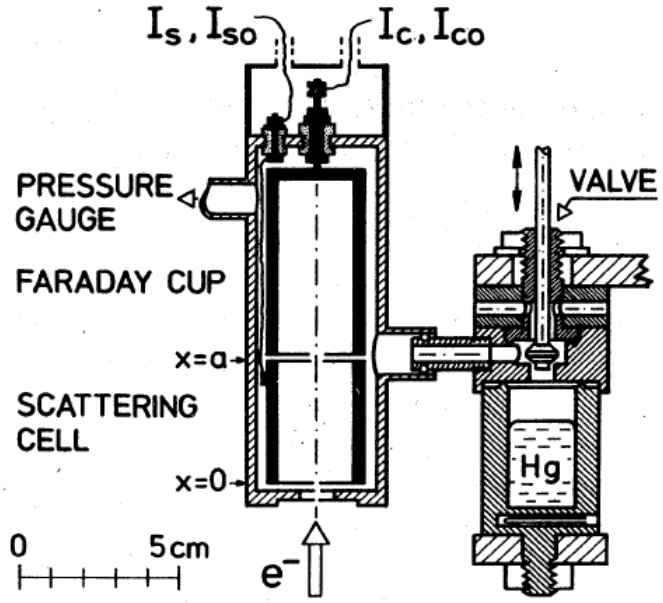


FIG. 3. Target cell for absolute measurements. This arrangement is used together with the electron optics of Fig. 1.

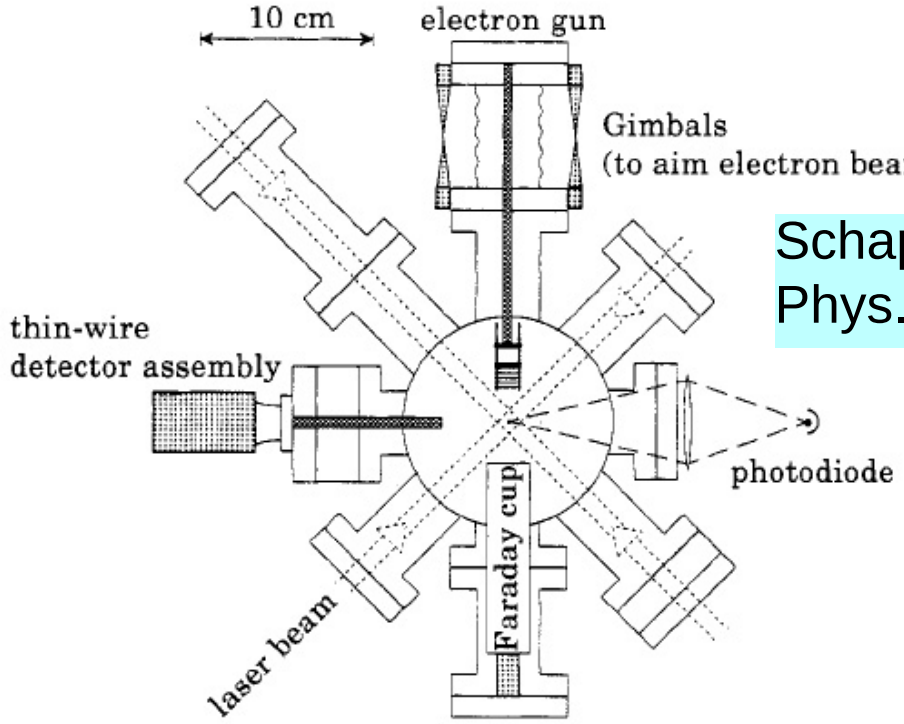
$$I = I_0 \exp(-nlQ)\,, \tag{1}$$

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

Trap Setup: Loss Rate $\Gamma_e = \sigma J/e$



Schappe, Walker, Anderson, Lin;
Phys. Rev. Lett. **76** (1996) 4328

further developed by
J.F. McConkey
and collaborators

Fig. 1. – Schematic diagram of the vacuum chamber. Not shown are two of the laser beams, the magnetic-field coils, and the diode laser with its stabilization and modulation equipment.

When the electron beam is turned on, atoms are ejected from the trap due to the electron-atom collisions at a rate

$$\Gamma_e = \sigma J/e\,, \qquad (1)$$

where σ is the cross-section for ejecting the atoms from the trap, J is the electron current density, and e the electron charge.
By measuring Γ_e and J, we determine σ directly from eq. (1).

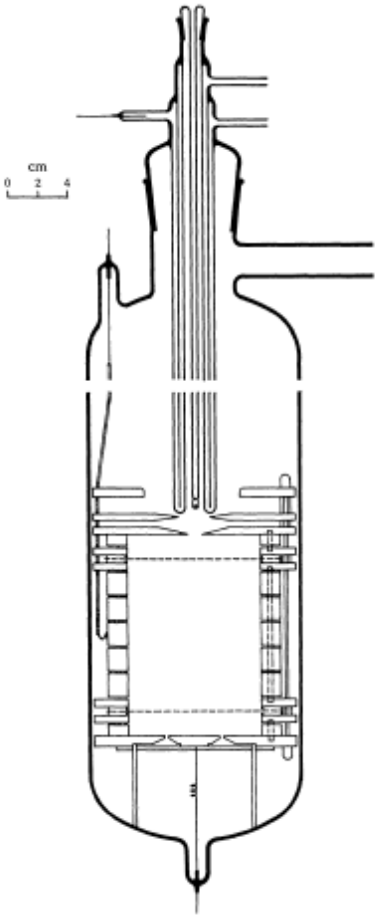
Note: The cross section is measured directly!

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 ...



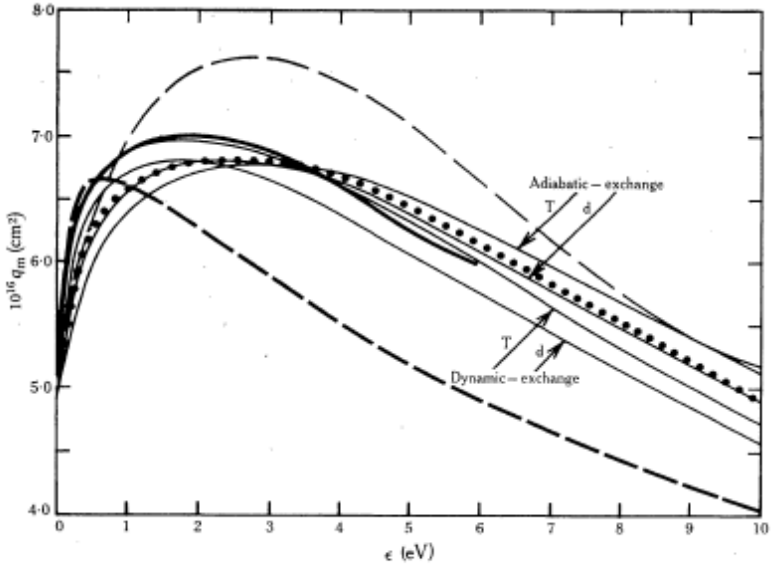


Fig. 7.—A comparison between theoretical and experimental momentum transfer cross sections. —— Crompton, Elford, and Jory; — — Frost and Phelps; — — Bauer and Browne; ——— La Bahn and Callaway; ••• Williamson and McDowell.

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

Will Allis did calculations for this in 1933!

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)

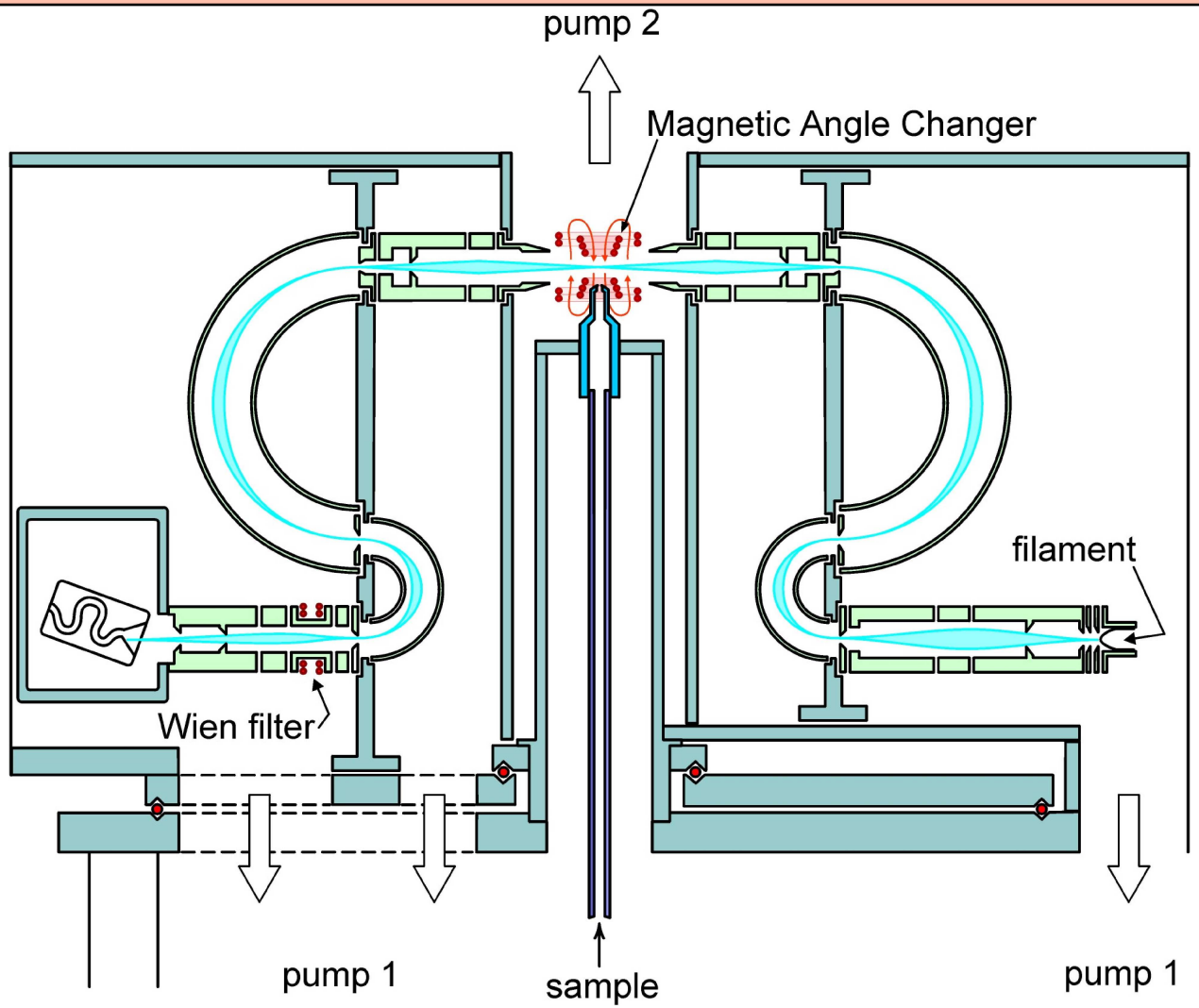
Recall:
This talk is NOT a comprehensive review!

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

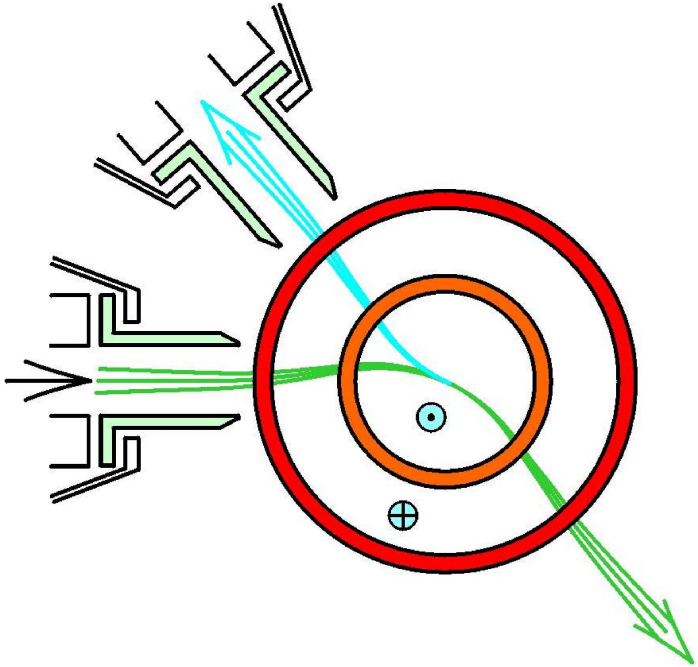
Angle-Differential Cross Sections

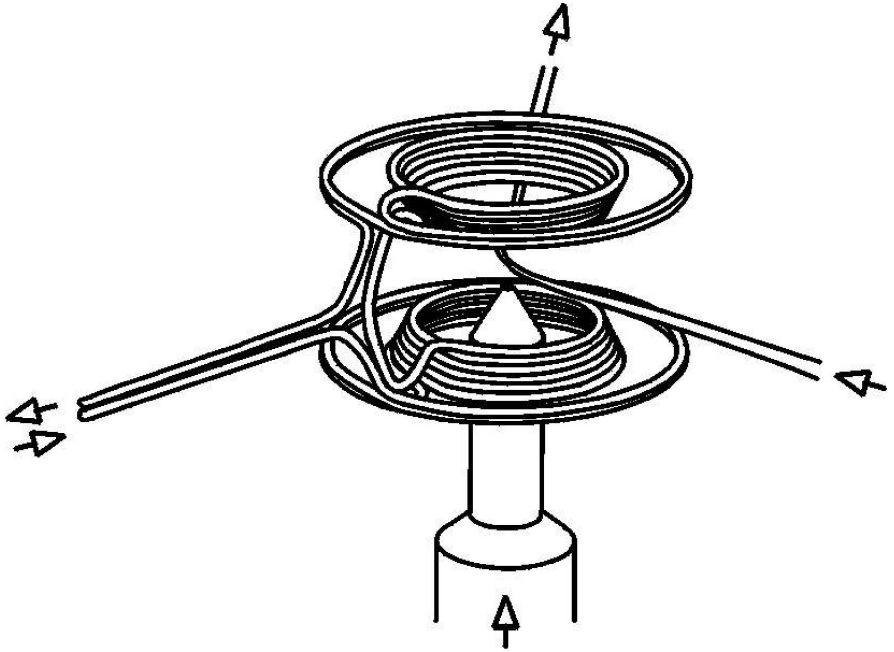
Michael Allan's high-resolution spectrometer to measure:

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



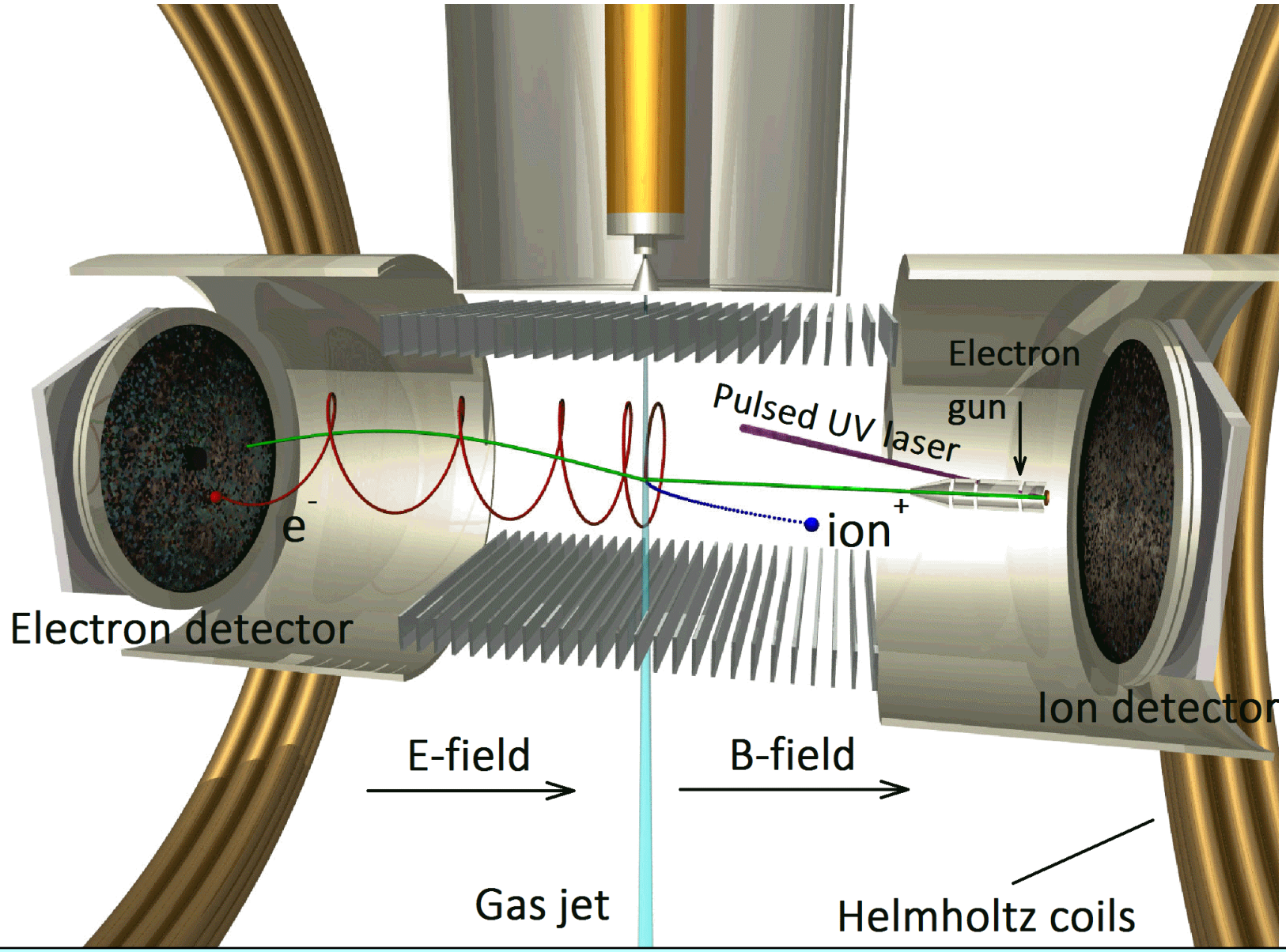
The "Magnetic Angle Changer" (MAC), developed by Reid and Channing, makes it possible to measure the full angular range, including 0º and 180º.





The Reaction Microscope

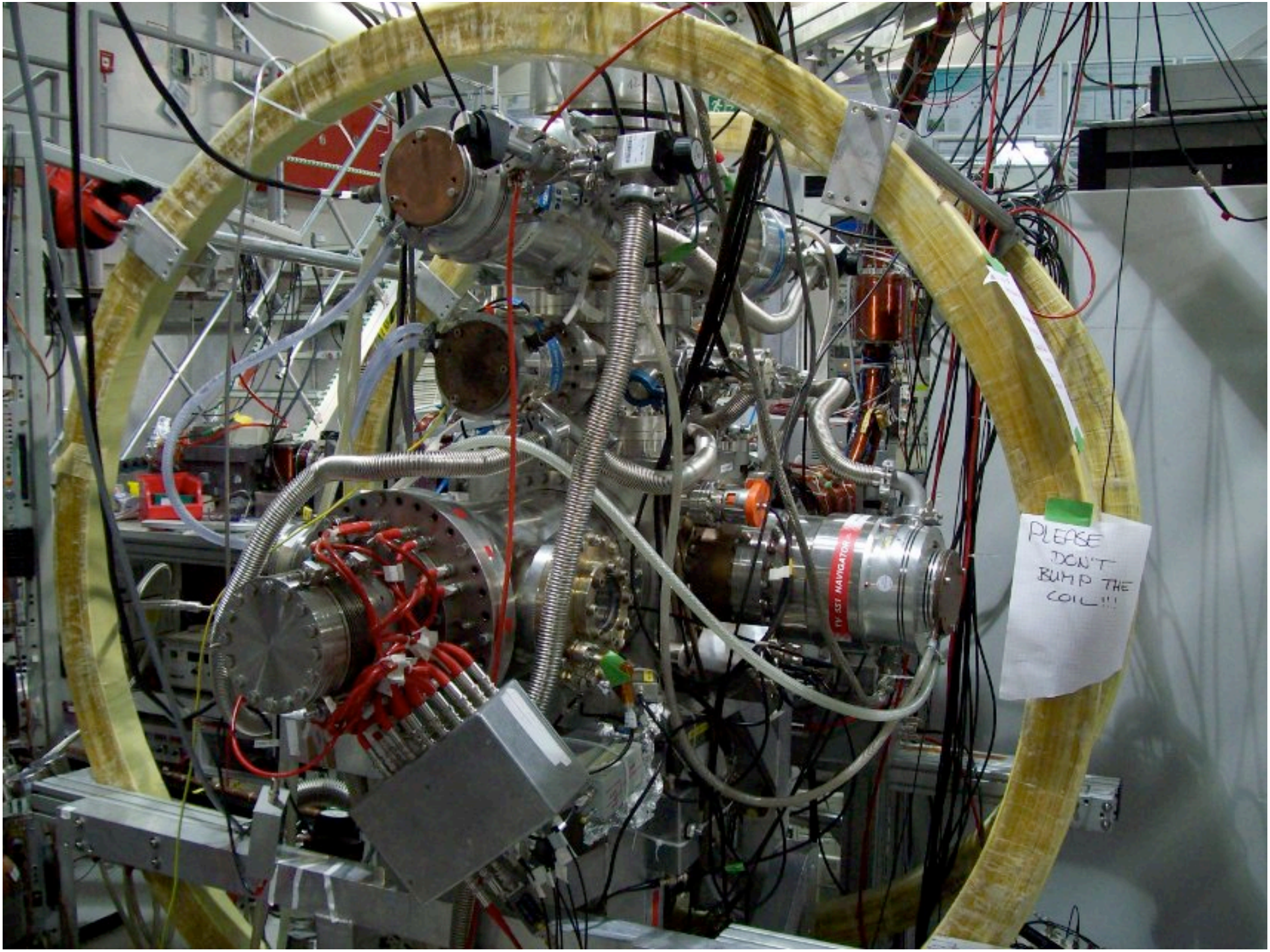
Ullrich, Moshammer, Dorn, *et al.*, Rep. Prog. Phys. 66 (2003) 1463



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!



Theoretical/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
- **(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**

Now come a few examples ...

Optical Model Potential (Blanco, Garcia) – a "Special Purpose" Approach

Numerical Methods: OMP for Atoms

- For electron-atom scattering, we solve the partial-wave equation

$$\left(\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} - 2V_{\rm mp}(k,r)\right) u_\ell(k,r) = k^2 u_\ell(k,r).$$

- The **local model potential** is taken as

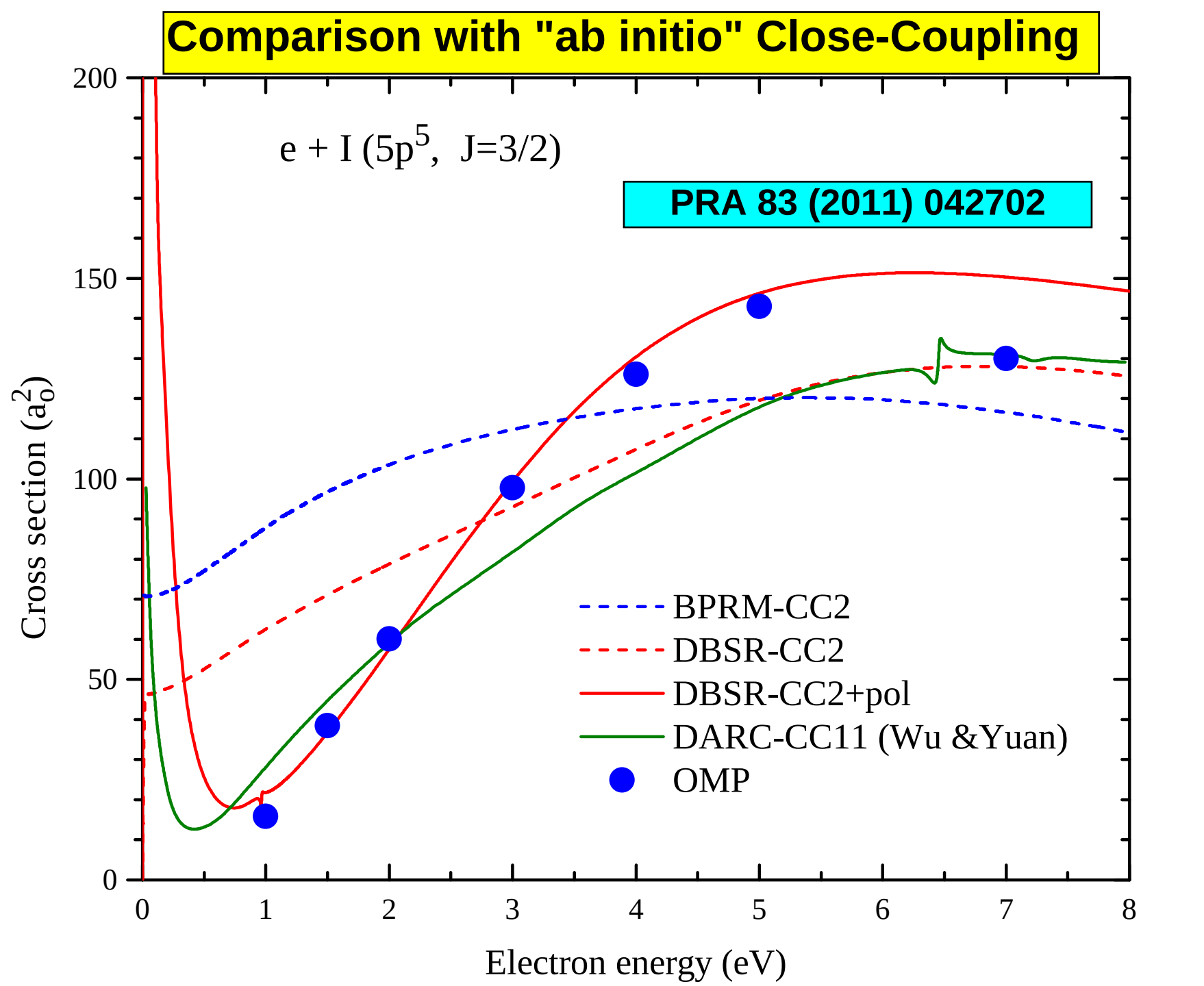
$$V_{\rm mp}(k,r) = V_{\rm static}(r) + V_{\rm exchange}(k,r) + V_{\rm polarization}(r) + iV_{\rm absorption}(k,r)$$

with

  - $V_{\rm exchange}(k,r)$ from Riley and Truhlar (J. Chem. Phys. **63** (1975) 2182);
  - $V_{\rm polarization}(r)$ from Zhang *et al.* (J. Phys. B **25** (1992) 1893);
  - $V_{\rm absorption}(k,r)$ from Staszewska *et al.* (Phys. Rev. A **28** (1983) 2740).

