The B-Spline R-Matrix Method:
Methodology and Implementation

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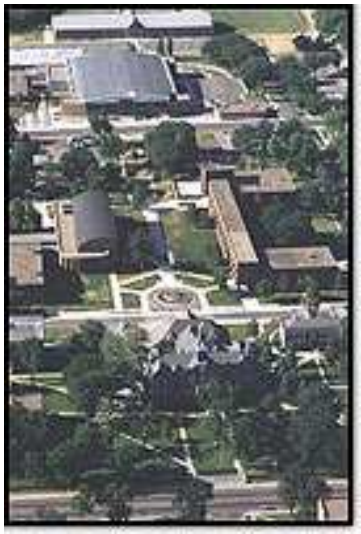
XSEDE (PHY-090031)



OVERVIEW:

I. Time-Independent Close-Coupling
II. General R-Matrix Idea / B-Spline R-Matrix Implementation
III. Examples of Atomic Data Production / Current Status
IV. Extensions to Time-Dependent Processes
V. Summary

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)!

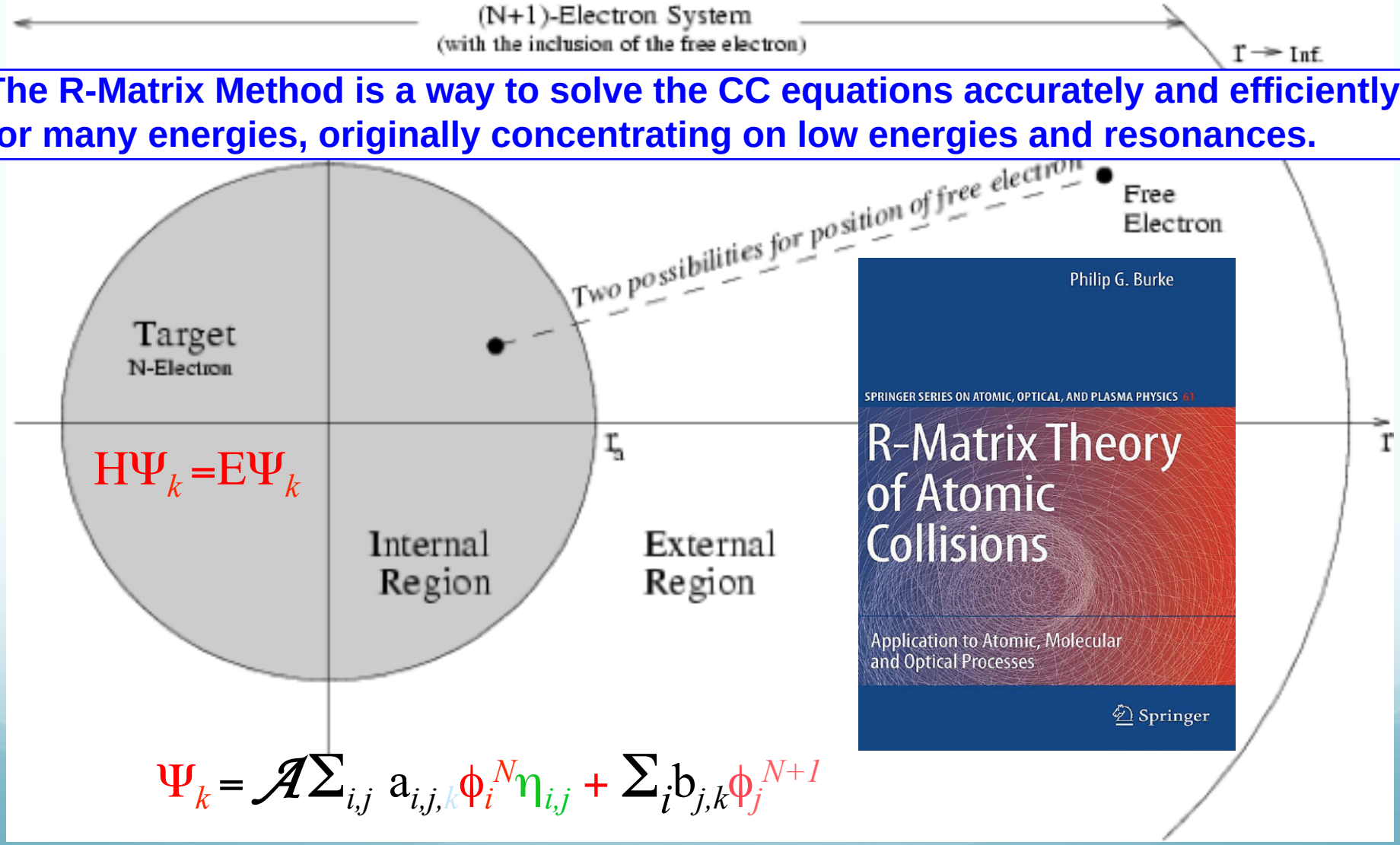
The R-Matrix Method:

Numerical Technique to solve the Close-Coupling Equations

- **Basic Idea**: indirect calculations – inner ($r < a$) and outer regions ($r > a$).
- **Complete set** of inner-region solutions is found from diagonalization of total Hamiltonian modified with the Bloch operator
- **Scattering parameters** can obtained from matching with solutions in the external region − allows cross sections at many energy points to be obtained cheaply

Theory: Atomic R-Matrix Method

[Original slide from Brendan McLaughlin with some modifications by K.B.]