- Due to the imaginary absorption potential, **the OMP method**
  - yields a complex phase shift $\delta_\ell = \lambda_\ell + i\mu_\ell$
  - allows for the calculation of ICS and DCS for
    - elastic scattering
    - inelastic scattering (all states together)
    - the sum (total) of the two processes

It's great if this is all you want!


Comparison with "ab initio" Close-Coupling
e + I (5p5, J=3/2)
PRA 83 (2011) 042702
BPRM-CC2
DBSR-CC2
DBSR-CC2+pol
DARC-CC11 (Wu &Yuan)
OMP
Cross section (a02)
Electron energy (eV)
0
50
100
150
200
0
1
2
3
4
5
6
7
8

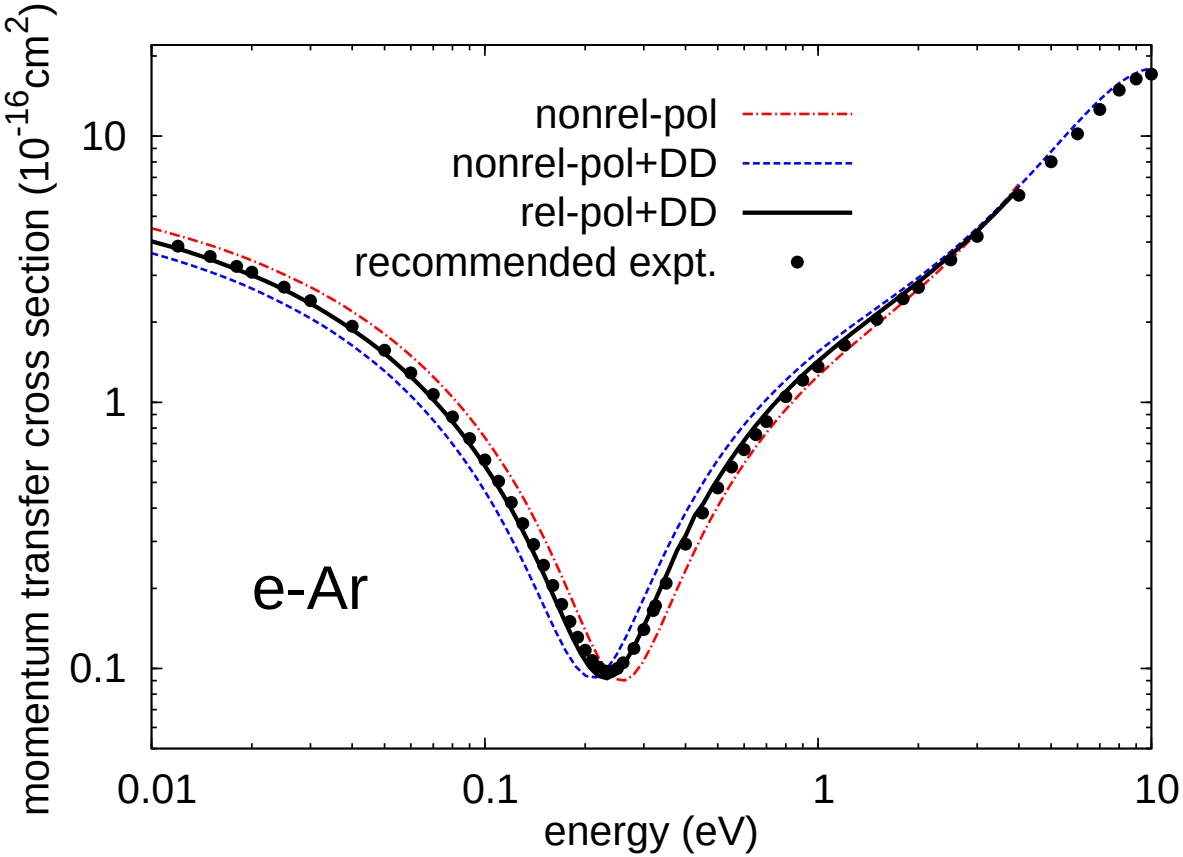
Polarized Orbital – an "Ab Initio Special Purpose" Approach

Aust. J. Phys., 1997, **50**, 511–24

Relativistic Effects in Low-energy Electron–Argon Scattering*

R. P. McEachran[A,B] *and A. D. Stauffer*[B]

We have performed a relativistic treatment at low energy of electron–argon scattering which includes both polarisation and dynamic distortion effects. Our results are in excellent agreement with the experimentally derived momentum transfer cross section and scattering length, as well as with very recent measurements of the elastic differential cross section.



Extension to account for inelastic effects:
J. Phys. B 42 (2009) 075202

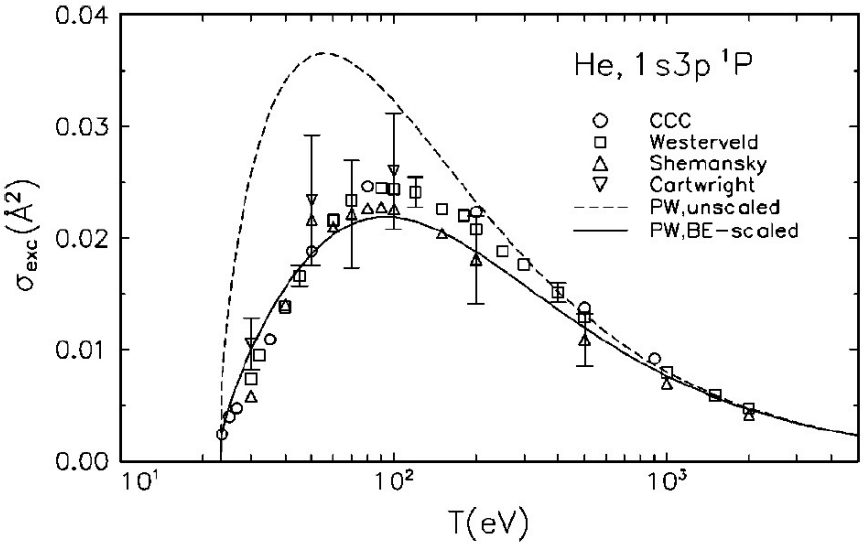
BEf-scaling; Plane-Wave Born with Experimental Optical Oscillator Strength and Empirical Energy Shift

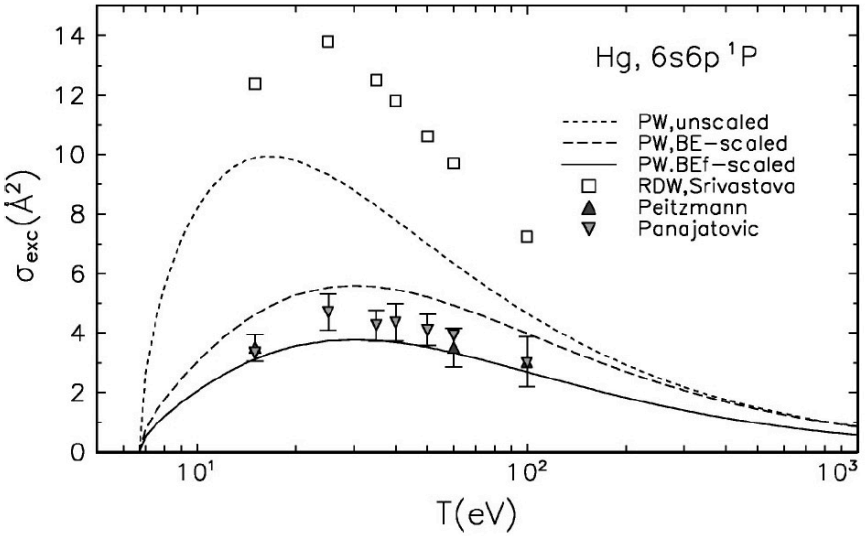
PHYSICAL REVIEW A, VOLUME 64, 032713

Scaling of plane-wave Born cross sections for electron-impact excitation of neutral atoms

Yong-Ki Kim
National Institute of Standards and Technology, Gaithersburg, Maryland 20899-8421
(Received 12 March 2001; published 20 August 2001)

Two methods to scale plane-wave Born cross sections for electron-impact excitations of neutral atoms are shown to produce excitation cross sections comparable in accuracy to those obtained by more sophisticated collision theories such as the convergent close-coupling method. These scaling methods are applicable to integrated cross sections for electric dipole-allowed transitions. Scaled cross sections are in excellent agreement with available theoretical and experimental data for excitations in H, He, Li, Be, Na, Mg, K, Ca, Rb, Sr, Cs, Ba, Hg, and Tl, indicating the possibility of rapid and reliable calculations of excitation cross sections for many other neutral atoms.





works well, but is limited to optically allowed transitions

Similar idea works even better for ionization of complex targets :=)

Semi-Relativistic DWBA

PHYSICAL REVIEW A, VOLUME 61, 022701

Excitation of Ar $3p^5 4s$-$3p^5 4p$ transitions by electron impact

C. M. Maloney,[1] J. L. Peacher,[1] K. Bartschat,[2] and D. H. Madison[1]
[1]*Physics Department, University of Missouri–Rolla, Rolla, Missouri 65409-0640*
[2]*Physics Department, Drake University, Des Moines, Iowa 50311*

Electron-impact excitation of argon from the $3p^5 4s$ ($J=0,2$) metastable states to the $3p^5 4p$ ($J=0,1,2,3$) manifold has been investigated in the semirelativistic first-order distorted-wave and plane-wave Born approximations. The results are compared with recent experimental data of Boffard *et al.* [Phys. Rev. A **59**, 2749 (1999)] and *R*-matrix predictions by Bartschat and Zeman [Phys. Rev. A **59**, R2552 (1999)]. In cases for which perturbative approaches are expected to be valid, the plane-wave Born approximation is found to be sufficiently accurate and thus allows for an efficient calculation of results over a wide range of collision energies.

The first-order distorted-wave T matrix for atomic excitation is given by

$$T_{fi}=(n+1)\langle \chi_f^-(r_0)\Psi_f(\xi)|V-U_f(r_0)|A\Psi_i(\xi)\chi_i^+(r_0)\rangle .$$

$$(K+U_f-E_f)\chi_f^-=0$$

$$U_f=\gamma V_f-\tfrac{1}{4}(\alpha V_f)^2-\frac{(j+1)}{r}\frac{\eta'}{\eta}+\frac{3}{4}\left(\frac{\eta'}{\eta}\right)^2-\frac{1}{2}\frac{\eta''}{\eta'},$$

$$\gamma=\sqrt{1+\alpha^2 E_f}, \qquad \eta=1+\gamma-\tfrac{1}{2}\alpha^2 V_f$$

polarization and absorption potentials may also be included

Ar $3p^5 4s$ –> $3p^5 4p$: DWBA vs. R-matrix

unitarization problem!

(can be fixed; e.g., Dasgupta's NRL code)

MALONEY, PEACHER, BARTSCHAT, AND MADISON

Phys. Rev. A 61 (2000) 022701

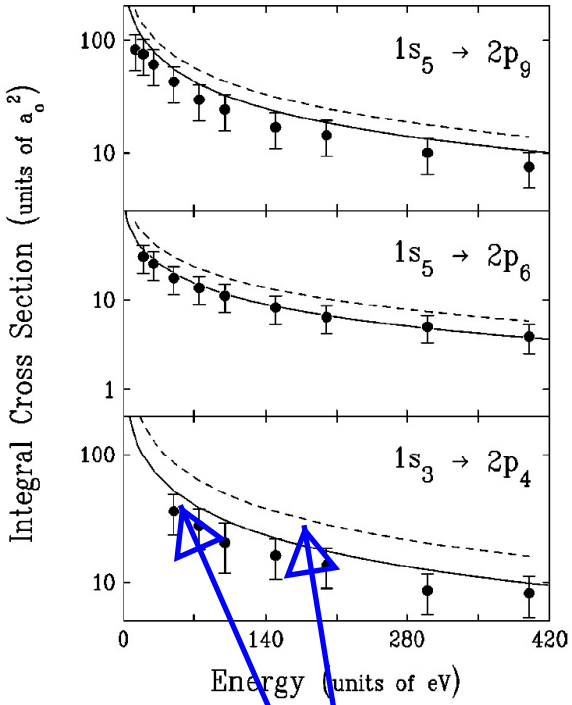


FIG. 1. Integral cross sections for electron-impact excitation of three states in the $2p$ manifold of argon from the metastable states in the $1s$ manifold as a function of incident electron energy. The experimental data are those of Boffard *et al.* [7]. The theoretical SRDW results are SS wave functions (dashed curve) and CIV3 wave functions (solid curve).

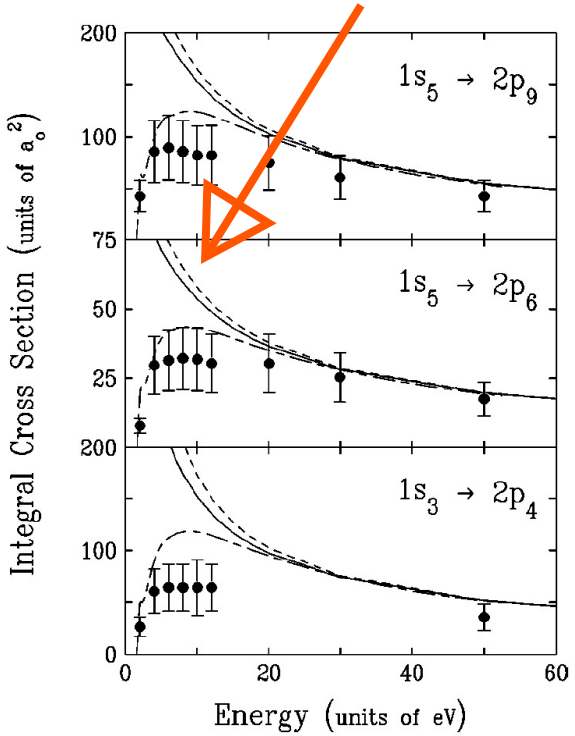


FIG. 2. Integral cross sections for electron-impact excitation of three states in the $2p$ manifold of argon from the metastable states in the $1s$ manifold as a function of incident electron energy. The experimental data are those of Boffard *et al.* [7]. The theoretical results are PWBA (dashed curve); 15-state R-matrix results (long-short dash); and SRDW with CIV3 wave functions (solid curve).

Theoretical results depend on wavefunctions and potentials

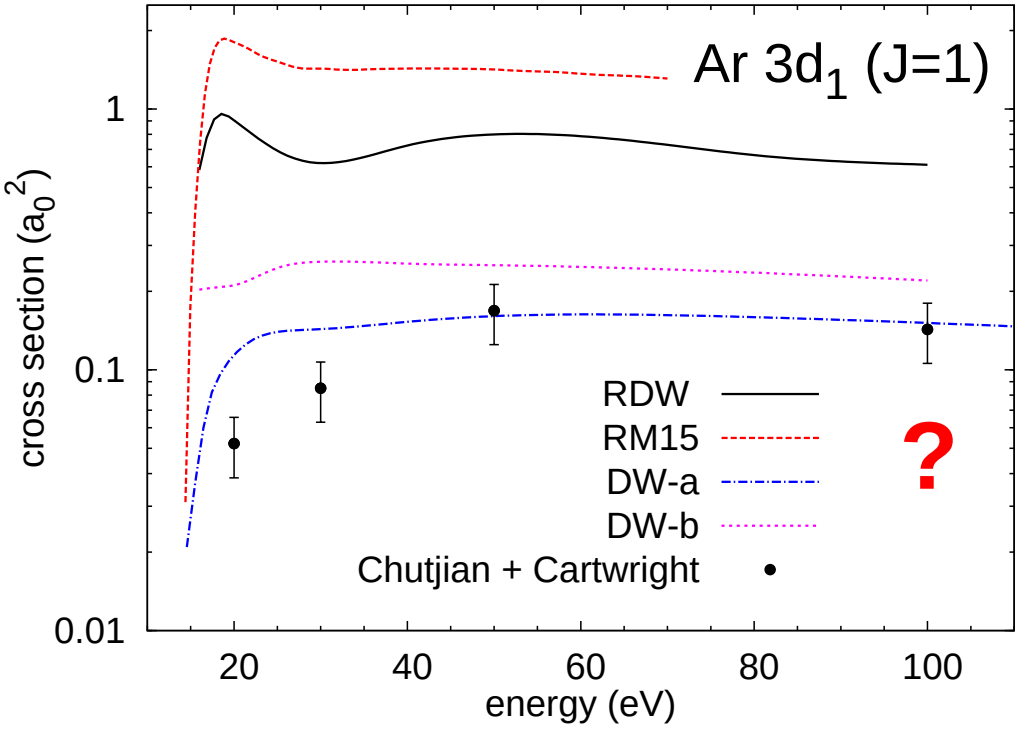
If you want to do your own calculations, check out
https://www-amdis.iaea.org/FAC/ or the
Los Alamos Atomic Collision Codes (if the site is accessible)

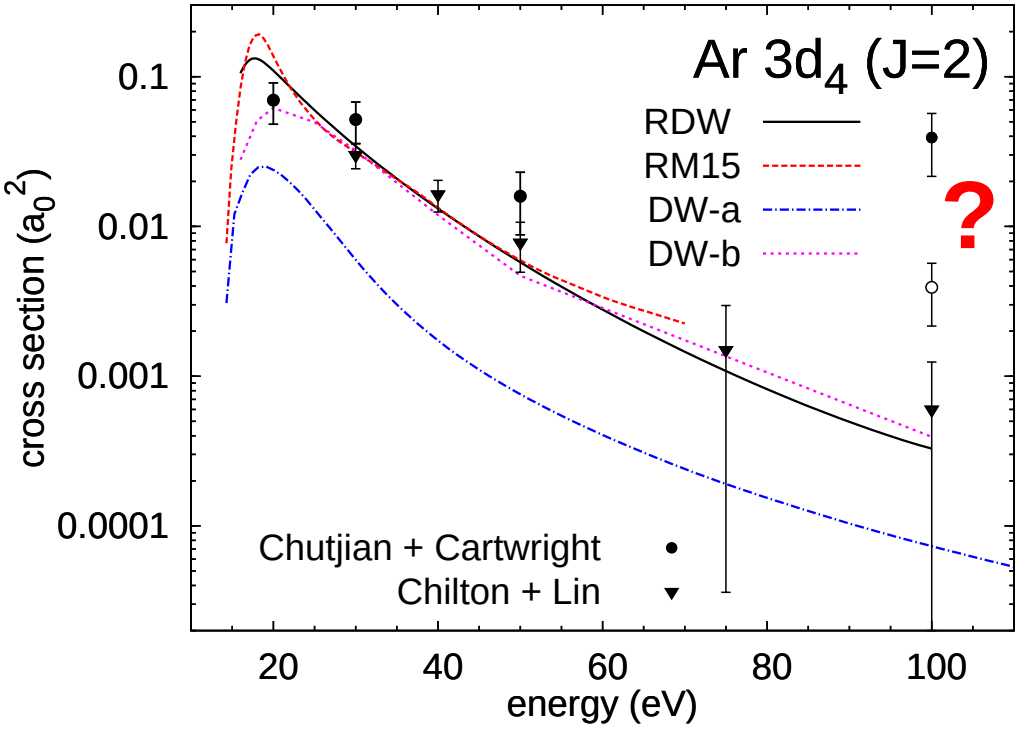
Relativistic DWBA; Semi-Relativistic DWBA; R-Matrix; Experiment

PHYSICAL REVIEW A **81**, 052707 (2010)

Electron-impact excitation of argon: Cross sections of interest in plasma modeling

R. K. Gangwar,[1] L. Sharma,[2] R. Srivastava,[1] and A. D. Stauffer[3]





Key Message:
Sometimes BIG Differences between Theories and HUGE Experimental Error Bars!

Which model, if any, can we trust?

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

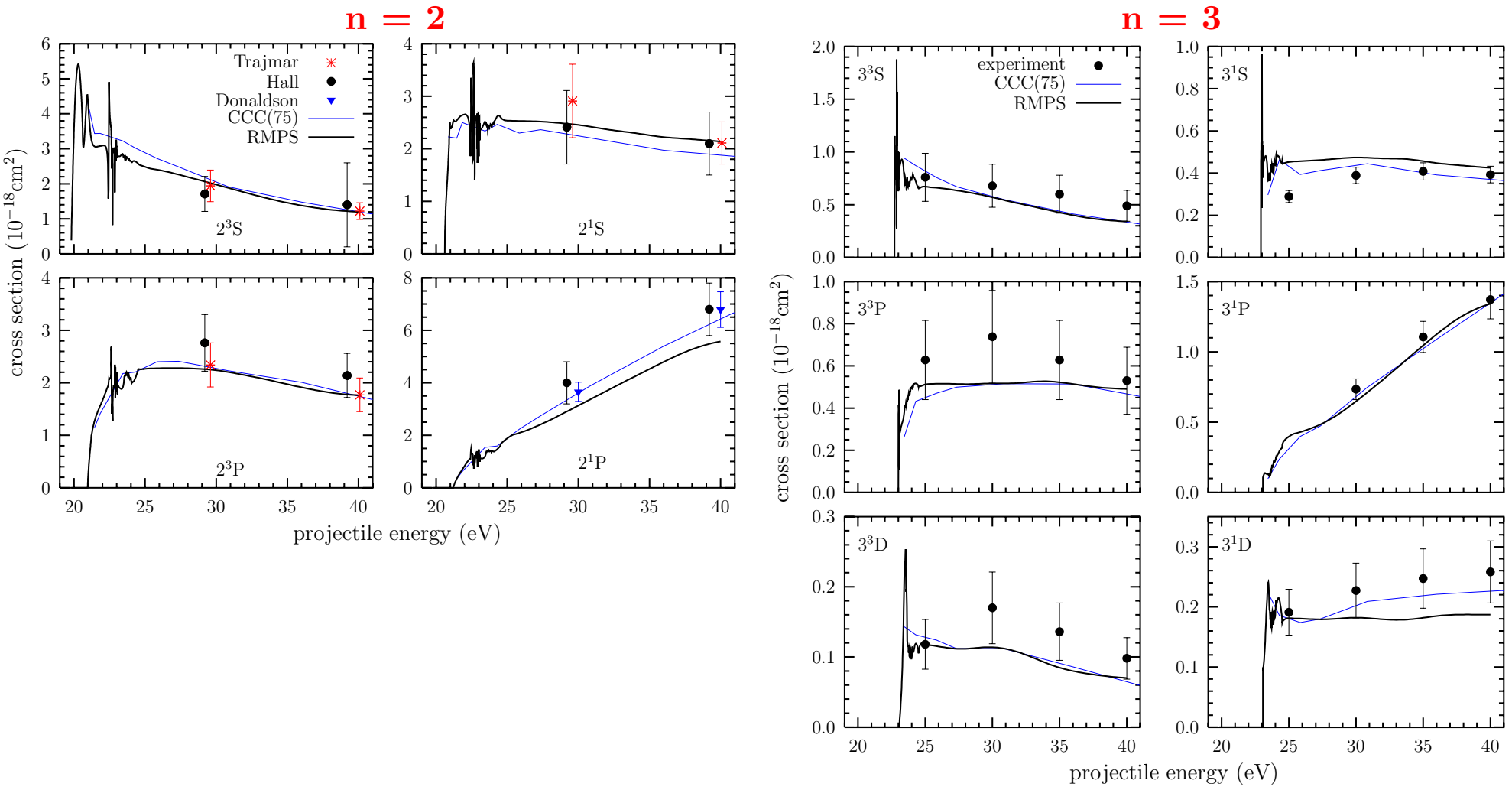
$$V_{ij}(r) = -\frac{Z}{r}\,\delta_{ij} + \sum_{k=1}^{N}\langle \Phi_i \mid \frac{1}{|\mathbf{r}_k - \mathbf{r}|} \mid \Phi_j \rangle$$

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

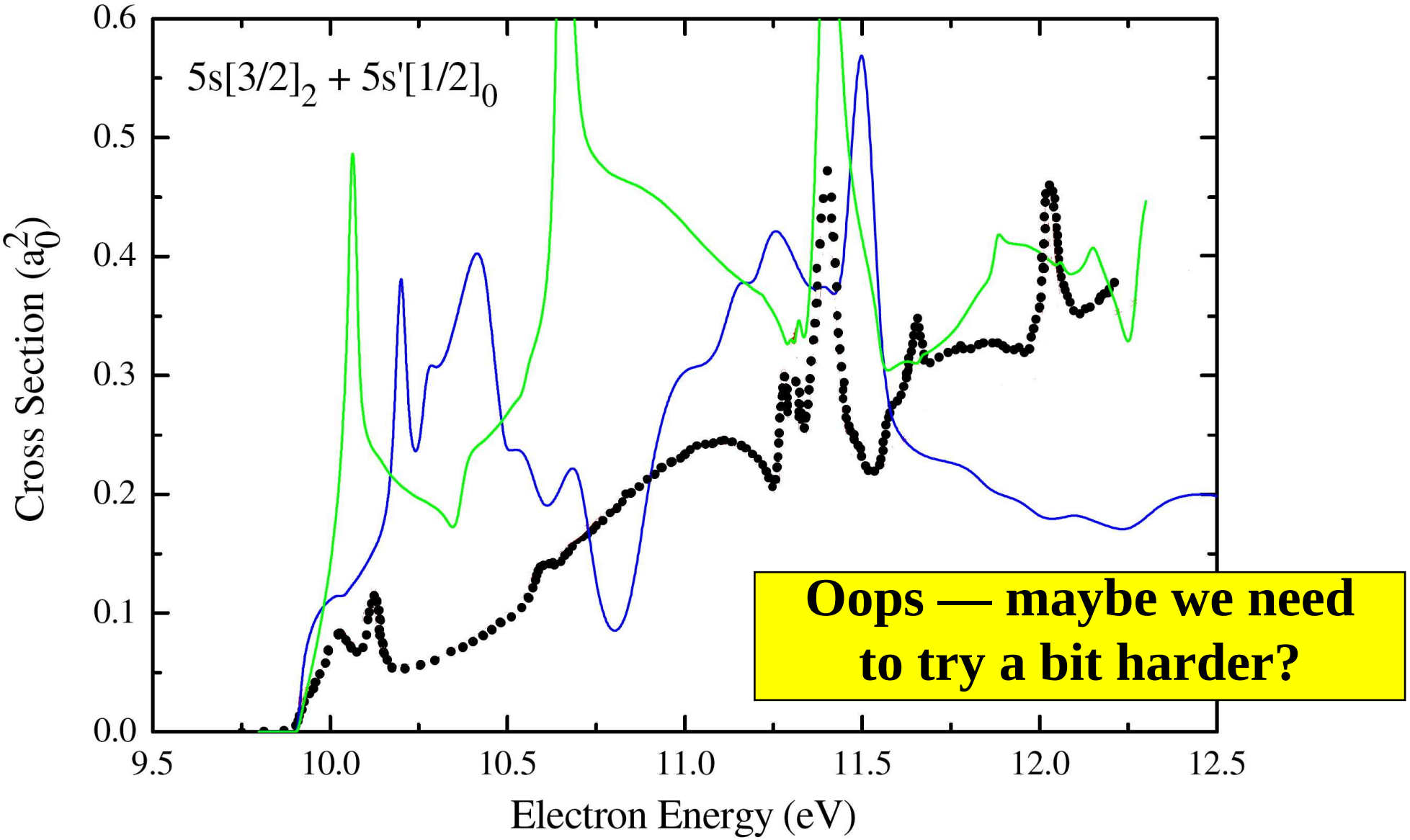


Already in 1998, de Heer recommends 0.5 x (CCC+RMPS) for uncertainty of 10% — independent of experiment!

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)



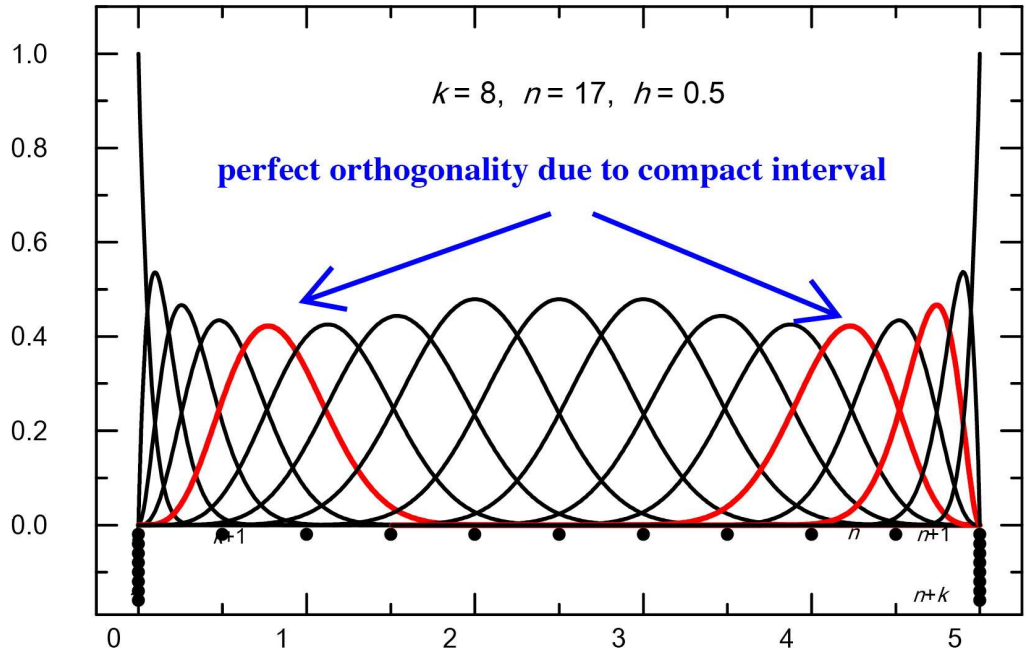
Oops — maybe we need to try a bit harder?

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 80 more since 2006

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

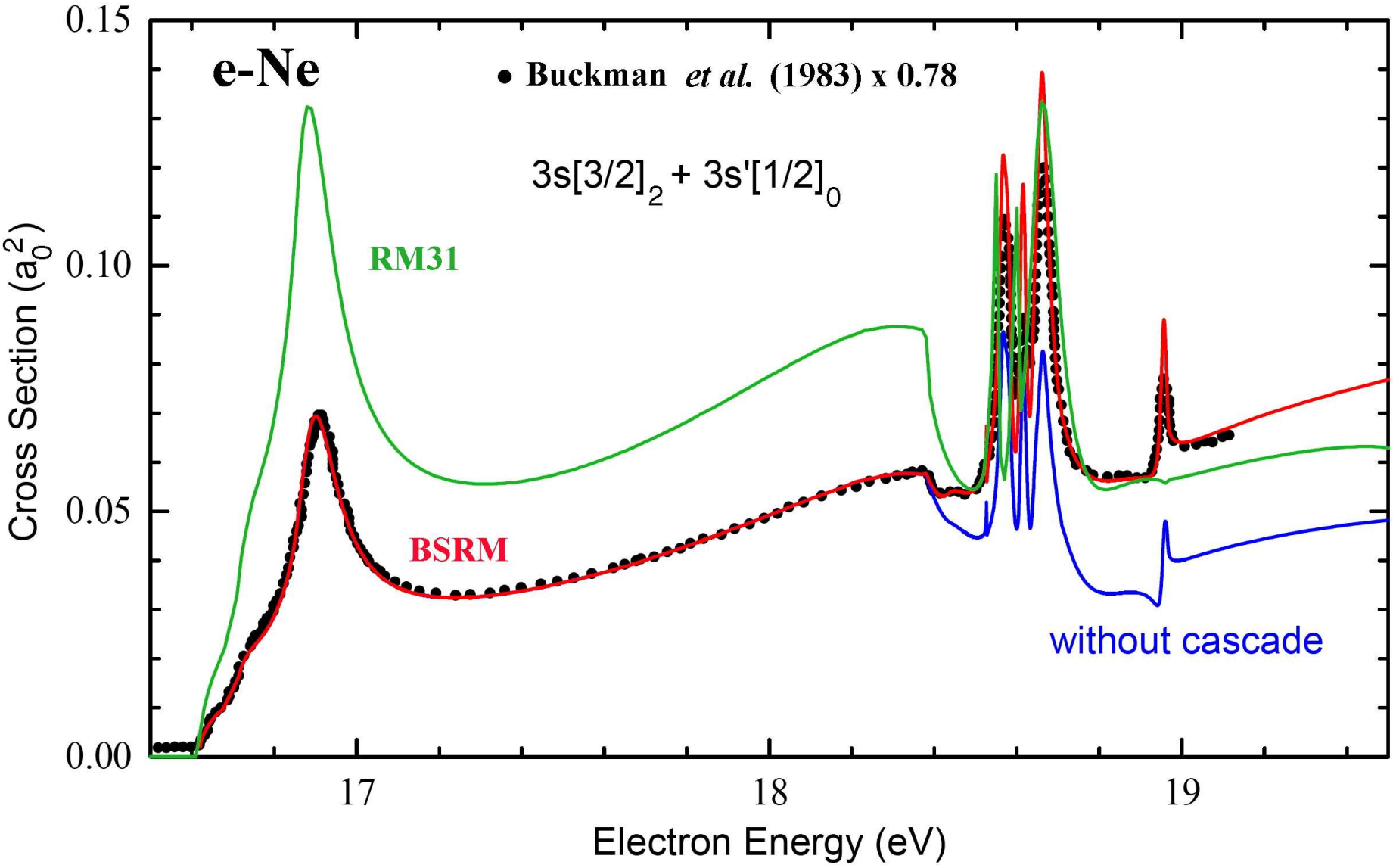
Our Apparatus — Supercomputers

Kraken (NICS)

TACC
TEXAS ADVANCED COMPUTING CENTER
Powering Discoveries That Change The World

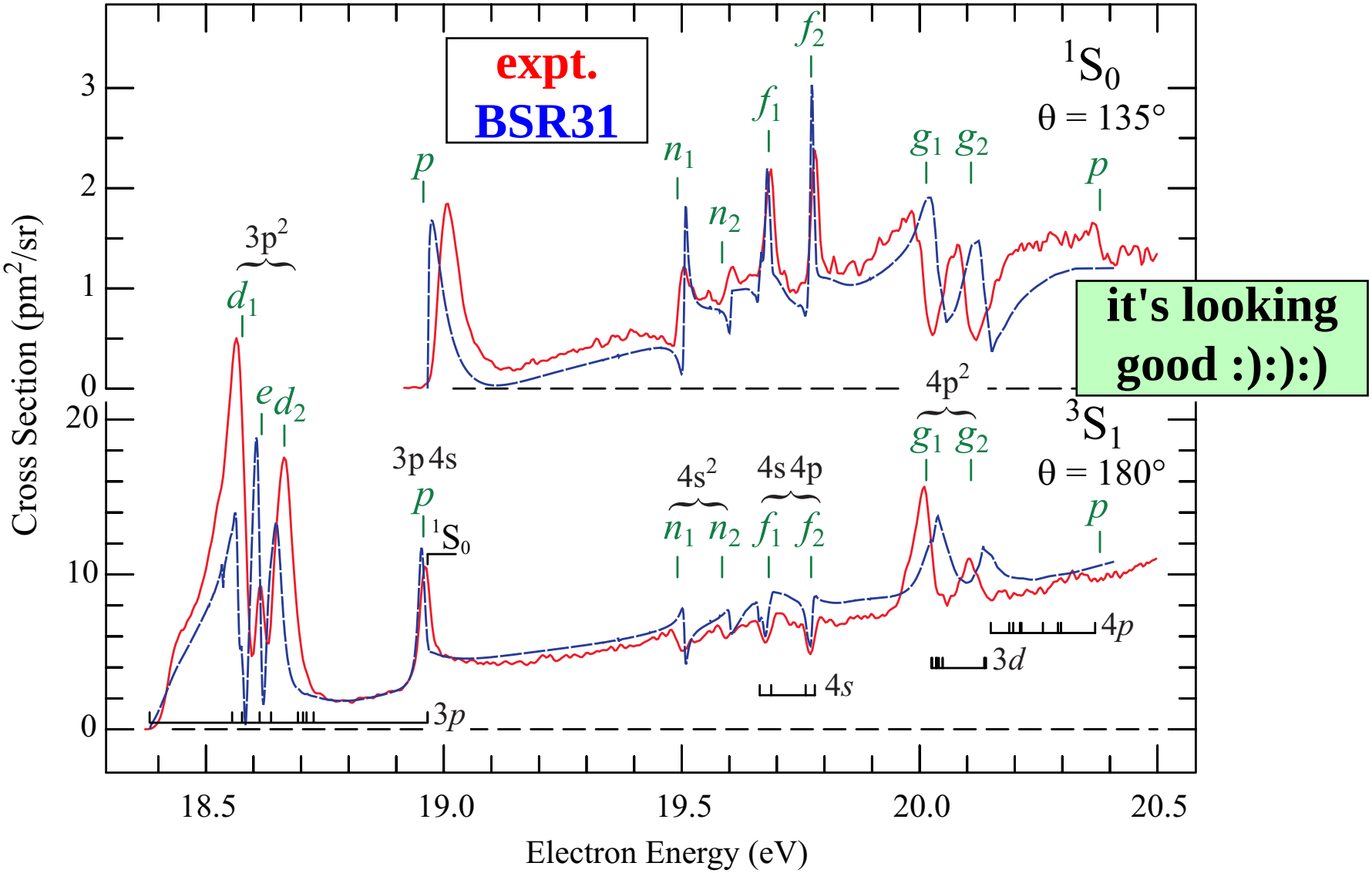
Metastable yield in e-Ne collisions

- 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



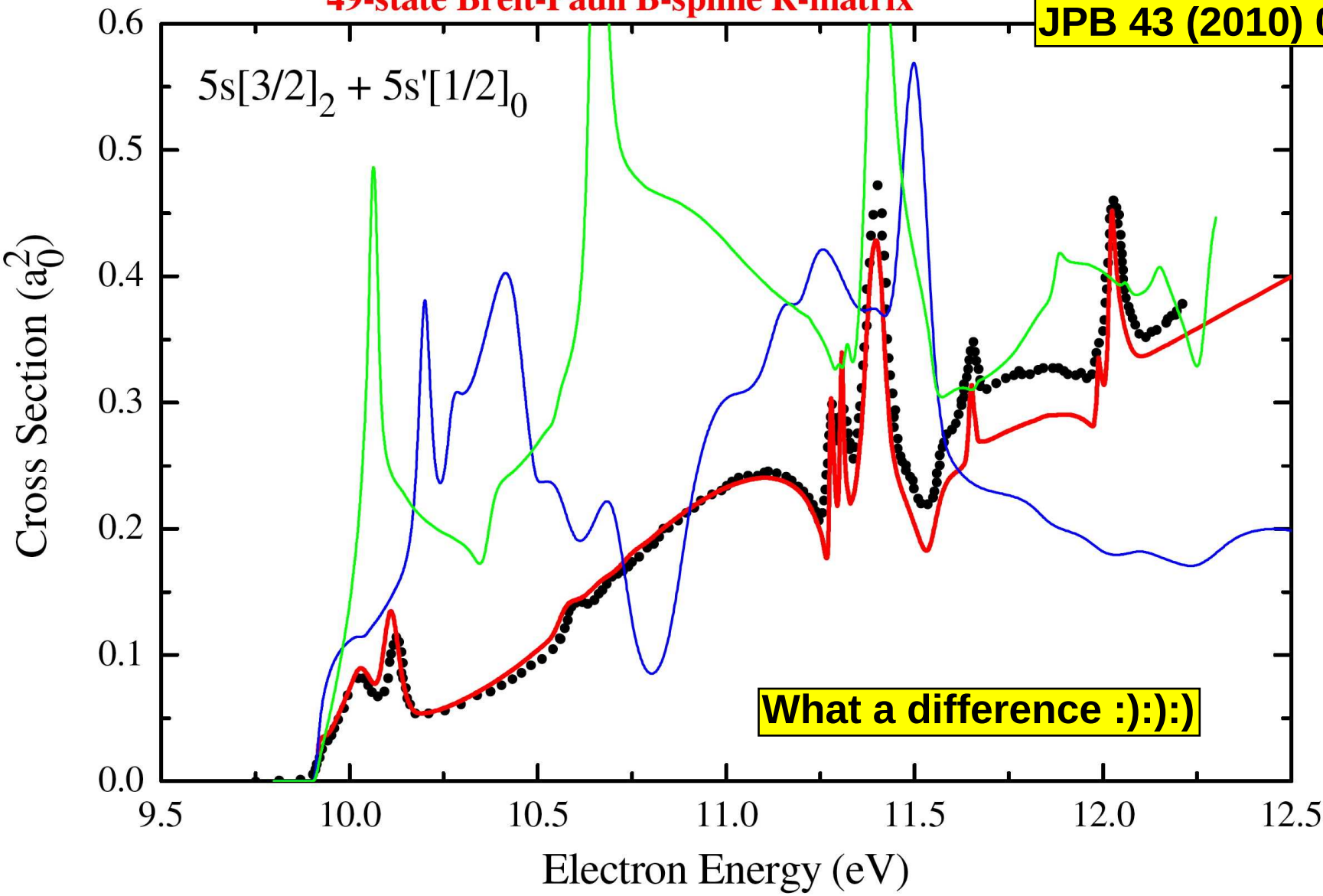
it's looking good :):):)

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

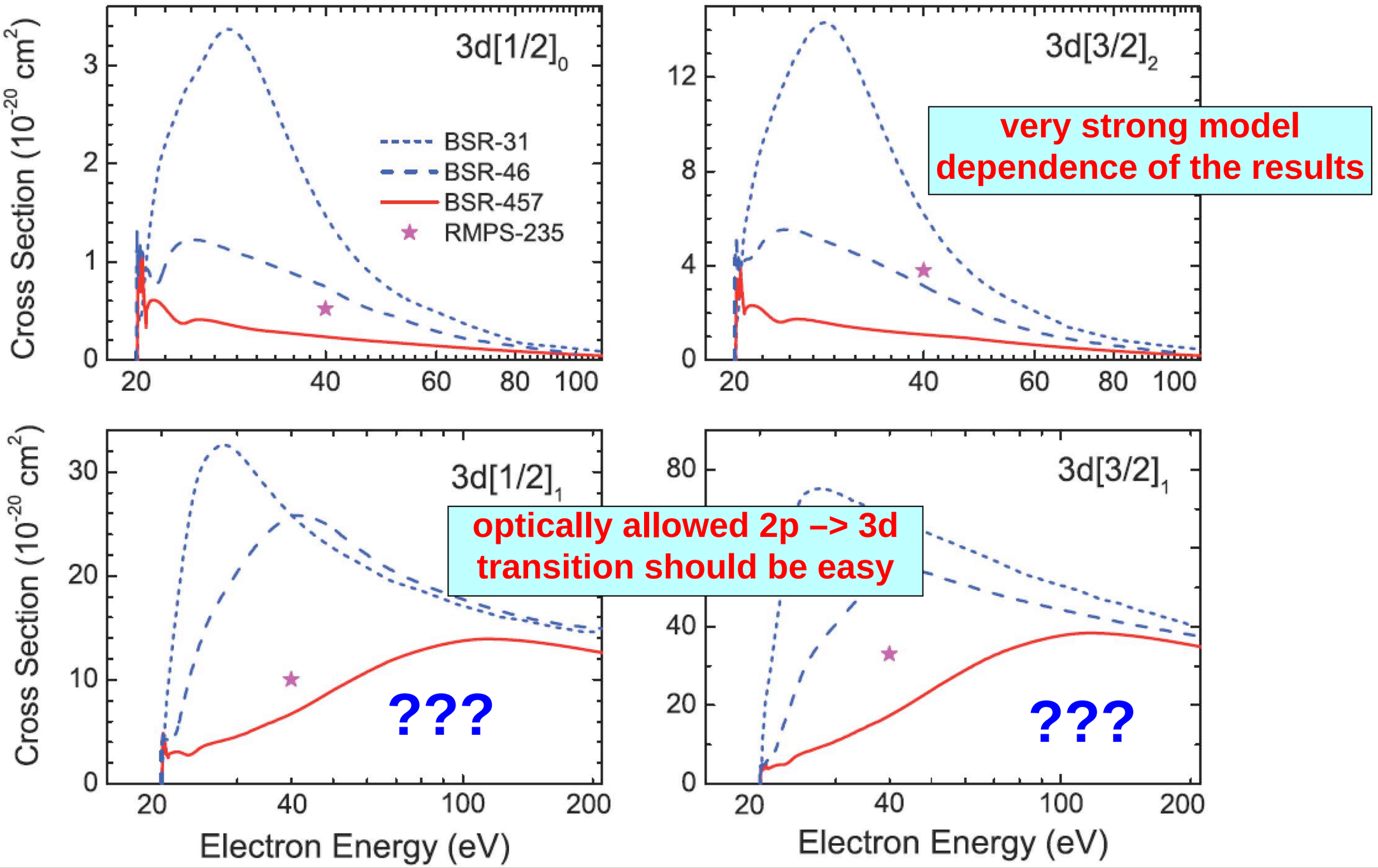


PHYSICAL REVIEW A **86**, 022717 (2012)

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.

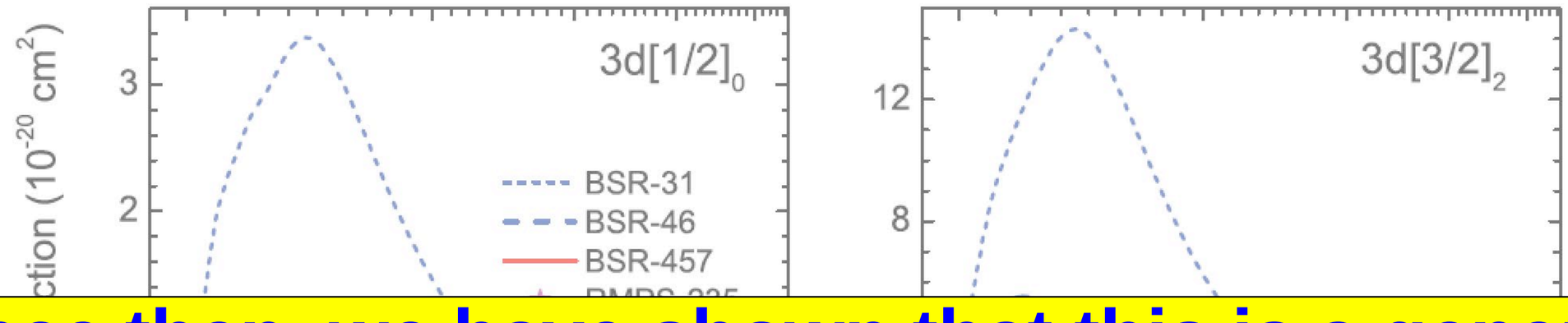
PHYSICAL REVIEW A **86**, 022717 (2012)

Electron-impact excitation of neon at intermediate energies

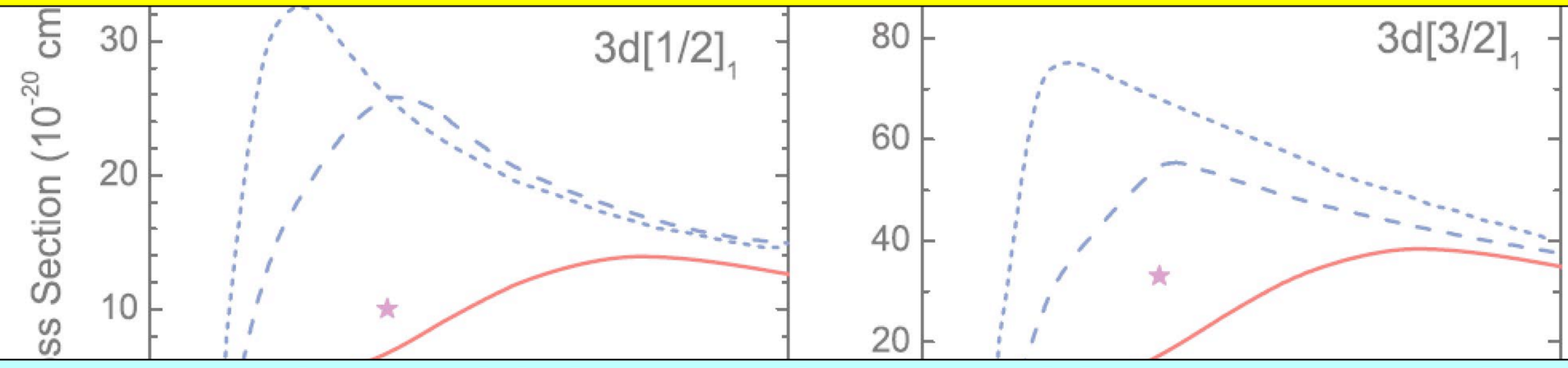
Oleg Zatsarinny and Klaus Bartschat

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, ...)