Phil Burke (18.10.1932 – 3.6.2019)

Phil taught me about computers and especially the R-matrix method. When I came to Belfast as a 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 R-Matrix Method:

Numerical Technique to solve the Close-Coupling Equations

- **Basic Idea**: indirect calculations – inner ($r < a$) and outer regions ($r > a$).
- **Complete set** of inner-region solutions is found from diagonalization of total Hamiltonian modified with the Bloch operator
- **Scattering parameters** can obtained from matching with solutions in the external region − allows cross sections at many energy points to be obtained cheaply

- **Computer Codes:**
  - RMATRX-I: Berrington *et al* (1995)
  - PRMAT: parallelized version of RMATRX-I
  - Badnell's R-matrix complex: http: //amdpp.phys.strath.ac.uk/, with possibility for radiative damping
  - DARC – relativistic version, http://web.am.qub.ac.uk/DARC/
  - Enormous number of calculations

Principal ingredient: a single set of orthogonal one-electron orbitals

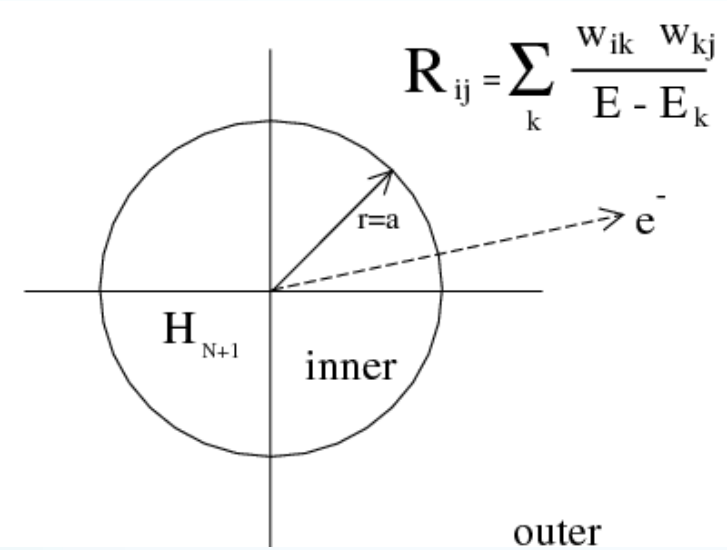
- $< P_{n\ell} \mid P_{n'\ell} > = 0 \rightarrow$ difficulties to achieve accurate target representation for different states
- $< P_{n\ell} \mid u_{k\ell} > = 0 \rightarrow$ large (N+1)-electron expansions needed for completeness (may lead to appearance of pseudo-resonances)

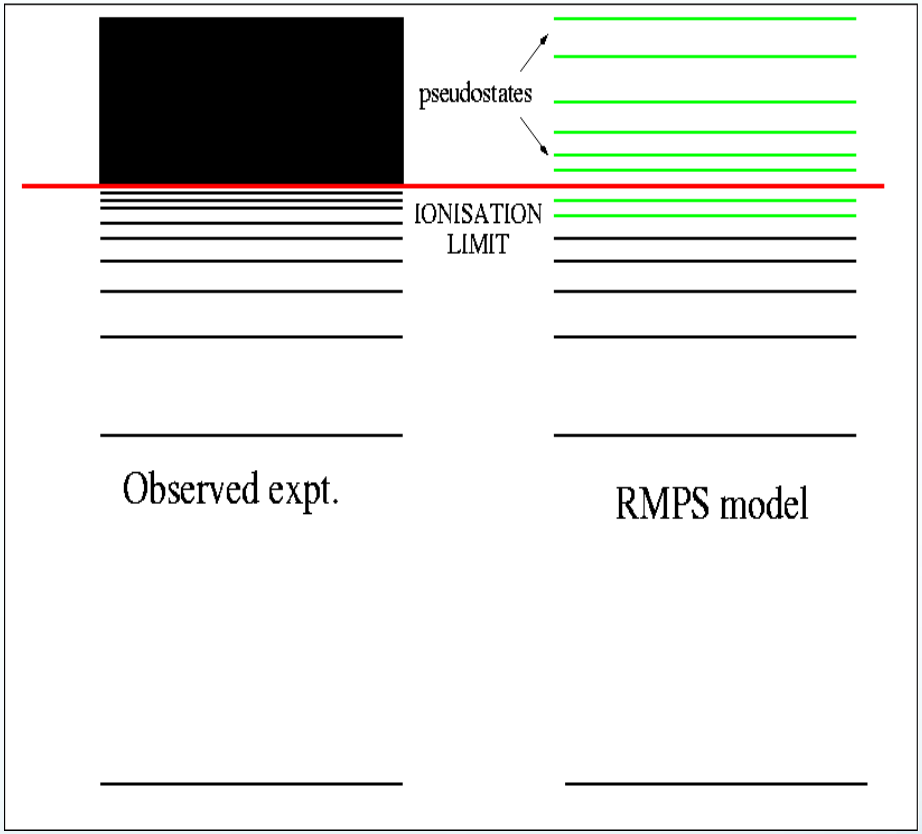
Inclusion of Target Continuum (Ionization)