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:**

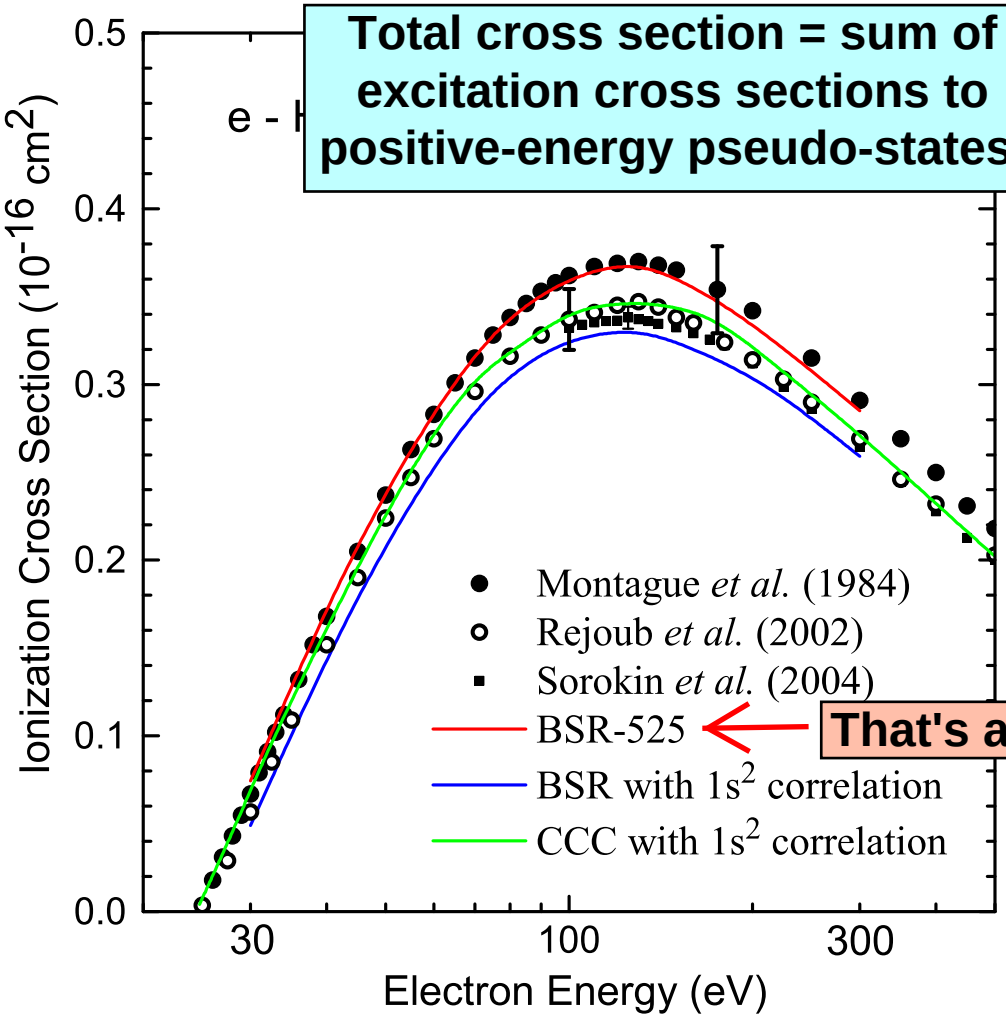
This direct projection is the essential idea – we'll see if it works.

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

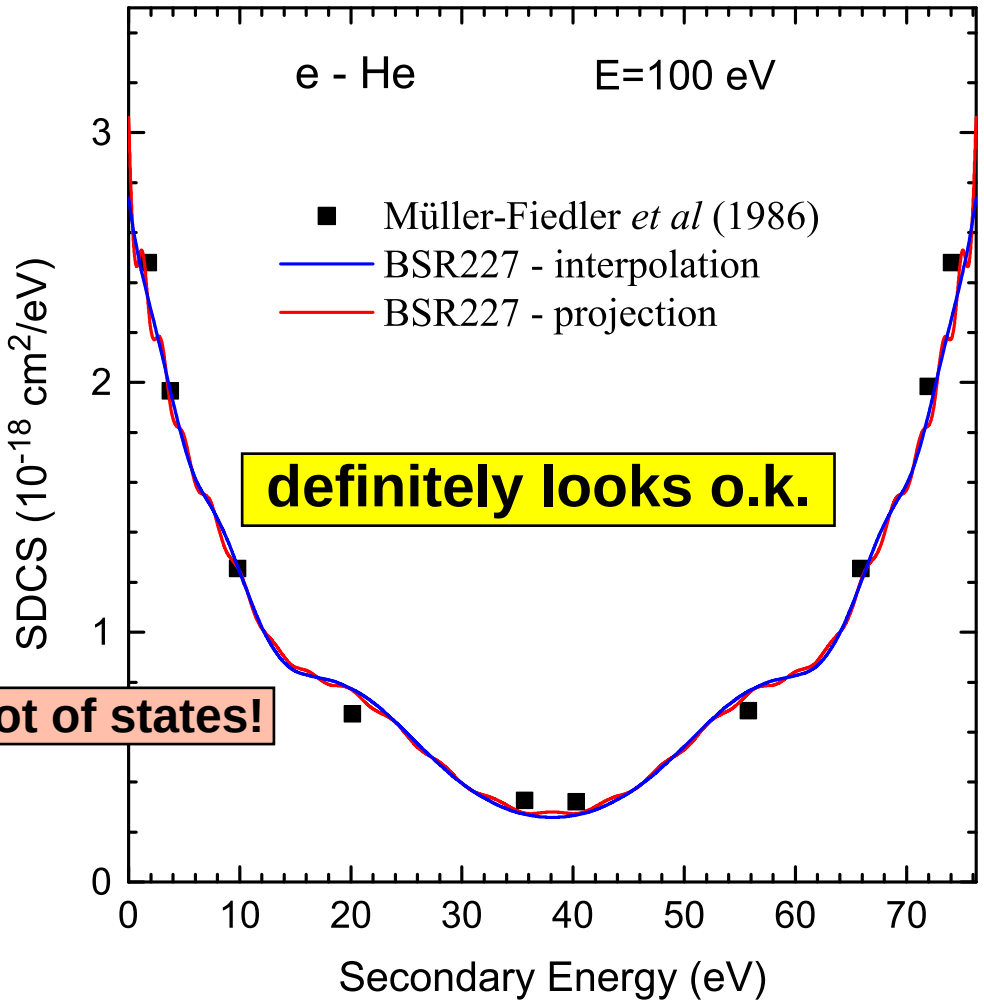
Some Checks: Ionization without Excitation (compare to CCC and TDCC)

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.

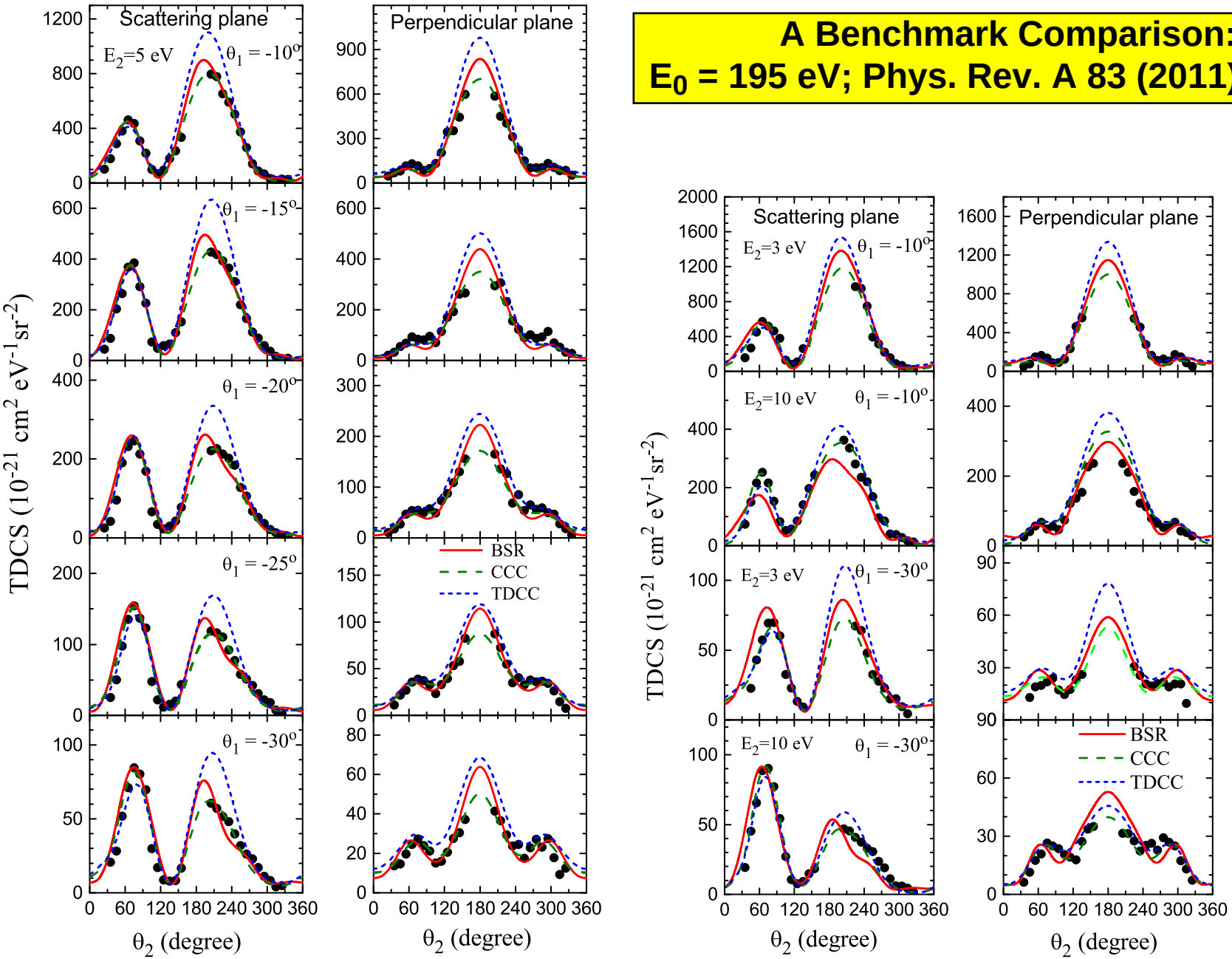
- **Including correlation in the ground state reduces the theoretical result.**
- **Interpolation yields smoother result, but direct projection is acceptable.**
- **DIRECT PROJECTION is NECESSARY for MULTI-CHANNEL cases!**

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

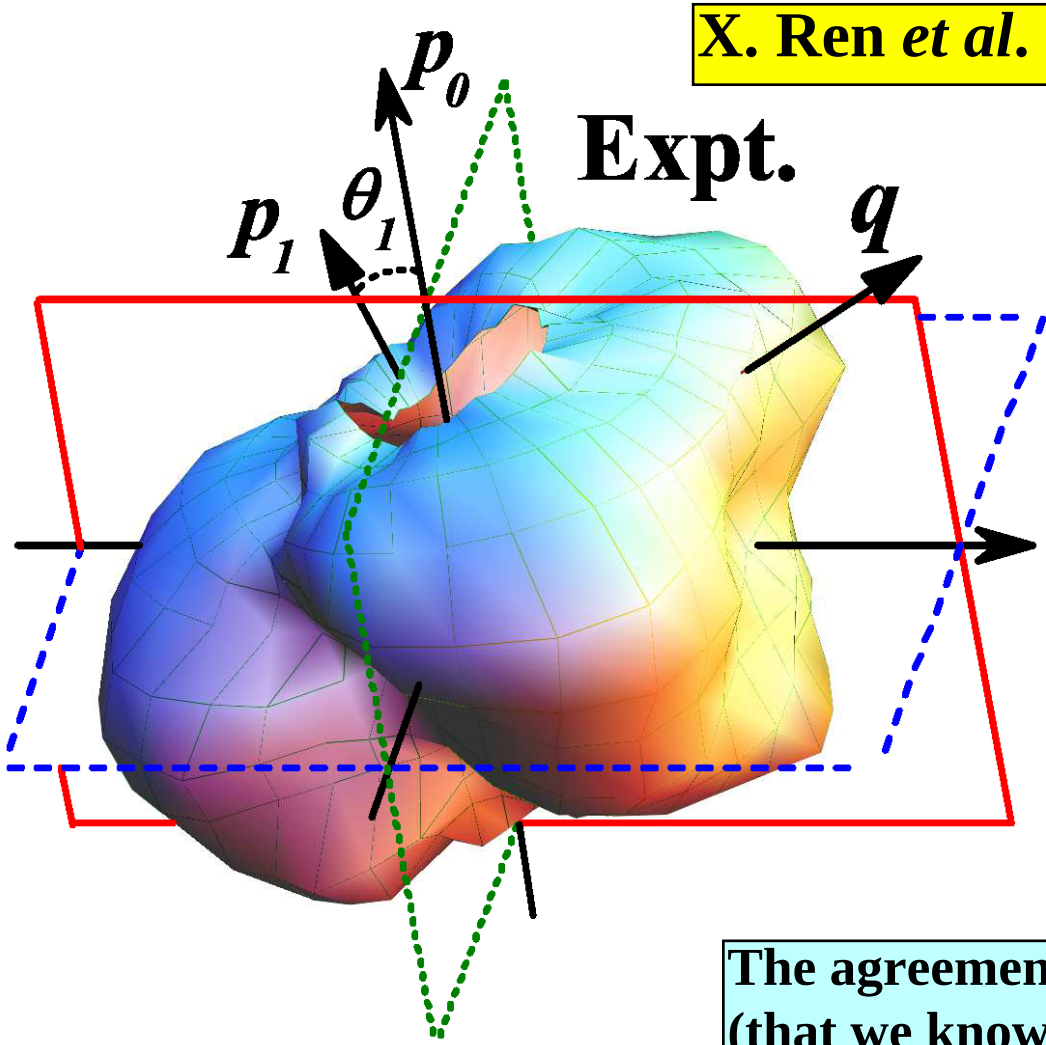


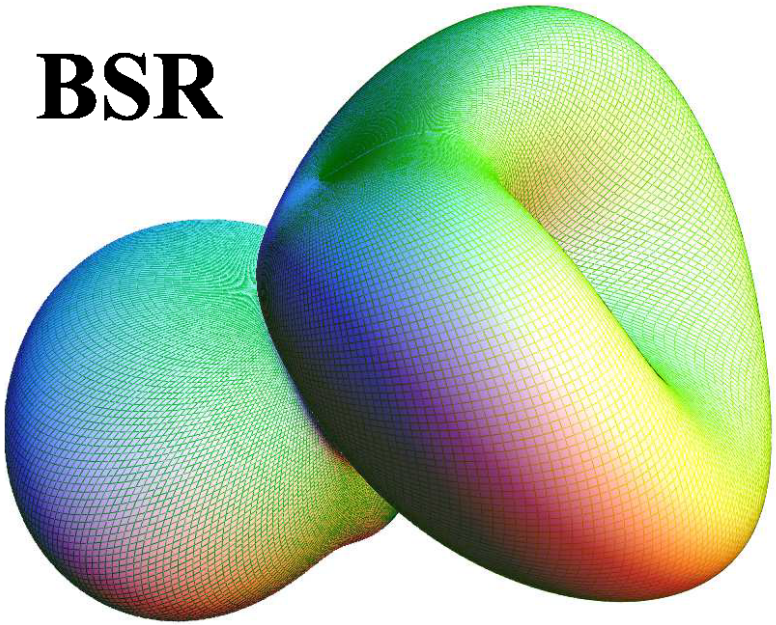
(e,2e) on Ar is a very l .. o .... n ..... g story. It includes the discovery of an error in the processing of the raw experimental data, which was found by the confidence gained in BSR predictions ...

(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

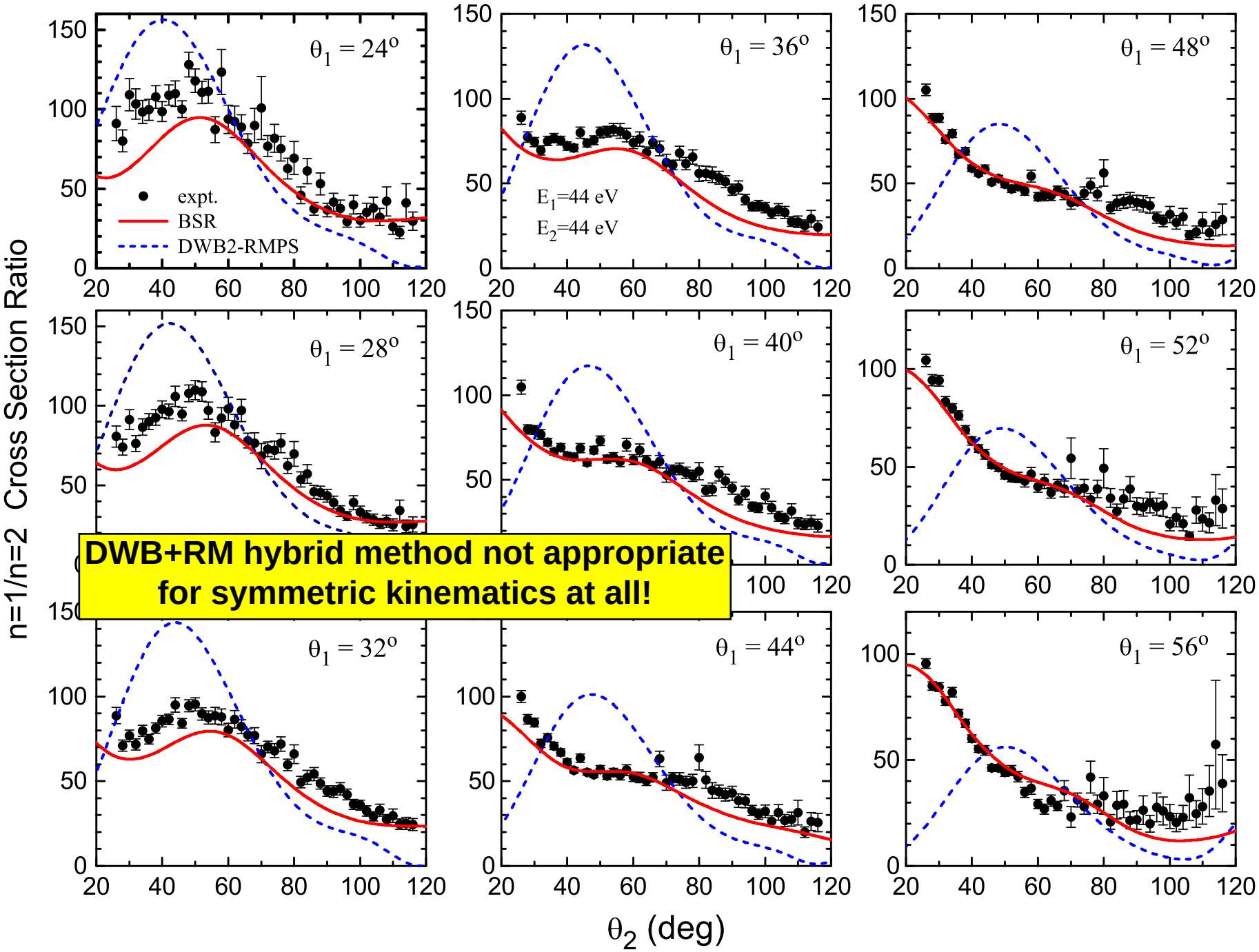
All Three Electrons Change Their Quantum State

(Movie by Allison Harris, Illinois State University)

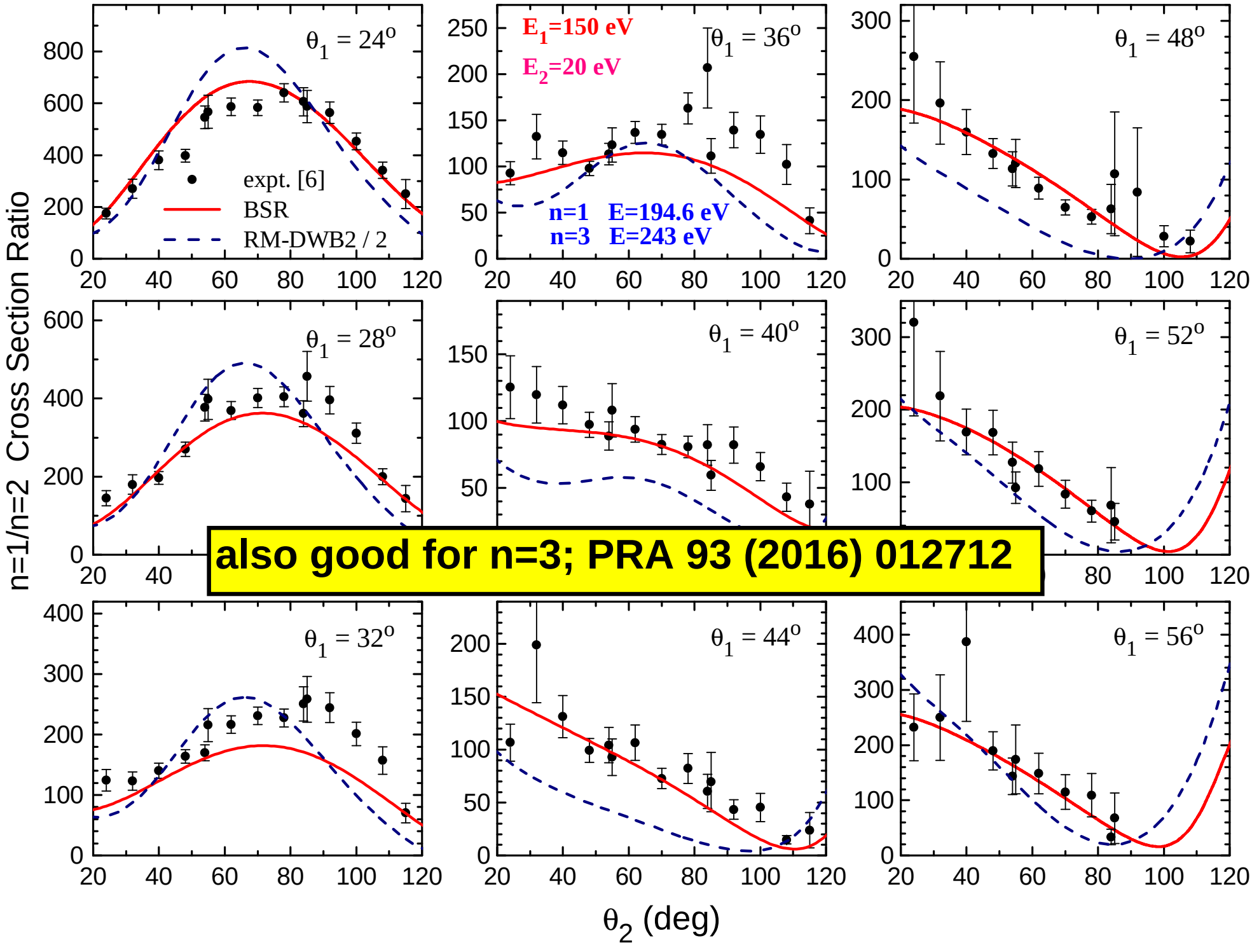
BSRMPS works great: PRL 107 (2011) 023203

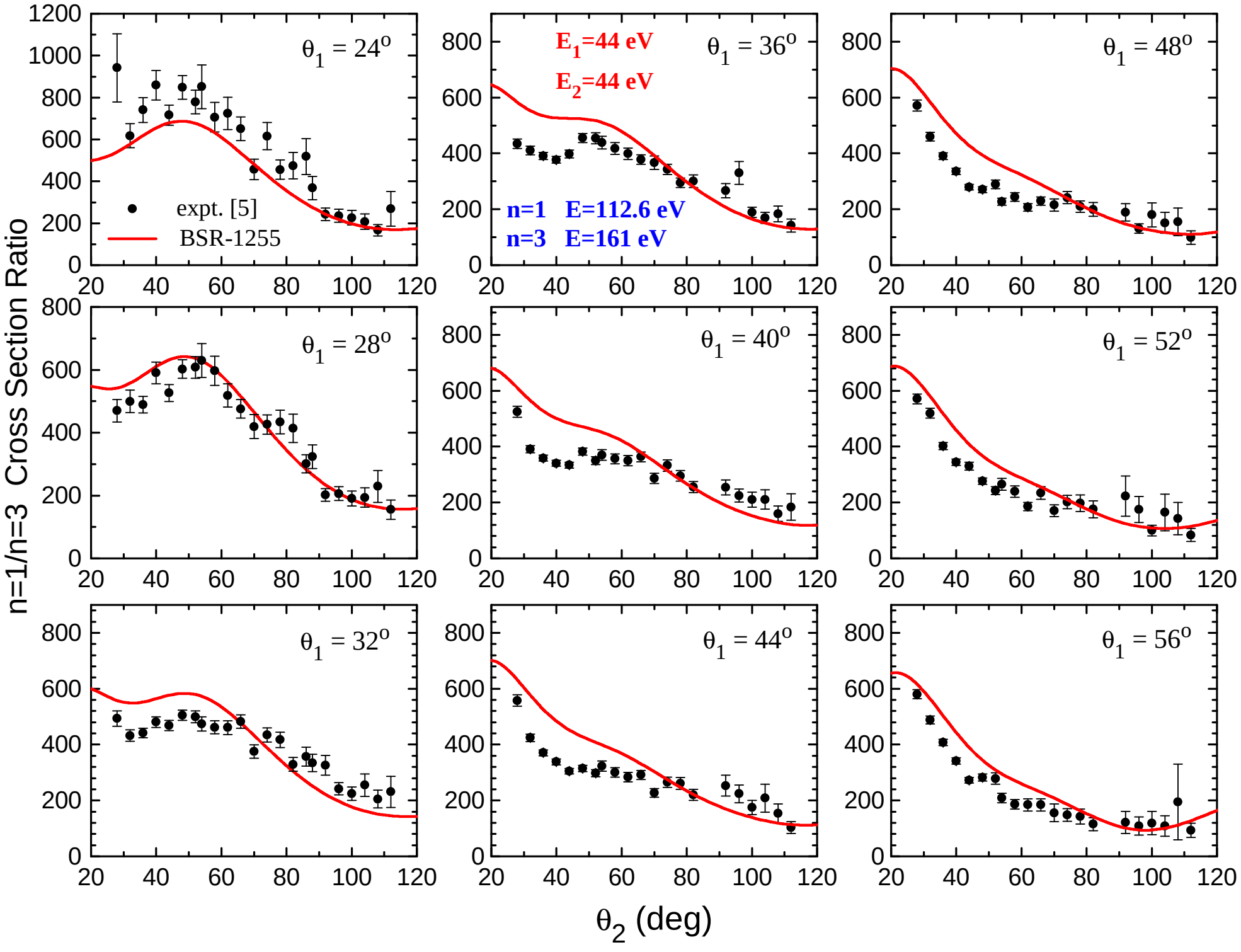
Triple-Differential Cross Section Ratio

experiment: Bellm, Lower, Weigold; measured directly



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


n=1/n=2 Cross Section Ratio
θ2 (deg)
θ1 = 24o
θ1 = 28o
θ1 = 32o
θ1 = 36o
θ1 = 40o
θ1 = 44o
θ1 = 48o
θ1 = 52o
θ1 = 56o
E1=150 eV
E2=20 eV
n=1 E=194.6 eV
n=3 E=243 eV
expt. [6]
BSR
RM-DWB2 / 2
also good for n=3; PRA 93 (2016) 012712


n=1/n=3 Cross Section Ratio
θ2 (deg)
θ1 = 24o
θ1 = 28o
θ1 = 32o
θ1 = 36o
θ1 = 40o
θ1 = 44o
θ1 = 48o
θ1 = 52o
θ1 = 56o
expt. [5]
BSR-1255
E1=44 eV
E2=44 eV
n=1 E=112.6 eV
n=3 E=161 eV

PHYSICAL REVIEW A **85**, 022701 (2012)

Topological angular momentum in electron exchange excitation of a single atom

J. F. Williams, L. Pravica, and S. N. Samarin

ARC Centre of Excellence for Antimatter and Matter Studies Centre for Atomic, Molecular and Surface Physics (CAMSP), School of Physics, M013, University of Western Australia, Perth 6009, Australia

Not everything is clear in electron scattering ...