- 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, ...)**

R-Matrix with Pseudo-States (RMPS)

K. Bartschat, E.T. Hudson, M.P. Sott, P.G. Burke, and V.M. Burke, J. Phys. B 29 (1996)





RMPS uses the same ideas as CCC (—> Igor Bray) to extend the applicability of close-coupling to "intermediate" energies, where coupling to the continuum can be very important. As a by-product, ionization processes can also be handled.

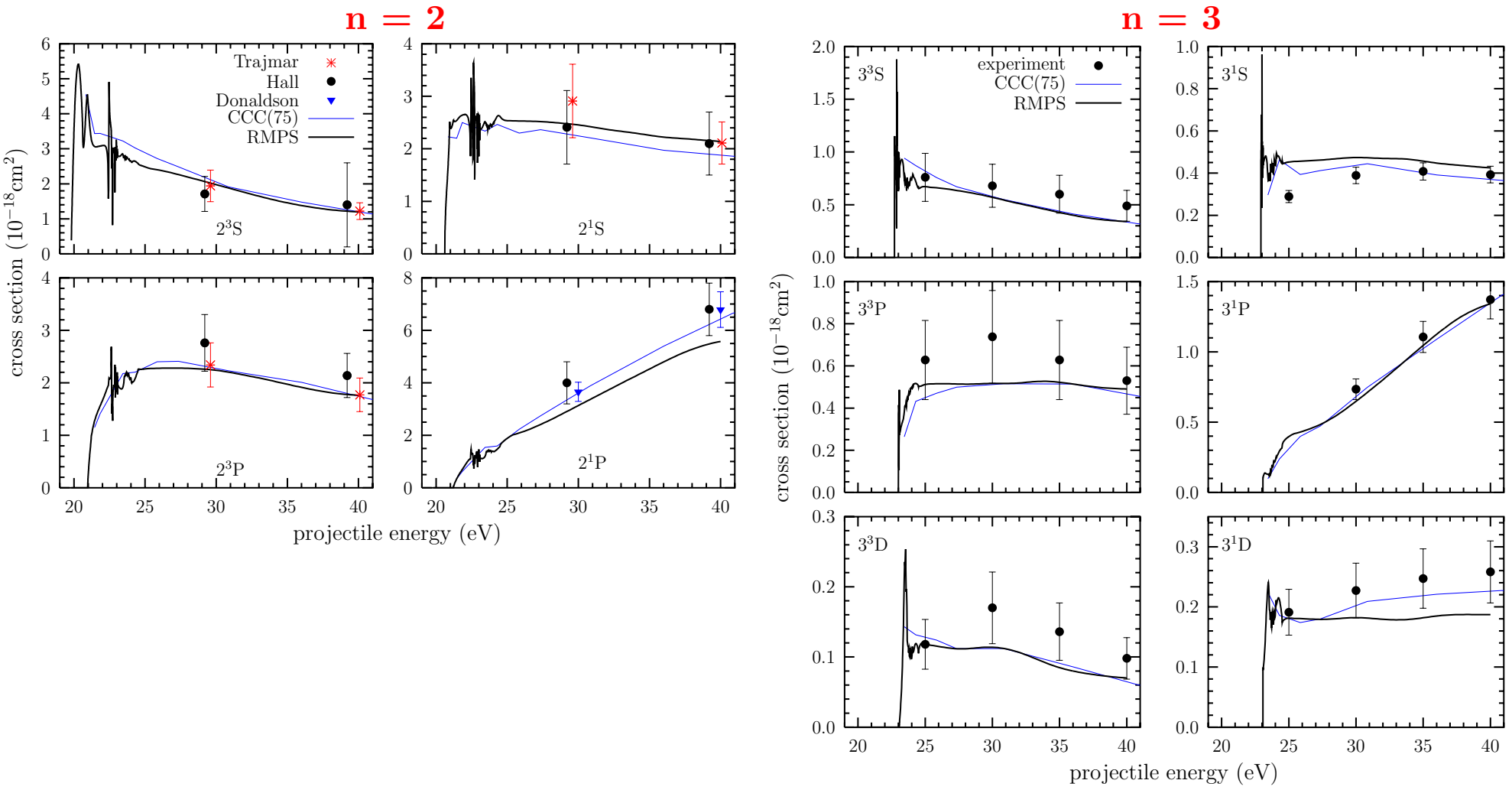
Inclusion of Target Continuum (Ionization)