In a single free two-valence-electron atom, the motion of the electron spin is a consequence of quantum statistics and the Pauli exclusion principle. Subsequently, during an electron impact exchange excitation from a $^1S_0\ M_S = 0$ to a $^3S_1\ M_S = 0$ state, the electron spin is "parallel transported" around a closed path with a geometrical Berry phase of π radians creating an aligned exchange spin angular momentum. This alignment is observed via the Stokes parameter P_2 of the photon decay into a ^3P state. The geometric phase is in addition to the dynamic phase. Measurements from zinc and mercury atoms in different laboratories show the effect close to the excitation threshold where there are no competing excitation processes. Similar effects are expected in other atomic and molecular quantum scattering processes where comparable geometrical or topological paths exist. Electron quantum scattering theories use antisymmetrized wave functions but none include this geometrical exchange angular momentum.

"The task remains for theory to include a topological nondynamical phase."

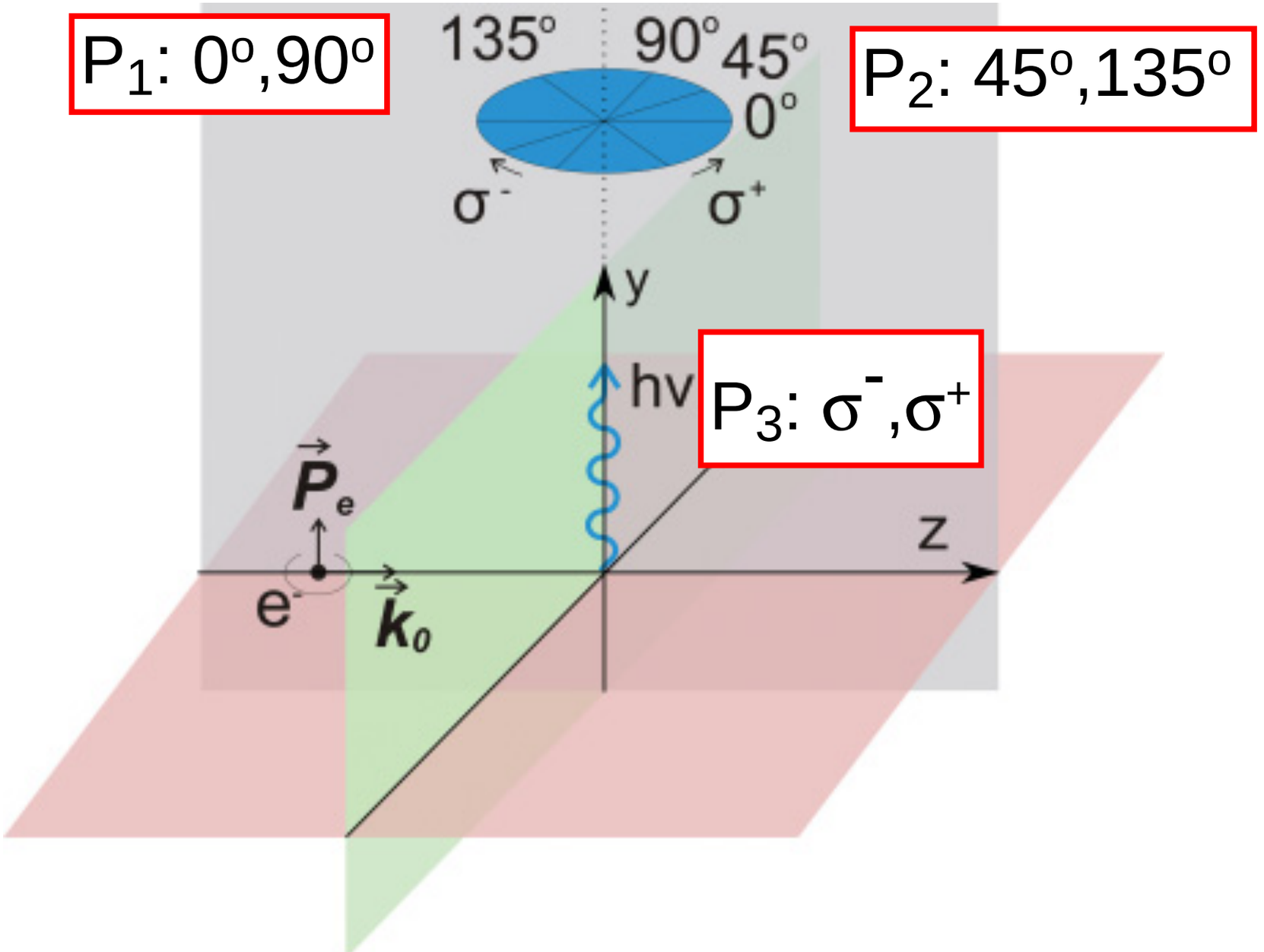


FIG. 1. (Color online) The geometrical (xyz) reference frame and scattering geometry. The spin $\boldsymbol{P_e}$ momentum $\boldsymbol{k_0}$ vectors of the incident electron beam define the scattering (yz) planar symmetry with the target atoms at the origin. Photons emitted along the y axis are analyzed with wavelength filters and linear and circular polarizers before detection with a photomultiplier.

$e + Zn(4s^2) \longrightarrow e + Zn(4s5s)^3S_1 \longrightarrow e + Zn(4s4p)^3P_{0,1,2} + h\nu$

Eminyan & Lampel (1980): P_3 = factor (J_f) x P_e (confirmed experimentally)
K.B. & K. Blum (1982): $P_1 = P_2 = 0$ (independent of P_e for this transition)

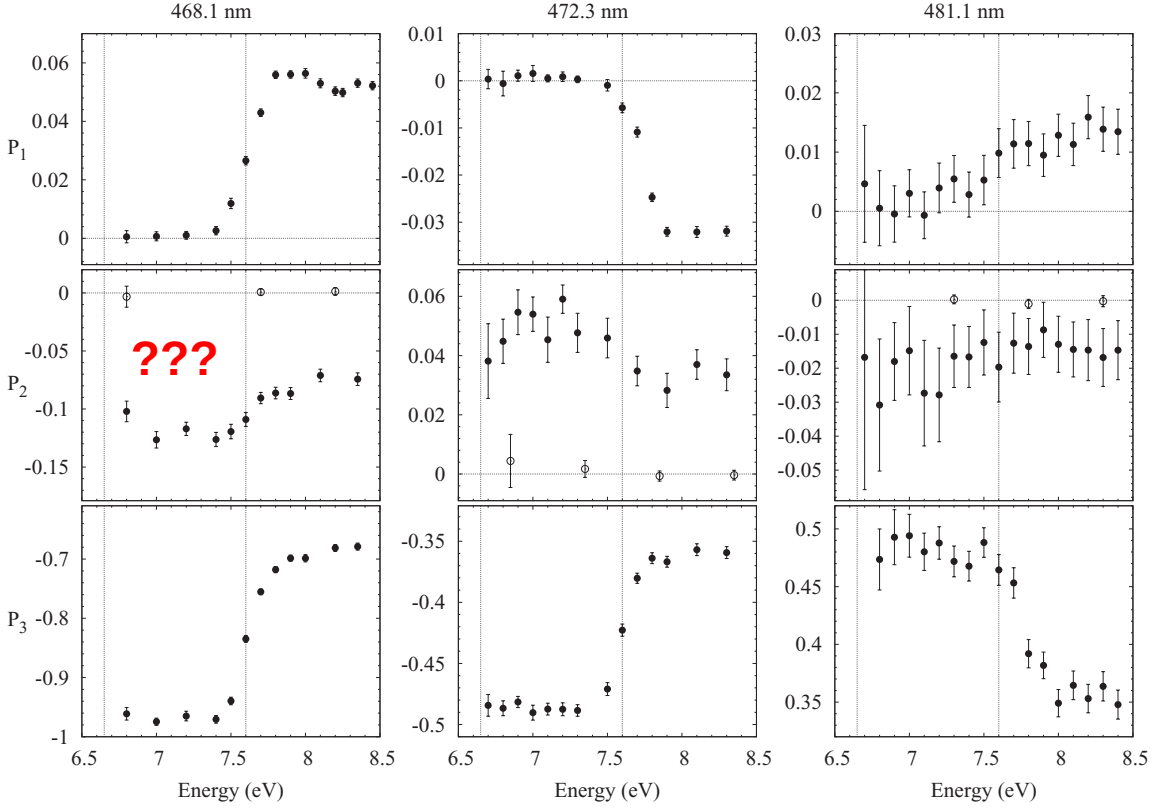


FIG. 2. The integrated Stokes parameters $P_{i=1,2,3}$ for zinc atoms excited from the ground $4s^1S_0$ state to the $5s^3S_1$ state and observed by the subsequent radiative decay to the $4p^3P_{0,1,2}$ states with photon wavelengths for $J = 0,1,2$ of 468.1, 472.3, and 481.1 nm, respectively. The data were normalized to an electron beam polarization which varied for different measurements but was normally of the order of 66 $\pm$ 0.5%. The threshold excitation energy for the $4s5s\ ^3S_1$ state is 6.65 eV and for the first cascading $5p\ ^3P$ state at 7.6 eV, as shown by the vertical lines. The open circles indicate measurements using unpolarized electrons and the closed circles using polarized incident electrons and normalized to the average incident spin P_e.

Comment I on "Topological angular momentum in electron exchange excitation of a single atom"

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(Received 4 April 2012; published 9 January 2013)

In their recent paper, Williams *et al.* [Phys. Rev. A **85**, 022701 (2012)] report on the apparatus and experimental method for the measurement of the Stokes parameter P_2 associated with spin-polarized electron impact $(3d^{10}s^2)\,{}^1S_0 \rightarrow (3d^{10}4s5s)\,{}^3S_1$ excitation of zinc. On the basis of a qualitative semiclassical argument, they make the following claim regarding the discrepancy between theory and experiment for P_2: "The task remains for theory to include a topological nondynamical phase." We analyze the validity of this assertion.

DOI: 10.1103/PhysRevA.87.016701 **Theorists were not happy ...** 4.80.Dp

Comment II on "Topological angular momentum in electron exchange excitation of a single atom"

Klaus Bartschat and Oleg Zatsarinny
Department of Physics and Astronomy, Drake University, Des Moines, Iowa 50311, USA
(Received 4 April 2012; published 9 January 2013)

A recent article by Williams *et al.* [Phys. Rev. A **85**, 022701 (2012)] highlights a discrepancy between experiment and theory for the linear light polarization P_2 measured after impact excitation of zinc atoms by a spin-polarized electron beam. The claim is made that current collision theories must be modified by including a geometric (Berry) phase in the calculations in order to reproduce the experimental data for Zn and similar data from the Münster group for Hg. We show that the *e*-Hg data can be qualitatively reproduced by our fully relativistic *B*-spline *R*-matrix approach *without* any further modification.

DOI: 10.1103/PhysRevA.87.016702

BSR gets nonzero P_2 for Hg, but not for Zn.

A serious discrepancy between experimental data and theoretical predictions was recently reported [1] for spin-polarized electron-impact excitation of the $(4s5s)\,^3S_1$ state in Zn atoms. The linear light polarization P_2, measured for optical decays to the $(4s4p)\,^3P_{0,1,2}$ states with a photon detector aligned along the direction of the spin polarization P_e of the incident electron beam, was found to be significantly (nearly 10% for the final state $^3P_0$) different from zero, whereas, all available numerical calculations predicted an effect of less than 0.01% in the cascade-free region just above the excitation threshold. In 1982, Bartschat and Blum [2] predicted a zero re
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interaction with terms of different L's and S's is negligible. The $(4s5s)\,^3S_1$ state in Zn seems to be a very good candidate for such a case, and Zn is sufficiently light that spin-orbit effects during the excitation process are likely small. Hence,

The experimental data from the Münster group (Goeke, Wolcke, Hanne, Kessler) were never published.

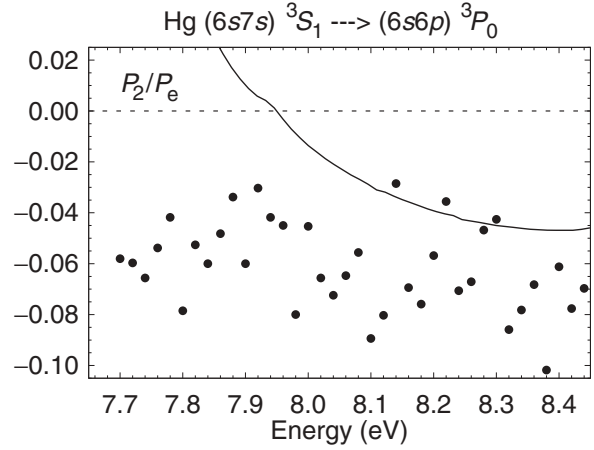

FIG. 1. P_2/P_e for spin-polarized electron-impact excitation of the $(6s7s)\,^3S_1$ st $^3P_0$ state. The e e DBSR prediction based on the model described in Ref. [6].

Tim Gay: Hg is not Zn!

The Solution?

PRL **119,** 093401 (2017) PHYSICAL REVIEW LETTERS week ending 1 SEPTEMBER 2017

Alignment of the $(3d^{10}4s5s)^3S_1$ State of Zn Excited by Polarized Electron Impact

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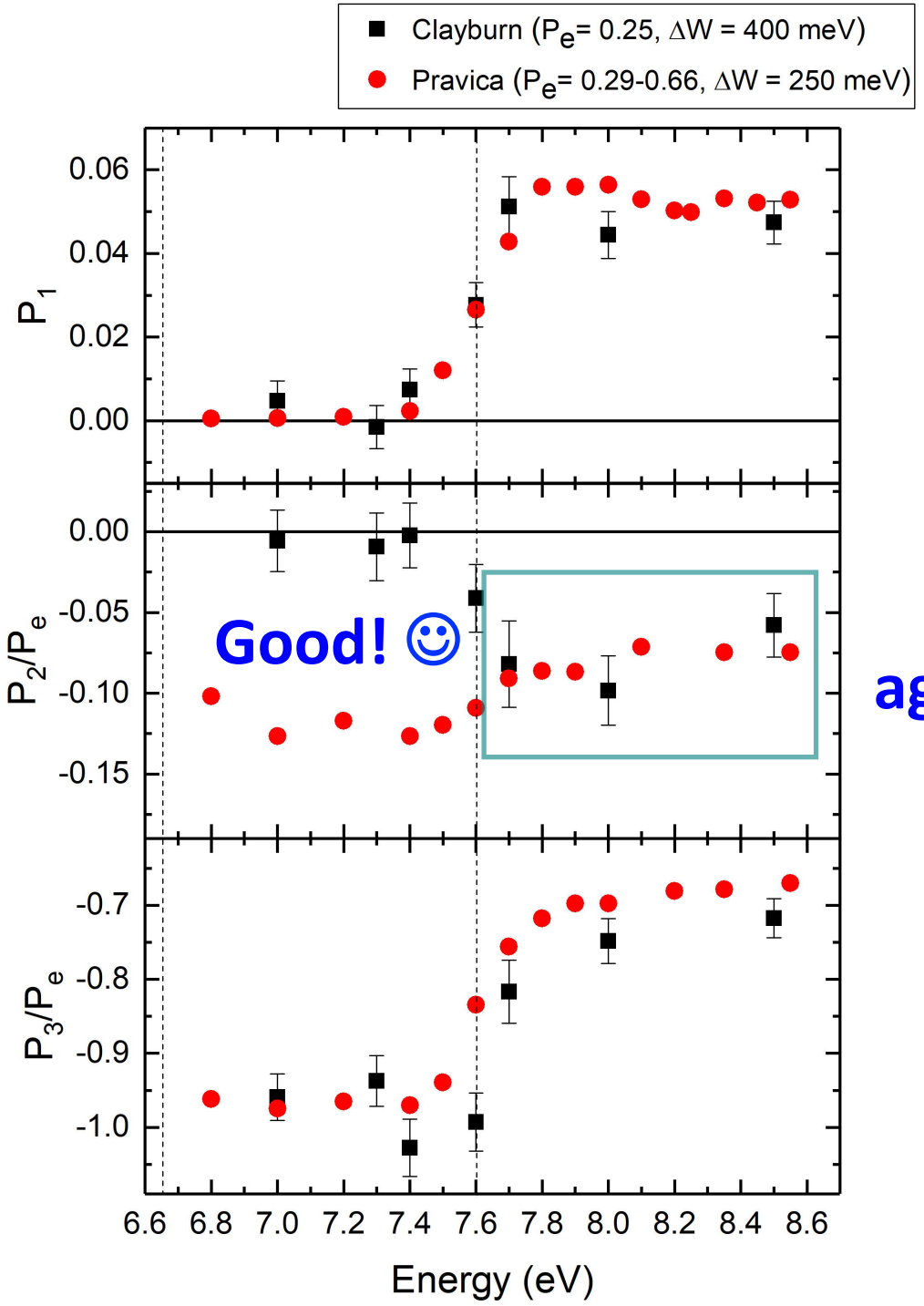
(Received 5 July 2017; published 31 August 2017)

We measure the integrated Stokes parameters of light from Zn $(4s4p)4^3P_{0,1}$-$(4s5s)5^3S_1$ transitions excited by a transversely polarized electron impact at energies between 7.0 and 8.5 eV. Our results for the electron-polarization-normalized linear polarization Stokes parameter P_2, between incident electron energies 7.0 and 7.4 eV, are consistent with zero, as required by basic angular-momentum coupling considerations and by recent theoretical calculations. They are in qualitative disagreement with previous experimental results for the P_2 parameter.

DOI: 10.1103/PhysRevLett.119.093401



Why is there agreement here?

The latest on this one: We stick with "zero" (below AND above the cascade threshold)!

Effect of cascade transitions on the polarization of light emitted after electron-impact excitation of Zn by spin-polarized electrons

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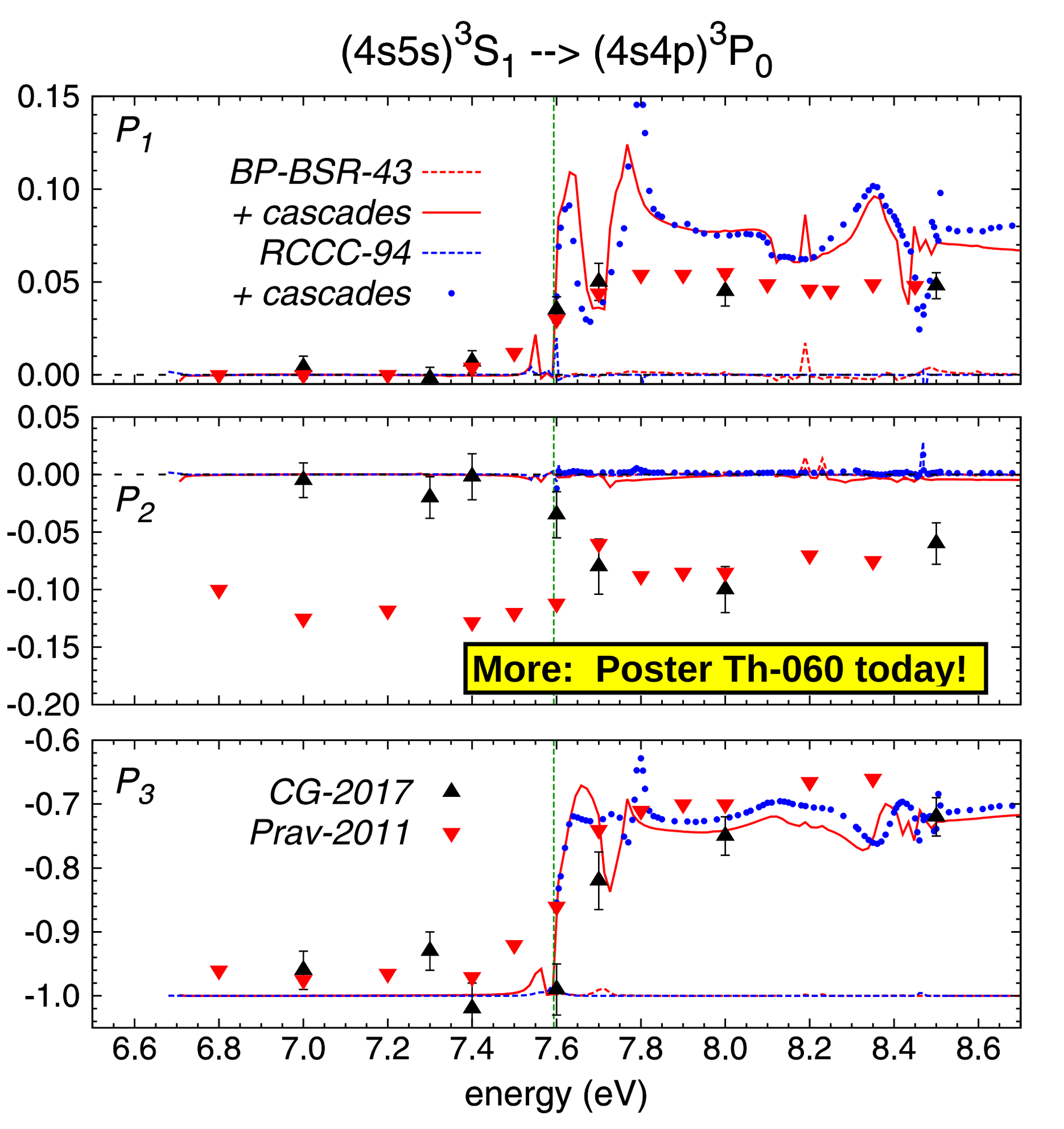
A. N. Grum-Grzhimailo
Skobeltsyn Institute of Nuclear Physics, Lomonosov Moscow State University, Moscow 119991, Russia

(Received 4 April 2019; published 3 July 2019)

We investigate the possible effect of cascade transitions from the $(4s5p)\,^3P_{0,1,2}$ states to the $(4s5s)\,^3S_1$ state of Zn. The polarization of the light emitted in the subsequent decay to the $(4s4p)\,^3P_{0,1,2}$ states has been the subject of recent controversy, with significant disagreement between the experimental data reported by Pravica *et al.* [Phys. Rev. A **83**, 040701 (2011)] and by Clayburn and Gay [Phys. Rev. Lett. **119**, 093401 (2017)] in the cascade-free region below ≈7.6 eV incident energy and relatively good agreement above. The cross sections for excitation of the $(4s5p)\,^3P_{0,1,2}$ states, as well as higher-lying triplet states, and the linear polarization of the cascade radiation seem too small to produce a significant alignment of the $(4s5s)\,^3S_1$ state, thereby raising additional questions regarding the origin of the relatively large linear polarizations measured above the cascade threshold.

DOI: 10.1103/PhysRevA.100.012702


$(4s5s)^3S_1$ --> $(4s4p)^3P_0$
P_1
BP-BSR-43
+ cascades
RCCC-94
+ cascades
P_2
More: Poster Th-060 today!
P_3
CG-2017
Prav-2011
0.15
0.10
0.05
0.00
0.05
0.00
-0.05
-0.10
-0.15
-0.20
-0.6
-0.7
-0.8
-0.9
-1.0
6.6
6.8
7.0
7.2
7.4
7.6
7.8
8.0
8.2
8.4
8.6
energy (eV)

Electron Collision Data for Applications:

About the proje

Where do the results go?

One (of many) databases: LXCat

https://fr.lxcat.net/home/

The **Plasma Data Exchange Project** is a c…aseous Electronics Conference (GEC), a leading int…at least in part, the well-recognized needs for the com… interpretation of experiments.

open-access website for collecting, displaying, and downloading electron and ion scattering cross sections, swarm parameters (*mobility*, *diffusion coefficients*, *etc.*), reaction rates, energy distribution functions, etc. and other data required for modeling low temperature plasmas.

This is a dynamic website, evolving as contributors add or upgrade data. Check back again frequently.

Supporting organizations

Laplace · CNRS · Plasmas Froids · Chatham University · Colorado Kinema · UNAM · Curtin University of Technology · CERN · Instituto Superior Técnico Lisboa · Drake University · Uppsala University · Quantemol · LPP · Institute of Space and Astronautical Science · York University · ABB · TU/e · STAE Toulouse · Australian National University · IIT · Plasma Matters.

FAST NAVIGATION

« PREV | NEXT »

NEWS AND EVENTS

2018-07-10 I New links to software
Links have been added to a multi-term Boltzmann solver, and to three tools by Mikhail Benilov and co-workers. Visit the recommended software page.

RECENT PUBLICATIONS

2019-03-05 I NEW UNPUBLISHED NOTES
Data needed for modeling low-temperature plasmas by LC Pitchford … read more »

PROJECT STATISTICS

Scattering cross sections: 24 databases I 94 x 415 species I 21.1k records I updated: 30 April 2019
Differential scattering cross sections: 4 databases I 29 species I 517 records I updated: 12 March 2019
Interaction potentials: 1 database I 78 x 8 species I 646 records I updated: 30 April 2019
Oscillator strengths: 1 database I 65 species I 150 records I updated: 25 November 2013
Swarm / transport data: 15 databases I 362 x 108 species I 169.4k records I updated: 30 April 2019
Publications, notes and reports: 5 databases I 30 records I updated: 5 March 2019

BSR (Quantum-mechanical calculations by O. Zatsarinny and K. Bartschat)

PERMLINK: www.lxcat.net/BSR

DESCRIPTION: The results in this database are from a semirelativistic Breit-Pauli B-spline R-matrix (close coupling) treatment of e-Ar collisions. An individually optimized, term-dependent set of non-orthogonal valence orbitals was used to account for the strong term dependence in the one-electron orbitals. The predictions have been validated against a number of benchmark experimental data measured in crossed-beam setups. Particularly good agreement was achieved in the near-threshold resonance regime, where the excitation process is dominated by negative-ion resonances.

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e-mails: oleg_zoi@@yahoo.com and klaus.bartschat@@drake.edu

HOW TO REFERENCE: O. Zatsarinny and K. Bartschat 2004 J. Phys. B: At. Mol. Opt. Phys. 37 4693 and
M. Allan, O. Zatsarinny, and K. Bartschat 2006 Phys. Rev. A 74 030701 (R).

SCATTERING CROSS SECTIONS

Species: e + **Ar {30}** , **Be {19}** , **C {63}** , **F {8}** , Kr [70], **N {27}** , Ne [34], Xe [76]
Updates: 2011-06-28 … 2017-09-09
Downloads: 5020 times from 2010-11-21

There is undoubtedly interest in these data.

DIFFERENTIAL SCATTERING CROSS SECTIONS

Species: e + Ar [62]
Updates: 2013-11-06 … 2016-05-29
Downloads: 1219 times from 2013-11-07

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

How good are the data?
[This question is not just for theory!]

Uncertainty estimates for theoretical atomic and molecular data

See also:
The Editors 2011 Phys. Rev. A 83 040001
and Gordon Drake's Tutorial on Tuesday

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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.

IOP PUBLISHING PHYSICA SCRIPTA

Phys. Scr. **T134** (2009) 014020 (9pp) doi:10.1088/0031-8949/2009/T134/014020

B-spline calculations of oscillator strengths in noble gases

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Abstract

B-spline box-based multi-channel calculations of transition probabilities in noble gases are reported for energy levels up to $n = 12$. Energy levels and oscillator strengths for transitions from the p^6 ground-state configuration, as well as for transitions between excited states, have been computed in the Breit–Pauli approximation. Individually optimized, term-dependent sets of non-orthogonal valence orbitals are used to account for the strong term dependence in the one-electron orbitals. The agreement in the length and velocity gauges of the transition data and the accuracy of the binding energies are used to estimate the accuracy of our results, which are also compared with experimental and other theoretical data. It is shown that the present method can be used for accurate calculations of oscillator strengths for states with intermediate to high n-values, for which it is difficult to apply standard multi-configuration Hartree–Fock (MCHF) methods. Recent developments based on the extension of our computer codes from the semi-relativistic Breit–Pauli Hamiltonian to the full relativistic Dirac–Breit Hamiltonian are also reported.

Summary of structure work

- The non-orthogonal orbital technique allows us account for **term-dependence** and **relaxation** effects practically to full extent. At the same time, this reduce the size of the configuration expansions, because we use **specific non-orthogonal sets of correlation orbitals** for different kinds of correlation effects.
- ***B***-spline multi-channel models allow us to treat entire Rydberg series and can be used for accurate calculations of oscillator strengths for states with **intermediate and high *n*-values**. For such states, it is difficult to apply standard CI or MCHF methods.
- The accuracy obtained for the low-lying states is close to that reached in large-scale MCHF calculations.
- **Good agreement with experiment** was obtained for the transitions from the ground states and also for transitions between excited states.
- **Calculations performed in this work**: s-, p-, d-, and f-levels up to ***n* = 12**.

```
Ne - 299 states  -  11300 transitions
Ar - 359 states  -  19000 transitions
Kr - 212 states  -   6450 transitions
Xe - 125 states  -   2550 transitions
```

- **All calculations are fully *ab initio*.**
- The **computer code BSR** used in the present calculations and the results for Ar were recently published:

BSR: O. Zatsarinny, Comp. Phys. Commun. **174** (2006) 273
Ar: O. Zatsarinny and K. Bartschat, J. Phys. B **39** (2006) 2145

A "simple"(?) collision problem. e-Be^+: coupling to continuum most important for i) optically forbidden transitions and/or ii) small cross sections

good agreement between CCC, RMPS, TDCC — no experiment !

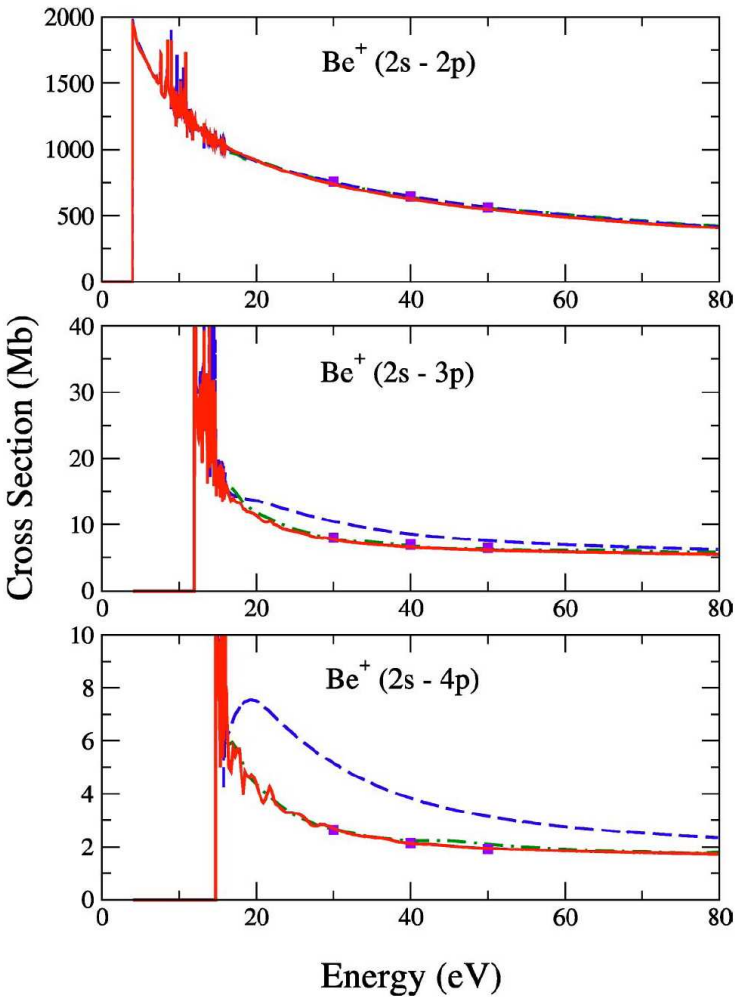

FIG. 4. Electron-impact excitation cross sections from the 2*s* ground term of Be^+ to the *np* excited terms. Dashed curves are from the present 14-term *R*-matrix calculation; solid curves are from the present 49-term RMPS calculation; solid squares are from the present TDCC calculation; dot-dashed curves from the CCC calculation by Bartschat and Bray [14].

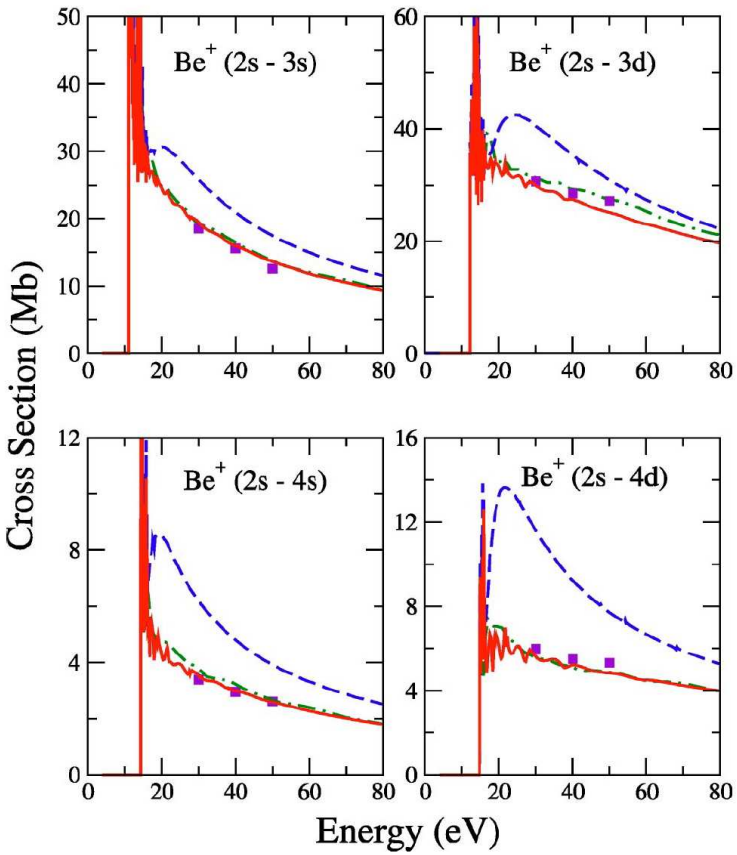

FIG. 5. Electron-impact excitation cross sections from the 2*s* ground term of Be^+ to the *ns* and *nd* excited terms. Dashed curves are from the present 14-term *R*-matrix calculation; solid curves are from the present 49-term RMPS calculation; solid squares are from the present TDCC calculation; dot-dashed curves from the CCC calculation by Bartschat and Bray [14].

This is a light quasi-one electron system. Essentially solved 15 years ago.

Phys. Rev. A 68 (2003) 062705

Another simple one. **e-Be: coupling to continuum most important for i) optically forbidden transitions and/or ii) small cross sections**

good agreement between CCC, RMPS, TDCC — no experiment !

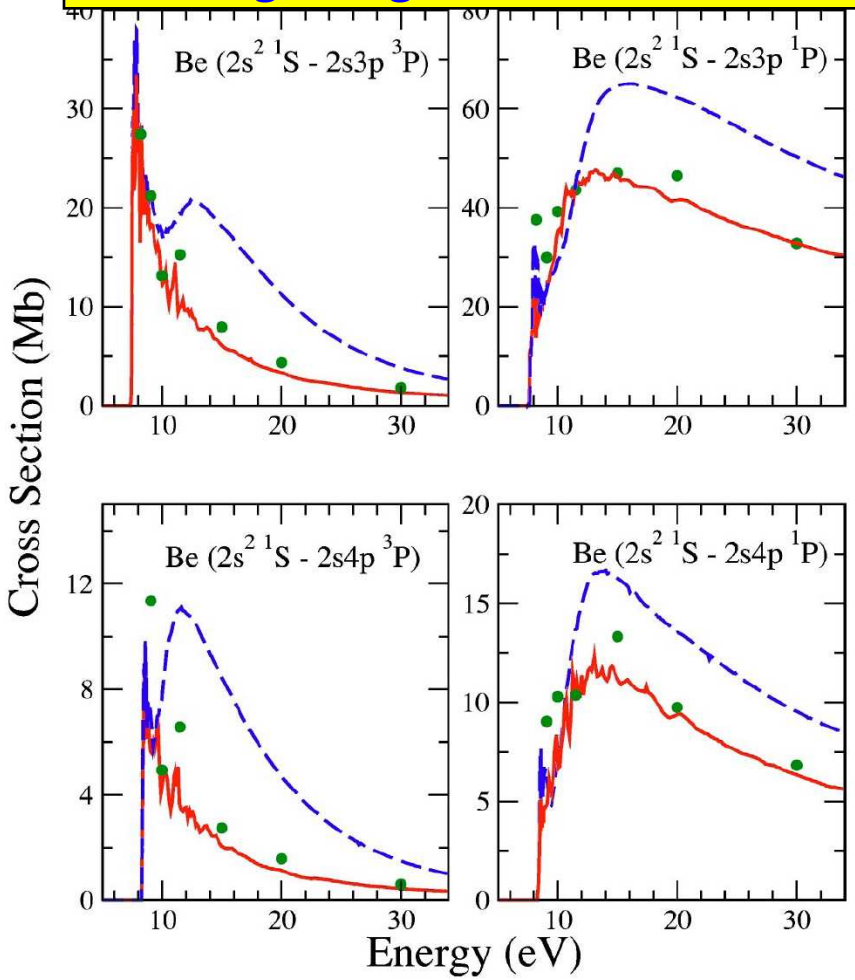

FIG. 2. Electron-impact excitation cross sections from the $2s^2\,{}^1S$ ground term of Be to the $2snp\,{}^3P$ and $2snp\,{}^1P$ excited terms for $n=3$ and 4. Dashed curves are from the present 29-term R-matrix calculation; solid curves are from the present 280-term RMPS calculation; solid circles are from CCC calculations as described in Fursa and Bray [10] and provided at the CCC database web site [11].

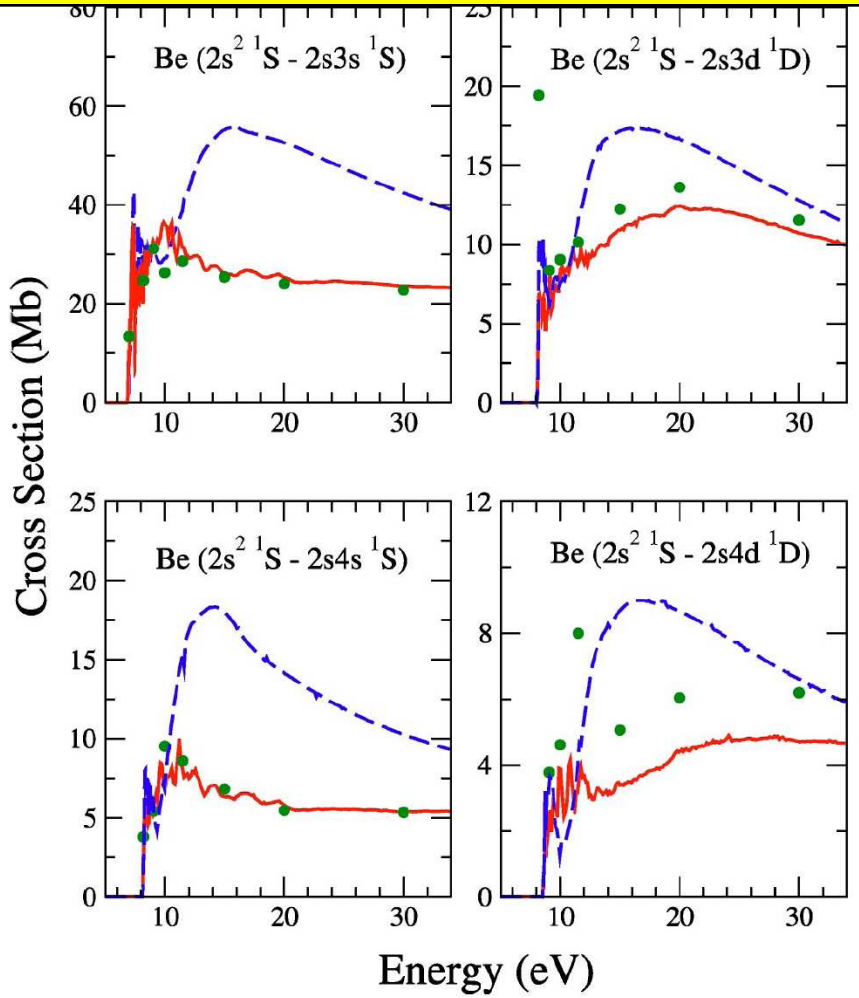

FIG. 3. Electron-impact excitation cross sections from the $2s^2\,{}^1S$ ground term of Be to the $2sns\,{}^1S$ and $2snd\,{}^1D$ excited terms. Dashed curves are from the present 29-term R-matrix calculation; solid curves are from the present 280-term RMPS calculation; solid circles are from CCC calculations as described in Fursa and Bray [10] and provided at the CCC database web site [11].

This is a light quasi-two electron system. Essentially solved 15 years ago.

Phys. Rev. A 68 (2003) 032712

Atomic Data and Nuclear Data Tables 127–128 (2019) 1–21

Contents lists available at ScienceDirect

Atomic Data and Nuclear Data Tables

journal homepage: www.elsevier.com/locate/adt

One can now safely recommend extensive datasets for this system.

Recommended electron-impact excitation and ionization cross sections for Be I

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ARTICLE INFO

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ABSTRACT

Analytic fits to the recommended electron-impact excitation and ionization cross sections for Be I are presented. The lowest 19 terms of configurations $2snl$ ($n \leq 4$) and $2p^2$ terms below the first ionization limit are considered. The fits are based on the accurate calculations with the convergent close coupling (CCC) method as well as the B-spline R-matrix (BSR) approach. The fitted cross sections provide rate coefficients that are believed to approximate the original data within 10% with very few exceptions. The oscillator strengths for the dipole-allowed transitions between all the considered states are calculated with the relativistic multi-configuration Dirac–Hartree–Fock (MCDHF) approach and compared with the CCC and BSR results. This comparison shows a very good agreement except for a handful of cases with likely strong cancellations.

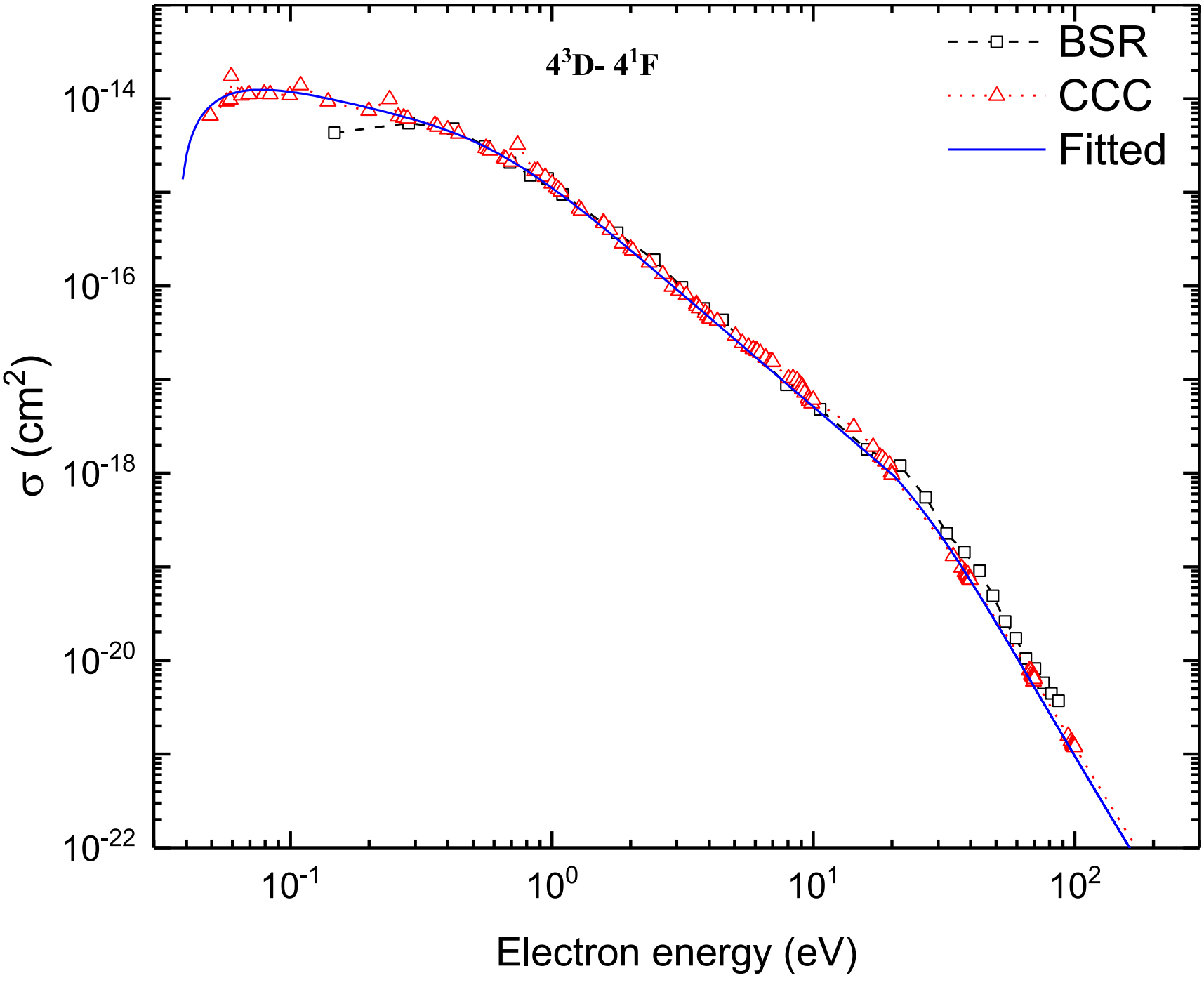

Fig. 4. Electron-impact excitation cross sections for the spin-forbidden ($4^3D \rightarrow 4^1F$) transition.

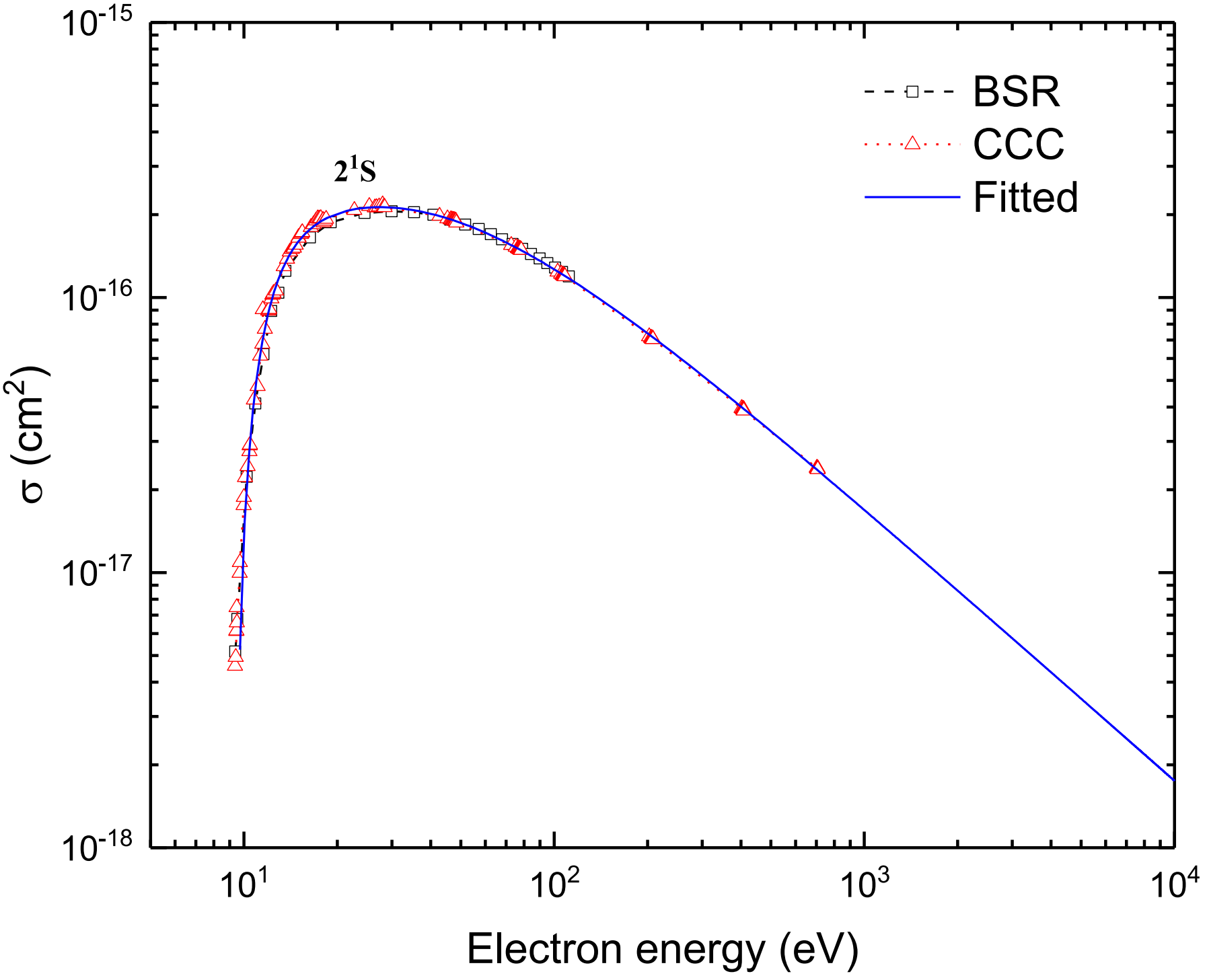

Fig. 6. Electron-impact ionization cross sections from the 2^1S state.