- **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**

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

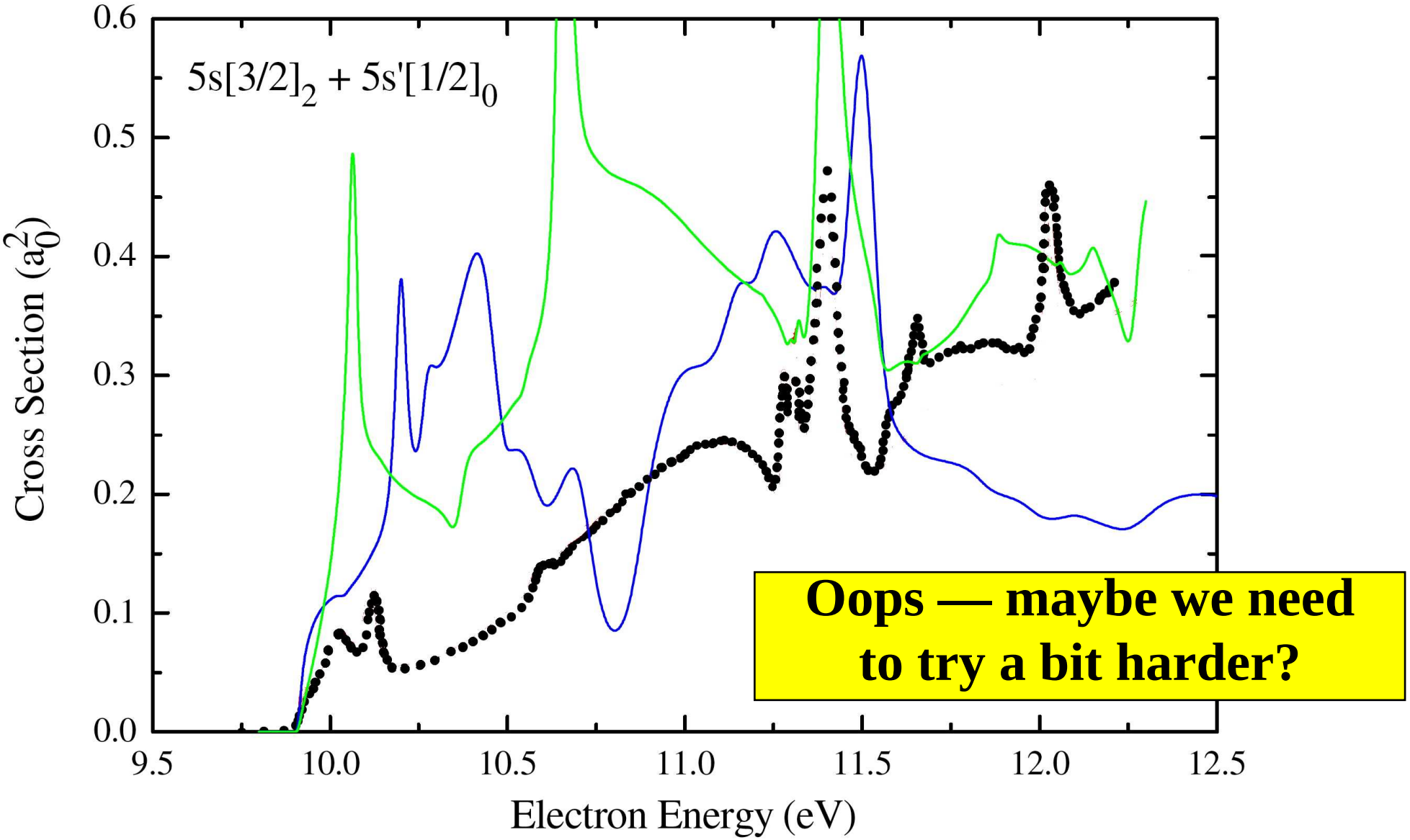


Already in 1998, de Heer recommends 0.5 x (CCC+RMPS) for uncertainty of 10% — independent of experiment!

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)



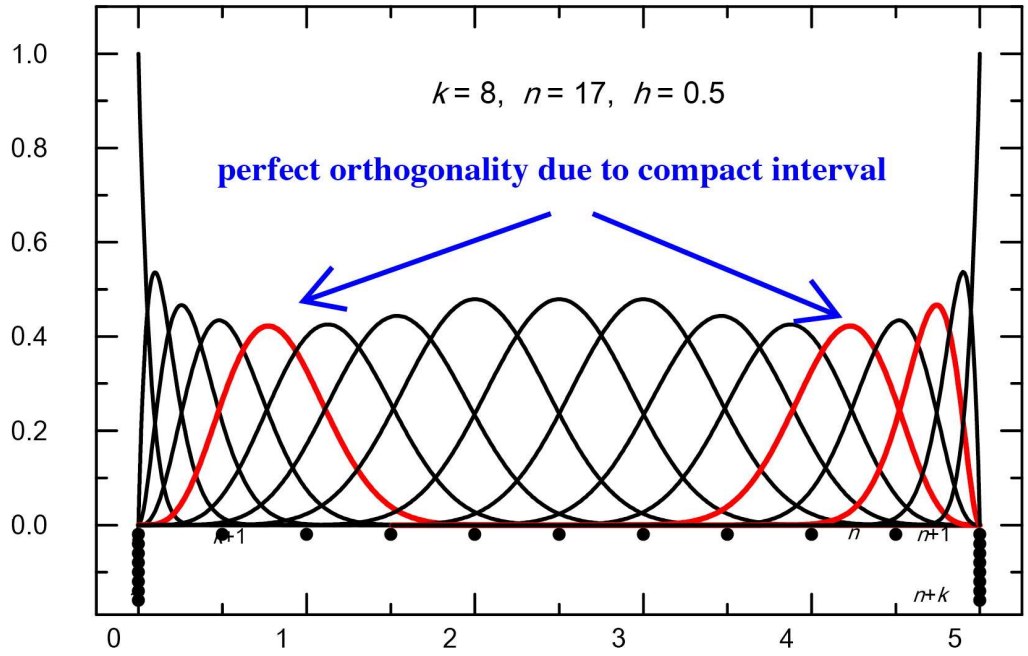
Oops — maybe we need to try a bit harder?

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;

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

The B-Spline R-Matrix (BSR) Method

[O. Zatsarinny, Comp. Phys. Commun. 174, 273 (2006)]

- The method is based on the non-perturbative **close-coupling** expansion.
- The close-coupling equations are solved using the **R-matrix method**.
- Atomic-structure calculations – **frozen-core approximation**

Distinctive feature:
Allows for **non-orthogonal orbital sets** to represent both bound and continuum radial functions

- **independent generation of target states** – much more accurate target representation (**term-dependence, relaxation effects, correlation**)
- **no artificial orthogonality constraints for continuum orbitals** – more consistent treatment of N-electron target and (N+1)-electron collision system –> **no pseudo–resonances** **[I wouldn't say it quite as strongly.]**
- **more recently extented to include large number of pseudo-states to handle ionization processes (BSRMPS) as well as a full-relativistic framework (DBSR).**

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

BSR – general B-spline R-matrix package

1. First implementation: Li photoionization (2000)
2. First presentation: ICPEAC XXX, Rosario, Argentina (2005)
3. First version published: Comp. Phys. Comm. (2006)
4. Fully-relativistic version: e–Cs scattering (2008)
5. RMPS extension, MPI intermediate energies;
   parallelization; ionization: (e,2e) on He,Ne,Ar (2011–present)
6. Topical review: J.Phys.B 46, 112001 (2013)
7. Sustainability Effort: CSSI project (funded since March 2019)

1a	2a	3b		4b	5b	6b	7b	VIII		1b	2b	3a	4a	5a	6a	7a	0
^{1}H																	^{2}He
^{3}Li	^{4}Be											^{5}B	^{6}C	^{7}N	^{8}O	^{9}F	^{10}Ne
^{11}Na	^{12}Mg											^{13}Al	^{14}Si	^{15}P	^{16}S	^{17}Cl	^{18}Ar
^{19}K	^{20}Ca	^{21}Sc		^{22}Ti	^{23}V	^{24}Cr	^{25}Mn	^{26}Fe	^{27}Co	^{28}Ni	^{29}Cu	^{30}Zn	^{31}Ga	^{32}Ge	^{33}As	^{34}Se	^{35}Br	^{36}Kr
^{37}Rb	^{38}Sr	^{39}Y		^{40}Zr	^{41}Nb	^{42}Mo	^{43}Tc	^{44}Ru	^{45}Rh	^{46}Pd	^{47}Ag	^{48}Cd	^{49}In	^{50}Sn	^{51}Sb	^{52}Te	^{53}I	^{54}Xe
^{55}Cs	^{56}Ba	^{57}La	*	^{72}Hf	^{73}Ta	^{74}W	^{75}Re	^{76}Os	^{77}Ir	^{78}Pt	^{79}Au	^{80}Hg	^{81}Tl	^{82}Pb	^{83}Bi	^{84}Po	^{85}At	^{86}Rn
^{87}Fr	^{88}Ra	^{89}Ac	+	^{104}Rf	^{105}Df	^{106}Sg	^{107}Bh	^{108}Hs	^{109}Mt	^{110}Uun	^{111}Uuu	^{112}Uub		^{114}Uuq				
* Lanthanides				^{58}Ce	^{59}Pr	^{60}Nd	^{61}Pm	^{62}Sm	^{63}Eu	^{64}Gd	^{65}Tb	^{66}Dy	^{67}Ho	^{68}Er	^{69}Tm	^{70}Yb	^{71}Lu	
+ Actinides				^{90}Th	^{91}Pa	^{92}U	^{93}Np	^{94}Pu	^{95}Am	^{96}Cm	^{97}Bk	^{98}Cf	^{99}Es	^{100}Fm	^{101}Md	^{102}No	^{103}Lr	