PHYSICAL REVIEW A **99**, 023430 (2019)

Big Challenge: Complex, heavy atoms and ions
Example: Photoionization of iron (—> astrophysics)

Photoionization of neutral iron from the ground and excited states

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(Received 21 January 2019; published 28 February 2019)

The *B*-spline *R*-matrix method is used to investigate the photoionization of neutral iron from the ground and excited states in the energy region from the ionization thresholds to 2 Ry. The multiconfiguration Hartree-Fock method in connection with adjustable configuration expansions and term-dependent orbitals is employed for an accurate representation of the initial states of Fe I and the target wave functions of Fe II. The close-coupling expansion contains 261 *LS* states of Fe II and includes all levels of the $3d^6 4s$, $3d^5 4s^2$, $3d^7$, $3d^6 4p$, and $3d^5 4s 4p$ configurations. Full inclusion of all terms from the principal configurations considerably changes both the low-energy resonance structure and the energy dependence of the background cross sections. Partial cross sections are analyzed in detail to clarify the most important scattering channels. Comparison with other calculations is used to place uncertainty bounds on our final photoionization cross sections and to assess the likely uncertainties in the existing data sets.

DOI: 10.1103/PhysRevA.99.023430

We need the structure of Fe II for the (half) collision ....

TABLE II. Excitation energies (in eV) of the Fe II final target levels included in the present photoionization calculations.

Index	Configuration	Term	Present	NIST [17]	Diff.	Index	Configuration	Term	Present	NIST [17]	Diff.
1	$3d^6(^5D)4s$	$a\ ^6D$	0.00000	0.00000	0.000	51	$3d^6(^3P)4p$	$y\ ^4D^o$	7.68767	7.67642	0.012
2	$3d^7$	$a\ ^4F$	0.22873	0.23746	−0.008	52	$3d^6(^3H)4p$	$z\ ^2I^o$	7.75384	7.68254	0.071
3	$3d^6(^5D)4s$	$a\ ^4D$	1.00085	0.98236	0.019	53	$3d^6(^3F)4p$	$x\ ^4D^o$	7.79919	7.78729	0.012
4	$3d^7$	$a\ ^4P$	1.61611	1.64122	−0.025	54	$3d^6(^3F)4p$	$z\ ^2F^o$	7.93216	7.92629	0.006
5	$3d^7$	$a\ ^2G$	1.97335	1.93060	0.042	55	$3d^6(^3F)4p$	$y\ ^4G^o$	7.96447	7.87869	0.086
6	$3d^7$	$a\ ^2P$	2.15249	2.25549	−0.102	56	$3d^6(^3P)4p$	$z\ ^2P^o$	7.98689	7.98813	−0.001
7	$3d^7$	$a\ ^2H$	2.45967	2.48451	−0.025	57	$3d^6(^3F)4p$	$y\ ^2G^o$	8.02078	7.99718	0.024
8	$3d^7$	$a\ ^2D$	2.52821	2.52757	0.000	58	$3d^6(^3H)4p$	$z\ ^2H^o$	8.05252	8.05993	−0.007
9	$3d^6(^3H)4s$	$a\ ^4H$	2.59340	2.60163	−0.009	59	$3d^6(^3G)4p$	$x\ ^4G^o$	8.14564	8.09909	0.047
10	$3d^6(^3P)4s$	$b\ ^4P$	2.62235	2.61313	0.009	60	$3d^54s^2$	^2I	8.16405		
11	$3d^6(^3F)4s$	$b\ ^4F$	2.78328	2.77477	0.008	61	$3d^6(^3G)4p$	$x\ ^4F^o$	8.16627	8.16450	0.002
12	$3d^54s^2$	$a\ ^6S$	2.94341	2.84212	0.101	62	$3d^6(^3P)4p$	$z\ ^2S^o$	8.18361	8.16489	0.019
13	$3d^6(^3G)4s$	$a\ ^4G$	3.12934	3.13143	−0.002	63	$3d^6(^3G)4p$	$y\ ^4H^o$	8.19170	8.19302	−0.001
14	$3d^6(^3P)4s$	$b\ ^2P$	3.13657	3.20920	−0.072	64	$3d^6(^3F)4p$	$y\ ^2D^o$	8.27347	8.26940	0.005
15	$3d^6(^3H)4s$	$b\ ^2H$	3.16495	3.20032	−0.035	65	$3d^6(^3G)4p$	$y\ ^2H^o$	8.35303	8.33407	0.019
16	$3d^6(^3F)4s$	$a\ ^2F$	3.33076	3.34805	−0.017	66	$3d^5(^6S)4s4p$	$x\ ^4P^o$	8.53341	8.53496	−0.001
17	$3d^6(^3G)4s$	$b\ ^2G$	3.77259	3.72956	0.043	67	$3d^6(^3G)4p$	$y\ ^2F^o$	8.58723	8.58270	0.004
18	$3d^6(^3D)4s$	$b\ ^4D$	3.84077	3.84398	−0.003	68	$3d^6(^3G)4p$	$x\ ^2G^o$	8.70428	8.67498	0.029
19	$3d^7$	$b\ ^2F$	3.88267	3.90300	−0.020	69	$3d^6(^1I)4p$	$z\ ^2K^o$	8.76101	8.76208	−0.001
20	$3d^6(^1I)4s$	$a\ ^2I$	3.97082	4.02791	−0.057	70	$3d^6(^3D)4p$	$w\ ^4P^o$	8.84826	8.88371	−0.036
21	$3d^6(^1G)4s$	$c\ ^2G$	4.08447	4.10141	−0.016	71	$3d^6(^1G)4p$	$x\ ^2H^o$	8.85140	8.89788	−0.047
22	$3d^6(^3D)4s$	$b\ ^2D$	4.43813	4.43693	0.001	72	$3d^6(^3D)4p$	$w\ ^4F^o$	8.90035	8.91993	−0.020
23	$3d^6(^1S)4s$	$a\ ^2S$	4.58154	4.56669	0.015	73	$3d^54s^2$	^2D	8.92103		
24	$3d^6(^1D)4s$	$c\ ^2D$	4.69523	4.68494	0.010	74	$3d^6(^3D)4p$	$y\ ^2P^o$	8.97058	9.02530	−0.054
25	$3d^6(^5D)4p$	$z\ ^6D^o$	4.75973	4.74993	0.010	75	$3d^6(^3D)4p$	$w\ ^4D^o$	8.99030	8.94838	0.042
26	$3d^6(^5D)4p$	$z\ ^6F^o$	5.16594	5.17773	−0.012	76	$3d^6(^1G)4p$	$x\ ^2F^o$	9.01599	9.00526	0.011

... and the structure of Fe I for the initial bound states

TABLE I. Excitation energies (in eV) of the Fe I target levels included in the present photoionization calculations.

Index	Configuration	Term	Present	NIST [17]	Diff.	Index	Configuration	Term	Present	NIST [17]	Diff.
1	$3d^64s^2$	$a\ ^5D$	0.00000	0.00000	0.000	23	$3d^7(^2H)4s$	$a\ ^1H$	3.52020	3.52326	−0.003
2	$3d^7(^4F)4s$	$a\ ^5F$	0.86082	0.87493	−0.014	24	$3d^64s^2$	$a\ ^1I$	3.48480	3.58439	−0.003
3	$3d^7(^4F)4s$	$a\ ^3F$	1.48145	1.48836	−0.007	25	$3d^6(^5D)4s4p$	$z\ ^5P^o$	3.54575	3.58639	0.005
4	$3d^7(^4P)4s$	$a\ ^5P$	2.16087	2.14265	0.018	26	$3d^64s^2$	$b\ ^3D$	3.56252	3.58977	−0.003
5	$3d^64s^2$	$a\ ^3P$	2.28122	2.30004	−0.019	27	$3d^64s^2$	$b\ ^1G$	3.60328	3.64464	−0.004
6	$3d^64s^2$	$a\ ^3H$	2.36601	2.37711	−0.011	28	$3d^6(^5D)4s4p$	$z\ ^3D^o$	3.77607	3.86382	−0.003
7	$3d^6(^5D)4s4p$	$z\ ^7D^o$	2.40412	2.38311	0.021	29	$3d^6(^5D)4s4p$	$z\ ^3F^o$	3.82394	3.87662	0.030
8	$3d^64s^2$	$b\ ^3F$	2.54367	2.53060	0.013	30	$3d^8$	$c\ ^3F$	4.05592	4.07445	0.015
9	$3d^64s^2$	$a\ ^3G$	2.67804	2.67132	0.007	31	$3d^7(^4F)4p$	$y\ ^5D^o$	4.13847	4.10398	−0.006
10	$3d^7(^4P)4s$	$b\ ^3P$	2.77262	2.78906	−0.016	32	$3d^7(^4F)4p$	$y\ ^5F^o$	4.16598	4.18009	−0.018
11	$3d^6(^5D)4s4p$	$z\ ^7F^o$	2.77755	2.79275	−0.015	33	$3d^6(^5D)4s4p$	$z\ ^3P^o$	4.16824	4.18450	−0.064
12	$3d^64s^2$	$a\ ^1S$	2.80530			34	$3d^7(^2D)4s$	$b\ ^1D$	4.23998	4.24445	0.005
13	$3d^7(^2G)4s$	$b\ ^3G$	2.93034	2.93053	−0.000	35	$3d^7(^4F)4p$	$z\ ^5G^o$	4.32527	4.30728	−0.017
14	$3d^6(^5D)4s4p$	$z\ ^7P^o$	2.93705	2.93277	0.004	36	$3d^7(^4F)4p$	$z\ ^3G^o$	4.37188	4.37506	−0.019
15	$3d^7(^2P)4s$	$c\ ^3P$	2.98683	2.99573	−0.009	37	$3d^7(^2F)4s$	$d\ ^3F$	4.51238	4.53713	−0.000
16	$3d^7(^2G)4s$	$a\ ^1G$	3.00166	2.99691	0.005	38	$3d^6(^5D)4s4p$	$y\ ^5P^o$	4.57776	4.54064	−0.014
17	$3d^6(^5D)4s4p$	$z\ ^5D^o$	3.17777	3.19232	−0.015	39	$3d^7(^4F)4p$	$y\ ^3F^o$	4.49736	4.54289	−0.062
18	$3d^7(^2H4s$	$b\ ^3H$	3.20414	3.21453	−0.010	40	$3d^7(^2F)4s$	^1F	4.53208		
19	$3d^7(^2D)4s$	$a\ ^3D$	3.21687	3.22250	−0.006	41	$3d^7(^4F)4p$	$y\ ^3D^o$	4.76043	4.72430	0.024
20	$3d^6(^5D)4s4p$	$z\ ^5F^o$	3.30659	3.32482	−0.018	42	$3d^8$	^1D	4.73248		
21	$3d^7(^2P)4s$	$a\ ^1P$	3.35960	3.36494	−0.005	43	$3d^6(^5D)4s4p$	$x\ ^5D^o$	4.86200	4.90585	−0.006
22	$3d^64s^2$	$a\ ^1D$	3.49993	3.49656	0.003	44	$3d^6(^5D)4s4p$	$x\ ^5F^o$	4.97766	4.98932	−0.012

some even-parity initial states: no experiment, so compare the two presumably best theories

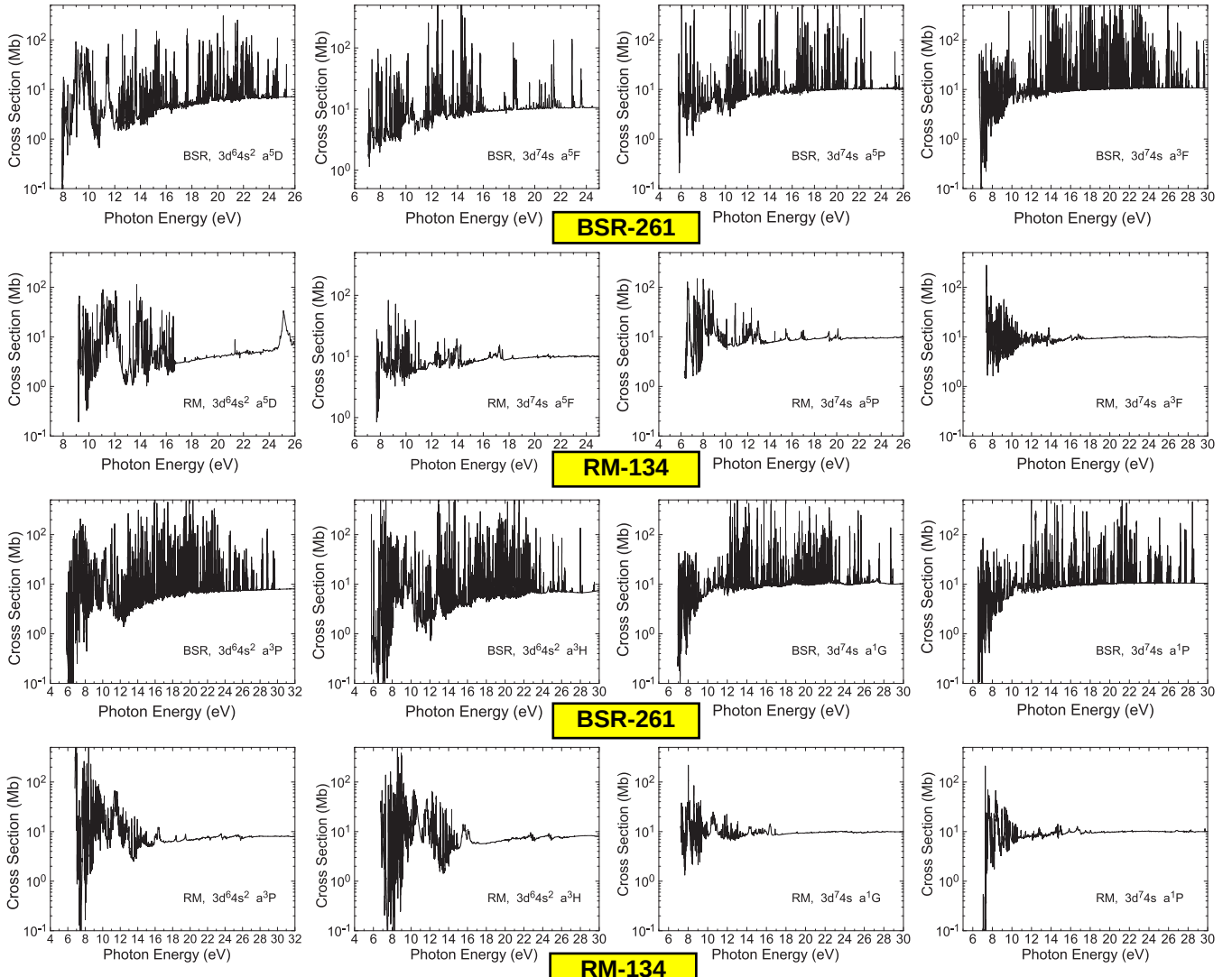


FIG. 1. Photoionization cross sections as a function of photon energy for a sample of low-lying even-parity states of Fe I. The present BSR-261 (BSR in the legend, first and third row) predictions are compared with the RM-134 (RM in the legend, second and fourth row) results of Bautista *et al.* [3].

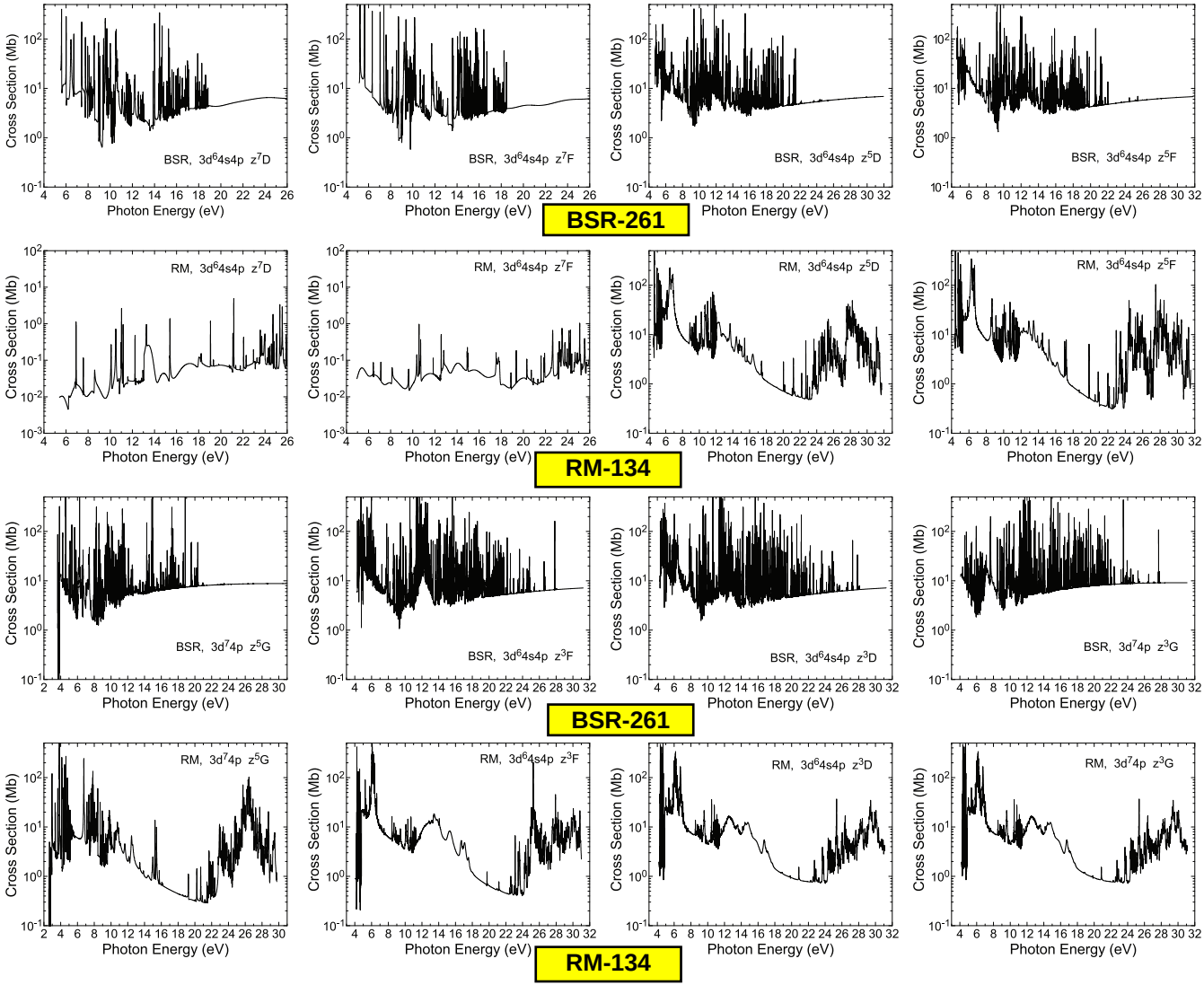


FIG. 4. Photoionization cross section for transitions from the first few odd-parity excited terms of Fe I. The present BSR-261 (BSR in the legend, first and third row) predictions are compared with the RM-134 (RM in the legend, second and fourth row) results of Bautista *et al.* [3].

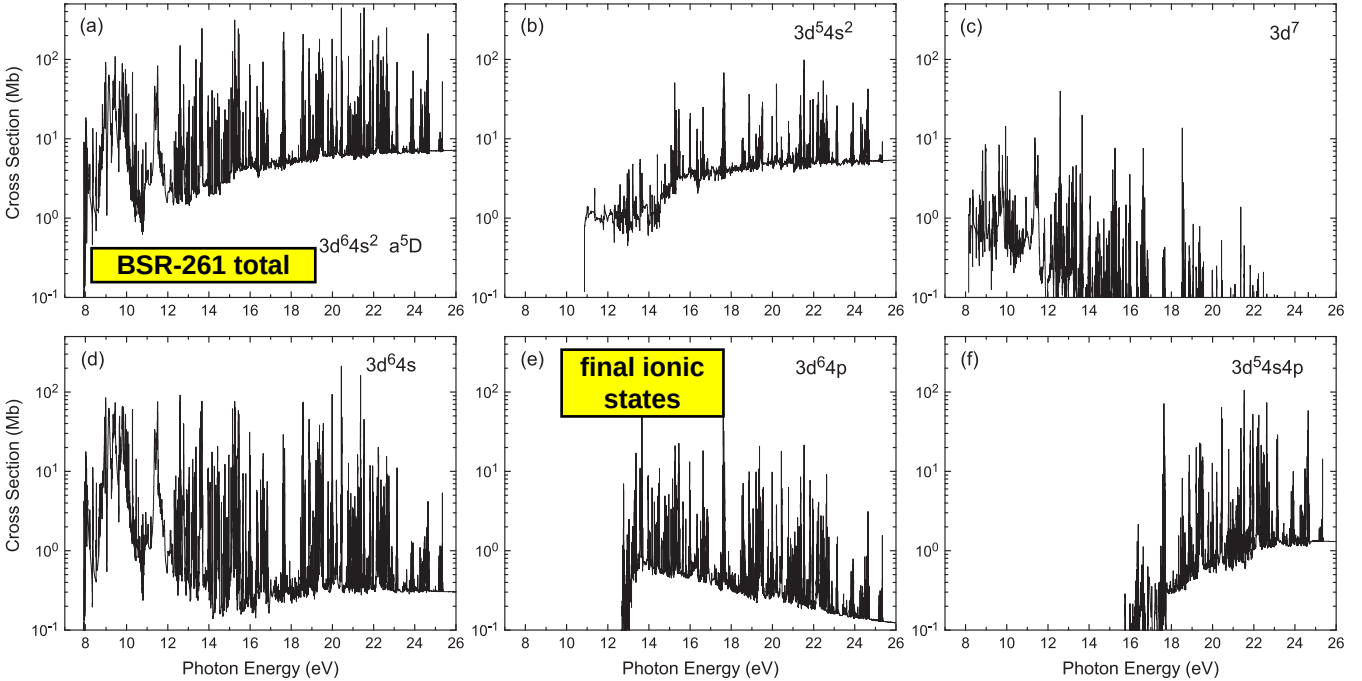


FIG. 2. Photoionization cross section of the $3d^6 4s^2\ ^5D$ ground state of Fe I (a), along with the contributions from different subsets (b)–(f) of final ionic configurations indicated in the legend.

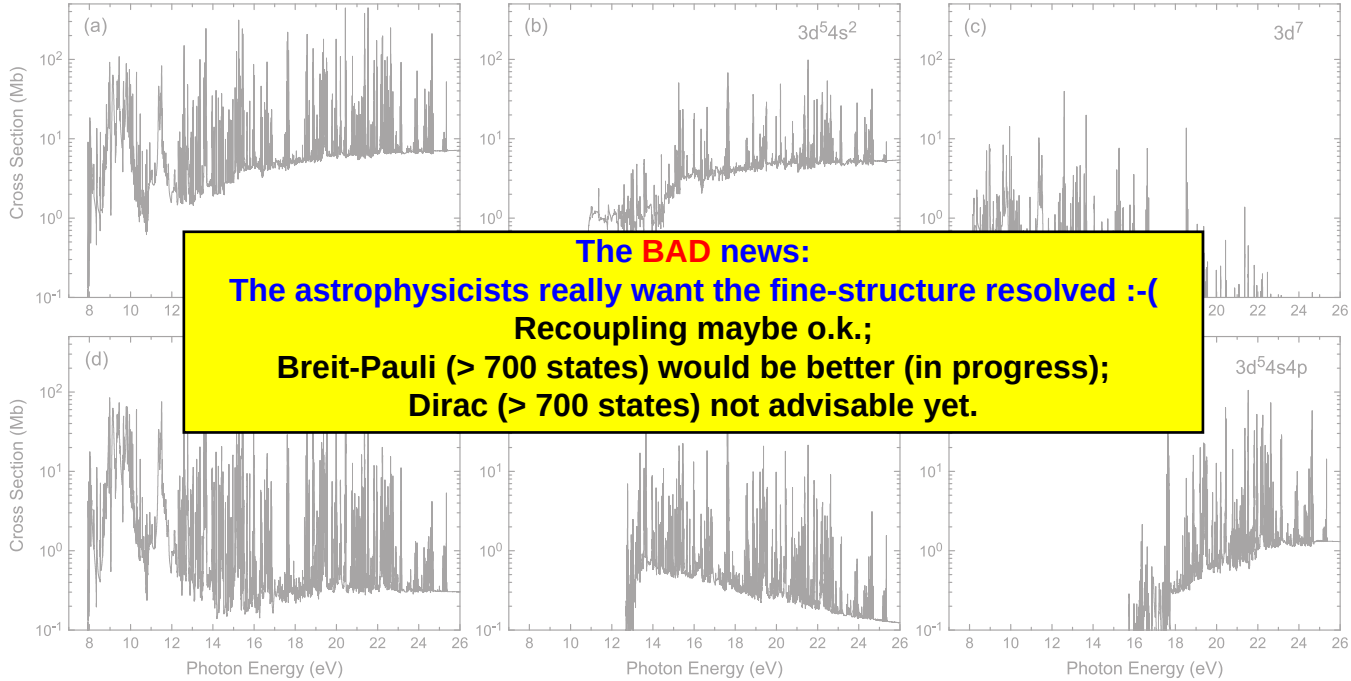


FIG. 2. Photoionization cross section of the $3d^6 4s^2\ ^5D$ ground state of Fe I (a), along with the contributions from different subsets (b)–(f) of final ionic configurations indicated in the legend.