Key point: The BSR package is *general*; the current version can, in principle, be applied to *any atomic/ionic target*.

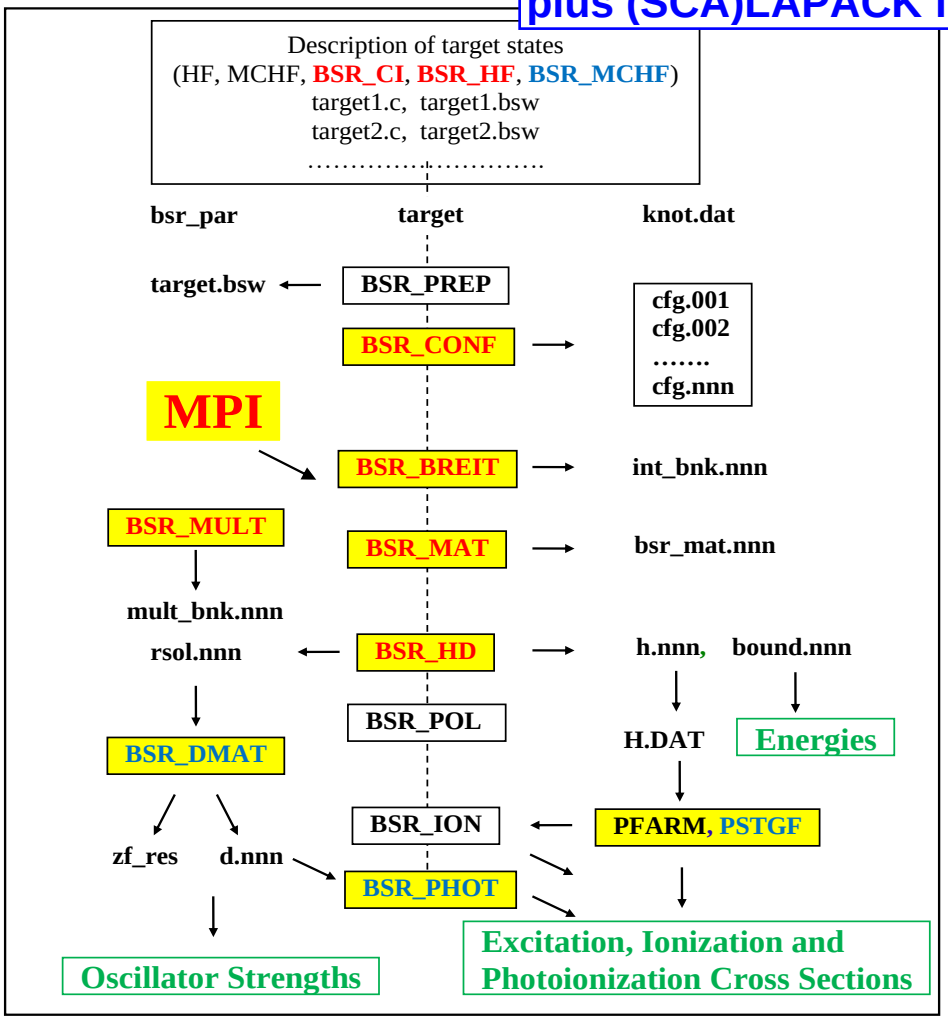
Our Apparatus — Supercomputers

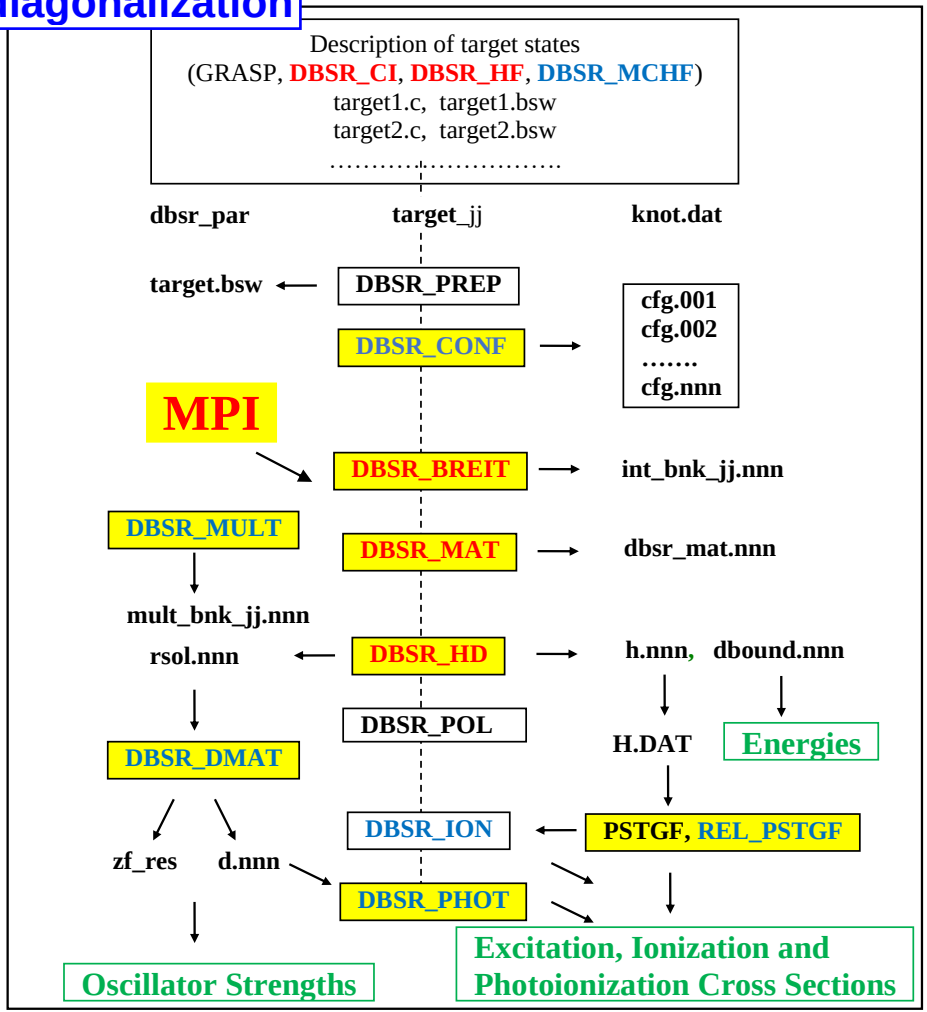
Kraken (NICS)

TACC
TEXAS ADVANCED COMPUTING CENTER
Powering Discoveries That Change The World

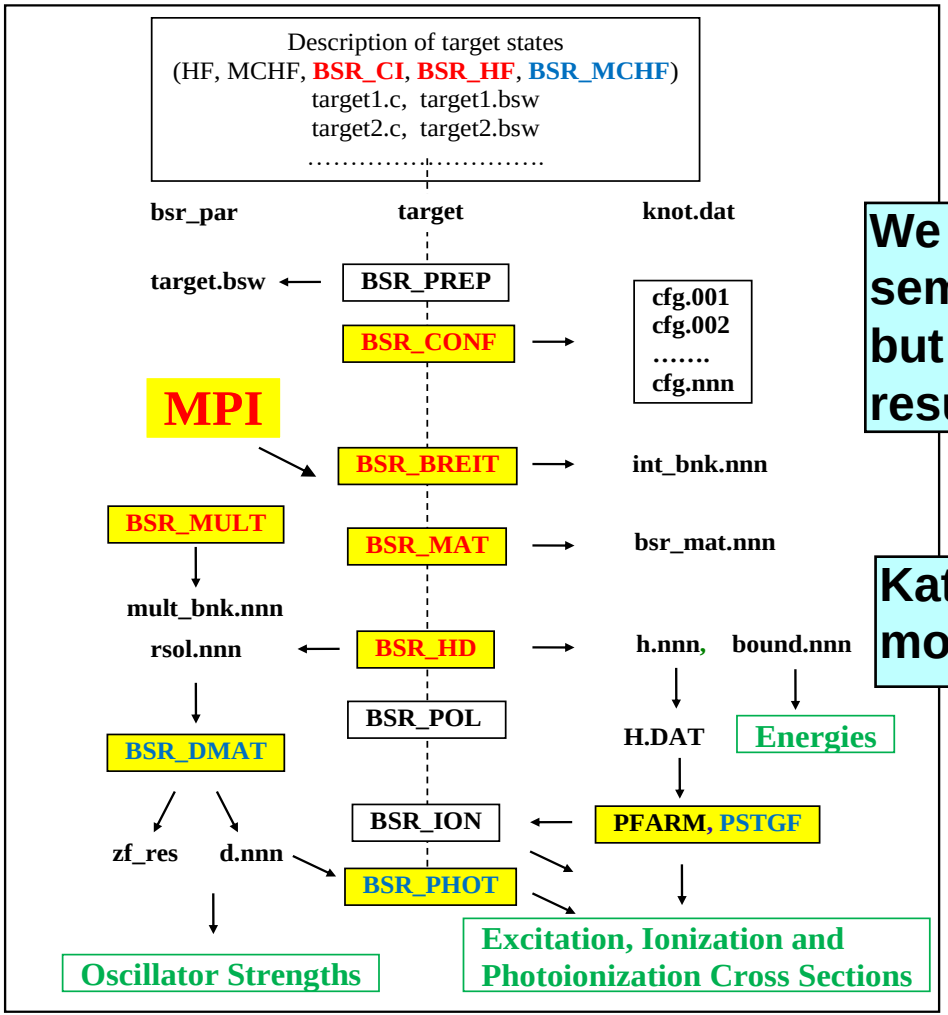
+ Comet at San Diego Supercomputer Center
+Bridges at Pittsburgh Supercomputer Center