And astrophysicists are not alone ... plasma modelers, too!

A xenon collisional-radiative model applicable to electric propulsion devices: I. Calculations of electron-impact cross sections for xenon ions by the Dirac *B*-spline *R*-matrix method

Yang Wang[1], Yan-Fei Wang[1], Xi-Ming Zhu[1,1], Oleg Zatsarinny[2], and Klaus Bartschat[2]

[1] Harbin Institute of Technology, Harbin, Heilongjiang 150001, People's Republic of China
[2] Department of Physics and Astronomy, Drake University, Des Moines, Iowa 50311, USA

Abstract

Xenon is the most important propellant in electric propulsion systems, including the widely-used Hall and ion thrusters. The performance of these devices critically depends on the kinetic processes involving xenon ions. However, in current numerical simulations of Hall and ion thrusters, excited states of xenon ions cannot be studied in detail due to the lack of fundamental cross-section data. Also, ionic emission lines are absent in the noninvasive diagnostic approach of optical emission spectroscopy, once again due to the lack of collisional-radiative (CR) models of xenon ions based on a reliable set of cross-section data.

In the present work, a fully relativistic Dirac *B*-spline *R*-matrix (DBSR) method is applied to calculate the oscillator strengths and electron-impact excitation cross sections involving the $5s^25p^5$, $5s5p^6$, $5p^46s$, $5p^45d$, $5p^46p$, and $5p^47s$ states of the Xe^+ ion. A fully relativistic approach is necessary for this problem, since the spin-orbit coupling is of the same order as electron correlations in the outer shells of Xe^+. Also, there is a complex open-shell structure with a strong term dependence in the one-electron orbitals. The calculated oscillator strengths are compared with those in the NIST database and some measured in plasma experiments reported in the literature, with overall good agreement between each other. The important excitation cross sections out of the ground, metastable, and quasi-metastable states of Xe^+ are compared and analyzed. In subsequent papers of this series of studies, the cross-section data for the Xe^+ ion, together with those for neutral Xe from our previous calculation, will be used to build a comprehensive CR model for electric propulsion systems involving xenon. The predictions of this model will then be examined by experiments in both Hall and ion thrusters.

What about really complex, heavy systems?

At a recent IAEA meeting, a scientist from the ITER project stated:
The three most important elements for us are …

tungsten, tungsten, and tungsten

Here are our best results for e–W^{n+} collisions:

NOTHING (yet)

Interested in a Post-Doc Position for BSR? Please talk to Oleg Zatsarinny or me!

Post-Doctoral Position in

Theoretical/Computational Atomic, Molecular, and Optical Physics

Drake University

A post-doctoral position in theoretical/computational AMO physics is available at Drake University. The appointment will be made on an annual basis, **beginning on or after September 1, 2019**. The position may be extended for up to three years, depending on performance and continued external funding. The successful candidate is expected to be involved in creating and maintaining a publicly available general suite of computer codes based on the B-spline R-matrix (close-coupling method) for atomic/ionic structure as well as electron and photon collisions with atoms and ions.

A significant portion of the work will involve the development of a web-based interface to enable interaction with potential users of the package. Consequently, excellent written and oral communication skills in English are required. The successful candidate will also assist in creating and testing parallelized versions of the package, preparing a number of example cases, and producing an extensive write-up. A portion of the workload will be allocated to allow for production calculations that should result in peer-reviewed publications to build the candidate's research record.

Review of applications will begin on June 1, 2019 and will continue until the position is filled. Drake University requires a formal application to be submitted through their HireTouch site:

https://drake.hiretouch.com/job-details?jobID=55293&job=research-scholar-999084

In addition, applicants should send a current C.V., including the names of three references, and a statement of their own research goals, directly to

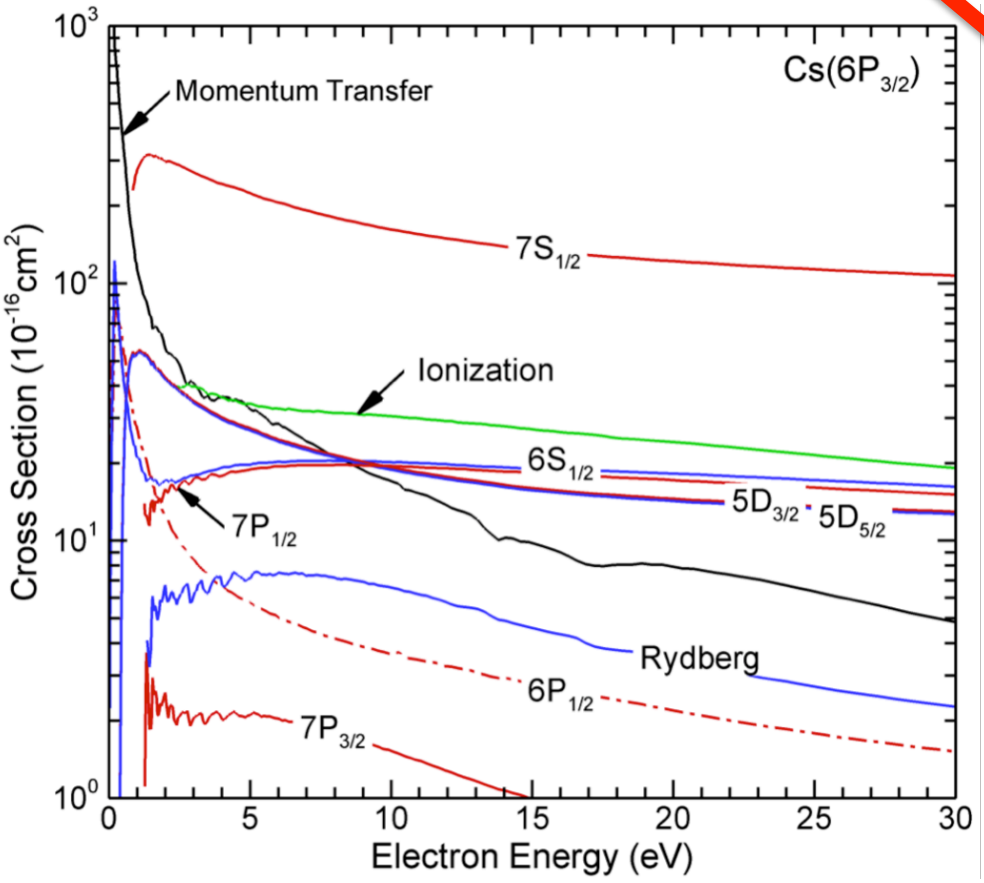
Dr. Oleg Zatsarinny (**oleg.zatsarinny@drake.edu**)
Department of Physics and Astronomy
Drake University
Des Moines, IA 50311, USA

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

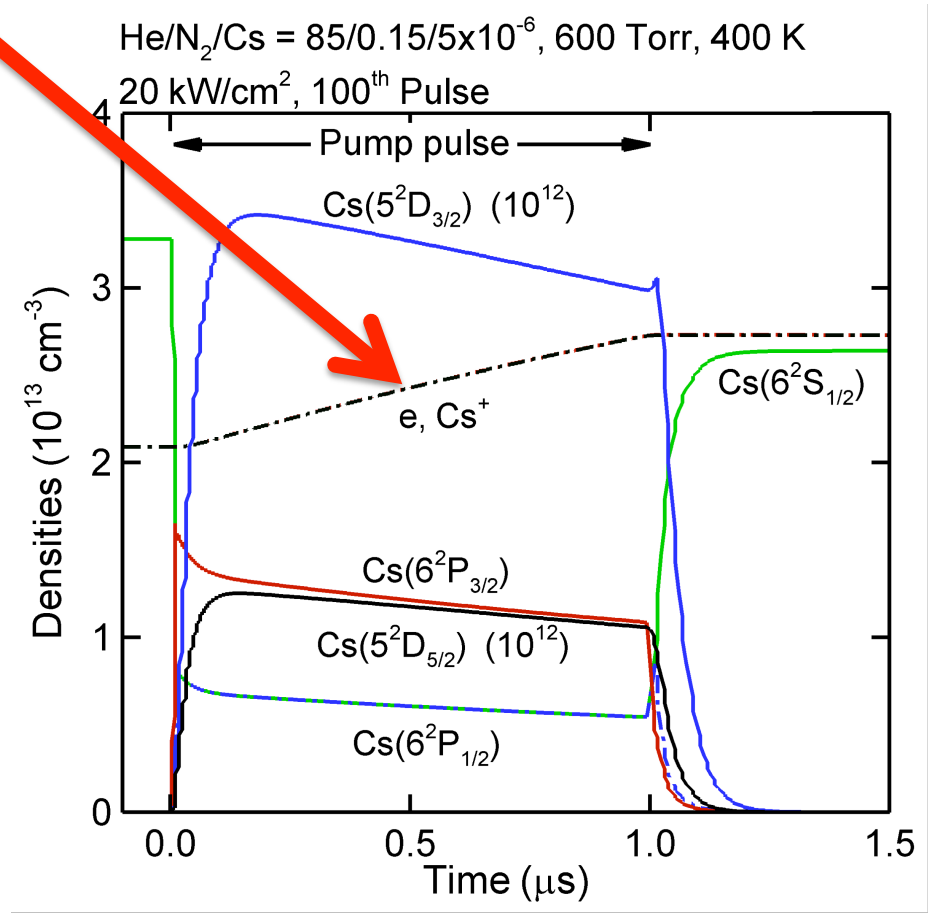
Modeling a Cs-based DPAL

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



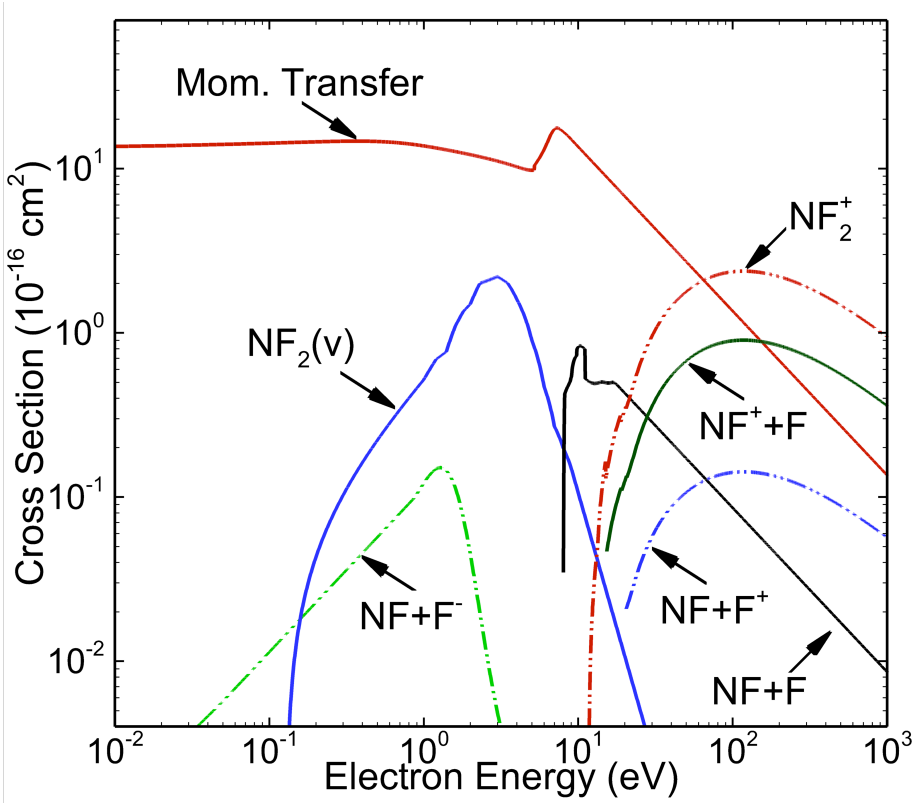
Output (M. J. Kushner's group): Densities of various species



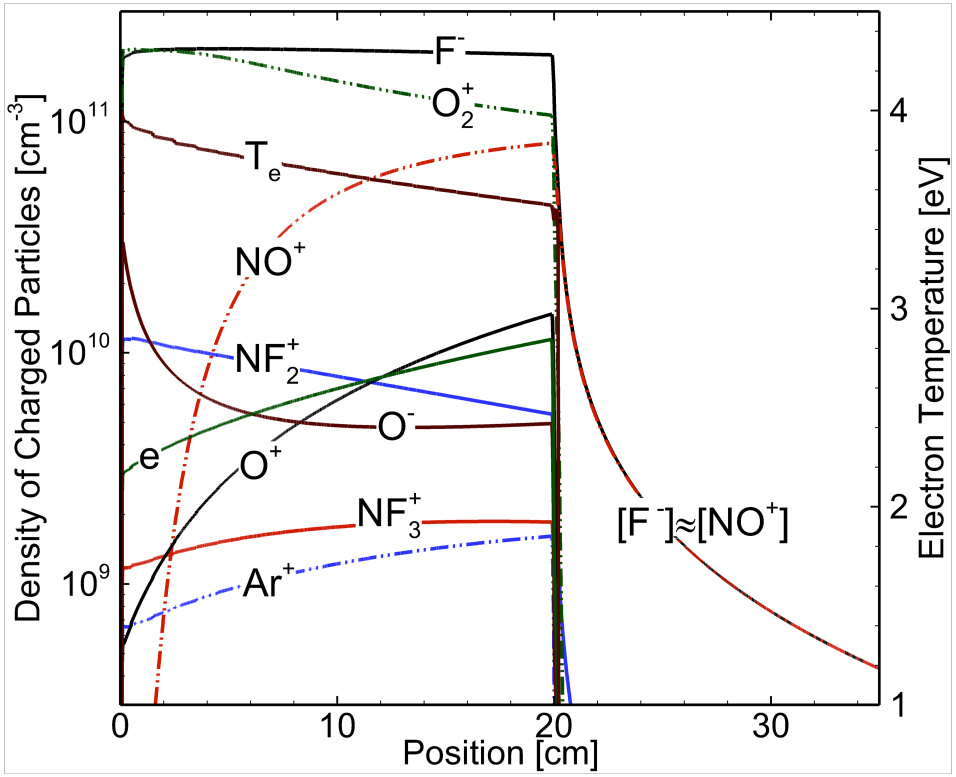
Remote plasma etching using an $Ar/NF_3/O_2$ mixture

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)



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



Conclusions and Outlook

+ Related Topics

- **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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(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

Conclusions and Outlook

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- **Knowledge about electron collisions also helps to understand photon-induced processes, in weak-field, strong-field, steady-state, and time-dependent cases.**

Time delays for attosecond streaking in photoionization of neon

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(Received 13 January 2014; published 14 March 2014)

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)

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

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[2]*Physics Division, National Science Foundation, Arlington, Virginia 22230, USA*
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[4]*Computational Science and Engineering Department, Daresbury Laboratory, Warrington WA4 4AD, United Kingdom*
(Received 24 April 2007; revised manuscript received 13 September 2007; published 15 November 2007)

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.

This projects needed e–Ne^+ collision data; others needed e–He^+, e–Ar^+

Pulse-duration dependence of the double-to-single ionization ratio of Ne by intense 780-nm and 800-nm laser fields: Comparison of simulations with experiments

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Toru Morishita
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C. D. Lin
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(Received 10 January 2019; revised manuscript received 14 March 2019; published 8 April 2019)

Accurate *ab initio* calculations of the ratio of double-to-single ionization of Ne atoms in strong laser fields are difficult due to the many-electron nature of the target. Here, with accurate total cross sections carefully evaluated by using the state-of-the-art many-electron *R*-matrix theory for both electron-impact ionization and electron-impact excitation of Ne^+, we simulate the total double-ionization yields of Ne^{2+} in strong laser fields at 780 and 800 nm for pulse durations in the range from 7.5 to 200 fs based on the improved quantitative rescattering model. The corresponding single-ionization yields of Ne^+ are calculated within the nonadiabatic tunneling model of Perelomov, Popov, and Terent'ev. The ratio of double-to-single ionization of Ne is then obtained from the calculated double- and single-ionization yields. By normalizing the ratio to the one calculated from solving the time-dependent Schrödinger equation for a short few-cycle pulse, we make quantitative comparisons of our results with experimental data to show that our model predicts the experimental findings very well. Finally, we analyze the pulse-duration dependence of the double-to-single ionization ratio.

DOI: 10.1103/PhysRevA.99.043408

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!**
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- **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 ...**

Electron scattering for quantum state engineering

Entanglement and Bell Correlation in Electron-Exchange Collisions

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(Received 14 June 2015; published 21 January 2016)

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.

DOI: 10.1103/PhysRevLett.116.033201

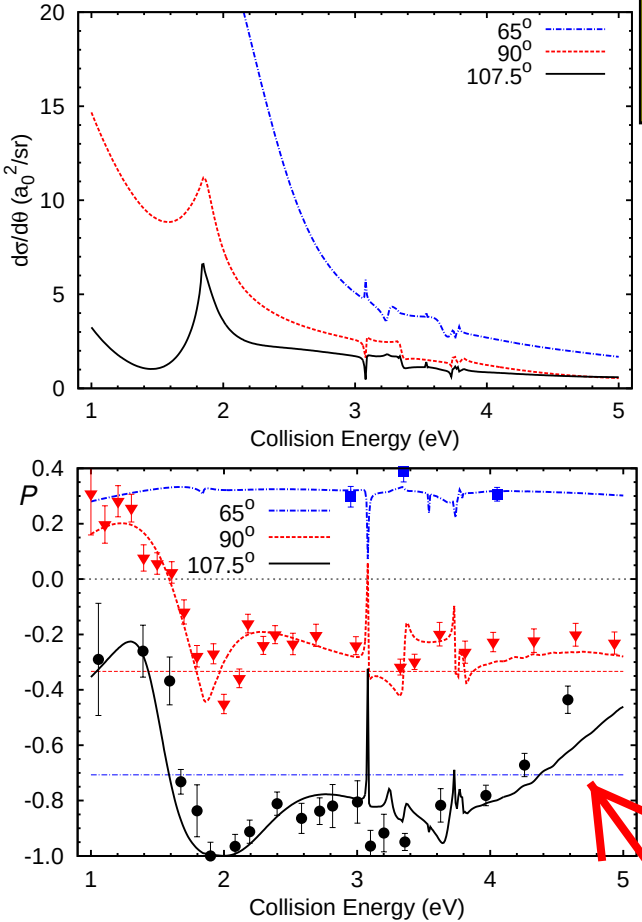


FIG. 1: Differential cross section (top) and spin correlation parameter P (bottom) for elastic electron scattering from Li atoms as a function of energy at scattering angles of $65°$, $90°$, and $107.5°$. The lines at $-1/3$ and $-1/\sqrt{2}$ in the panel for P mark the borders between separable and 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!

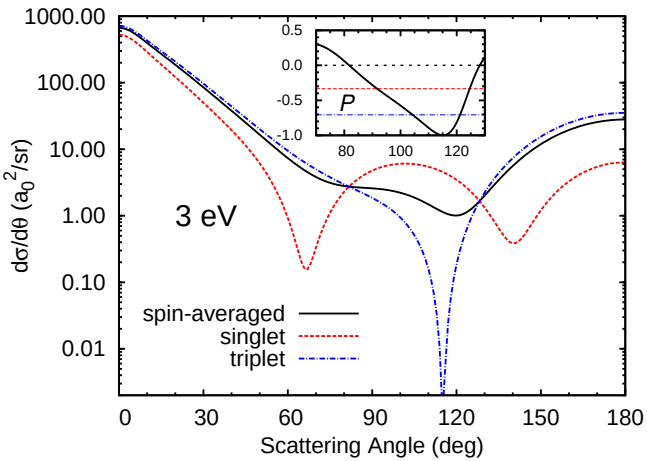
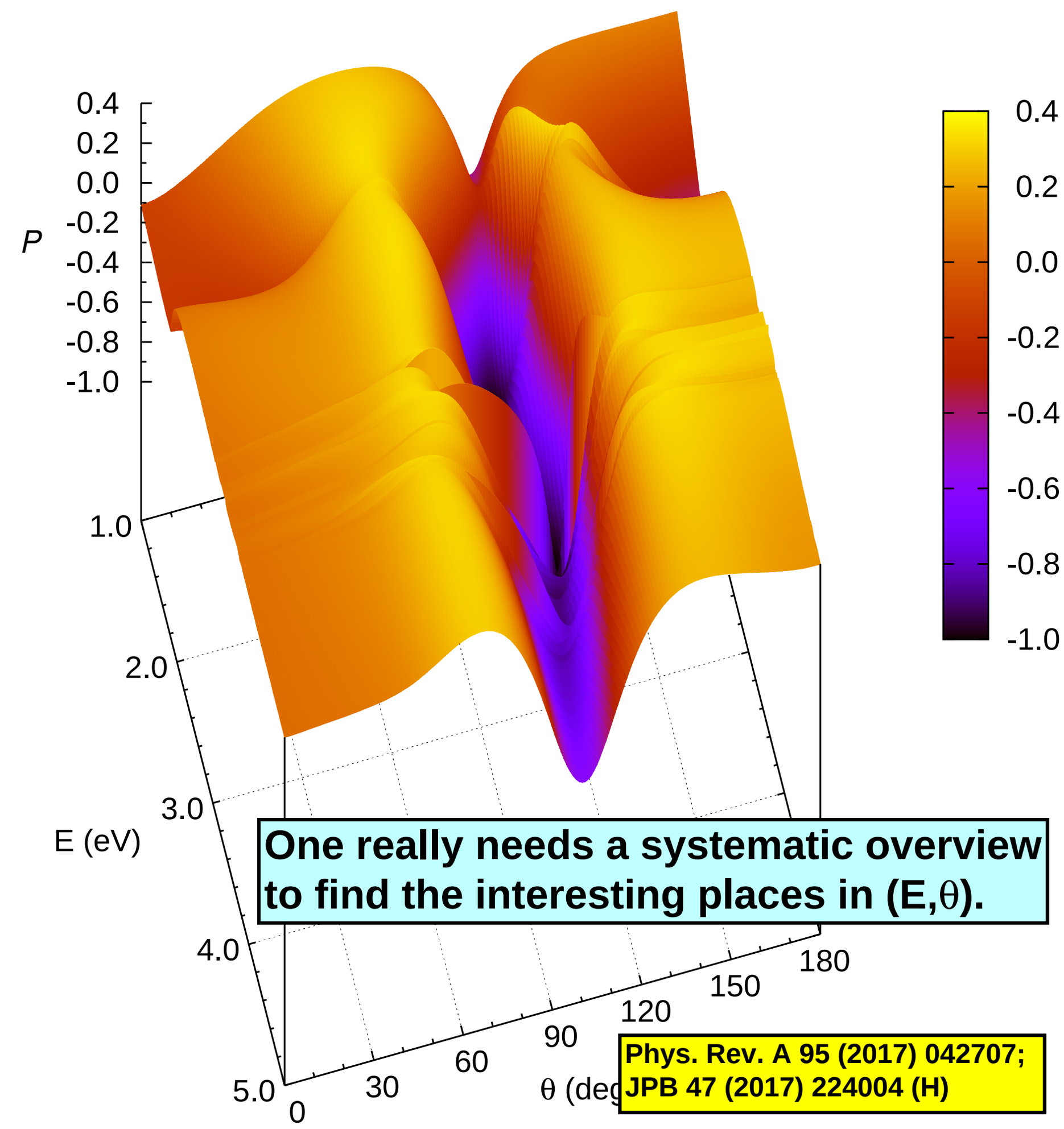


FIG. 2: Differential cross section as well as the individual contributions from the singlet and triplet total spin channels for elastic electron scattering from Li atoms at a collision energy of 3 eV. The insert shows the parameter P in the region $70° - 130°$. The lines at $-1/3$ and $-1/\sqrt{2}$ mark 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
0
30
60
90
120
150
180
θ (deg
One really needs a systematic overview to find the interesting places in (E,θ).
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JPB 47 (2017) 224004 (H)

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).
- 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!

And Please Remember: Electron Collisions Save the World!