about 30,000 – 50,000 lines of code;
plus (SCA)LAPACK for diagonalization





BSR

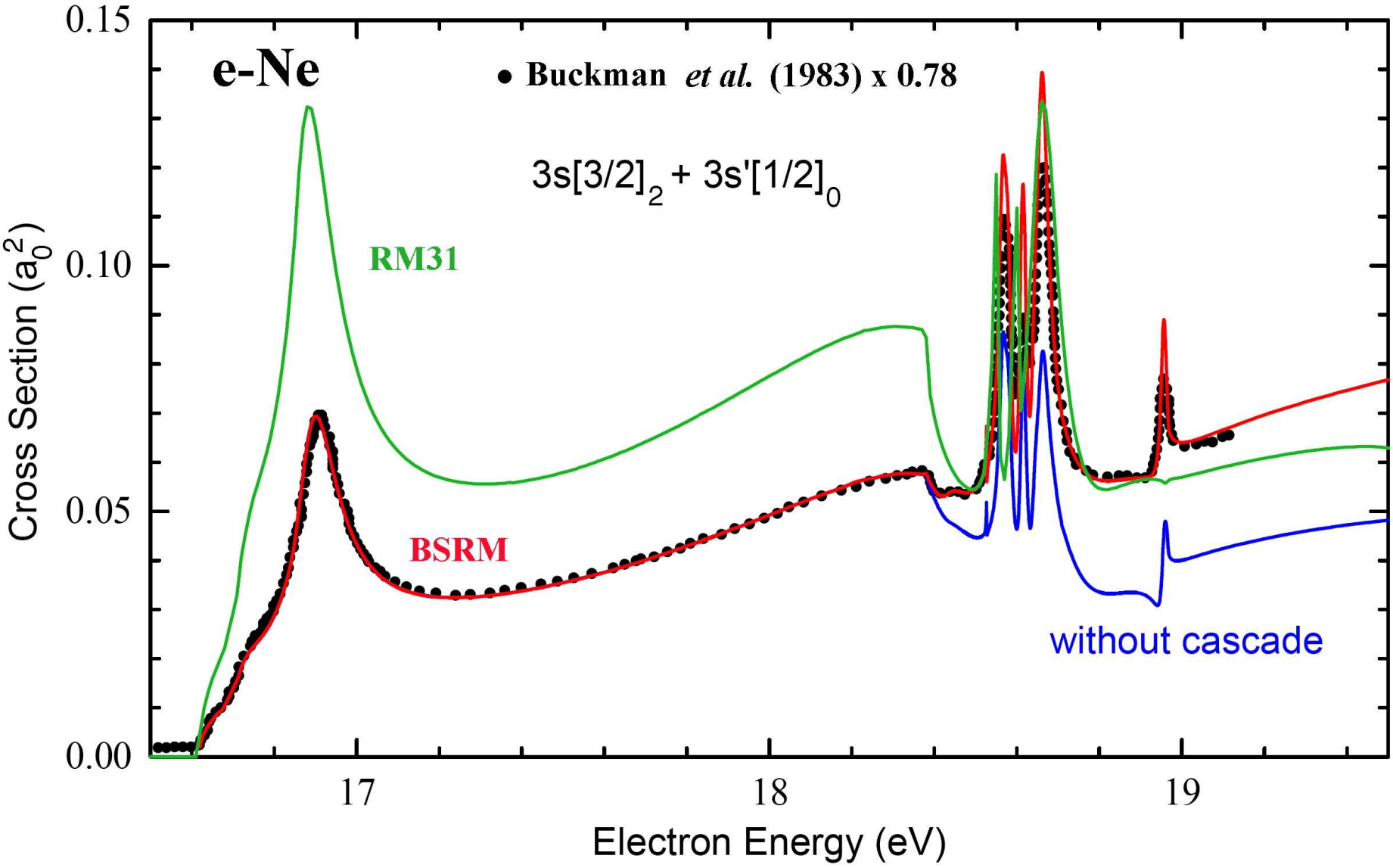


We will focus on the semi-relativistic version, but I'll show some DBSR results as well.

Kathryn Hamilton will present more details tomorrow.

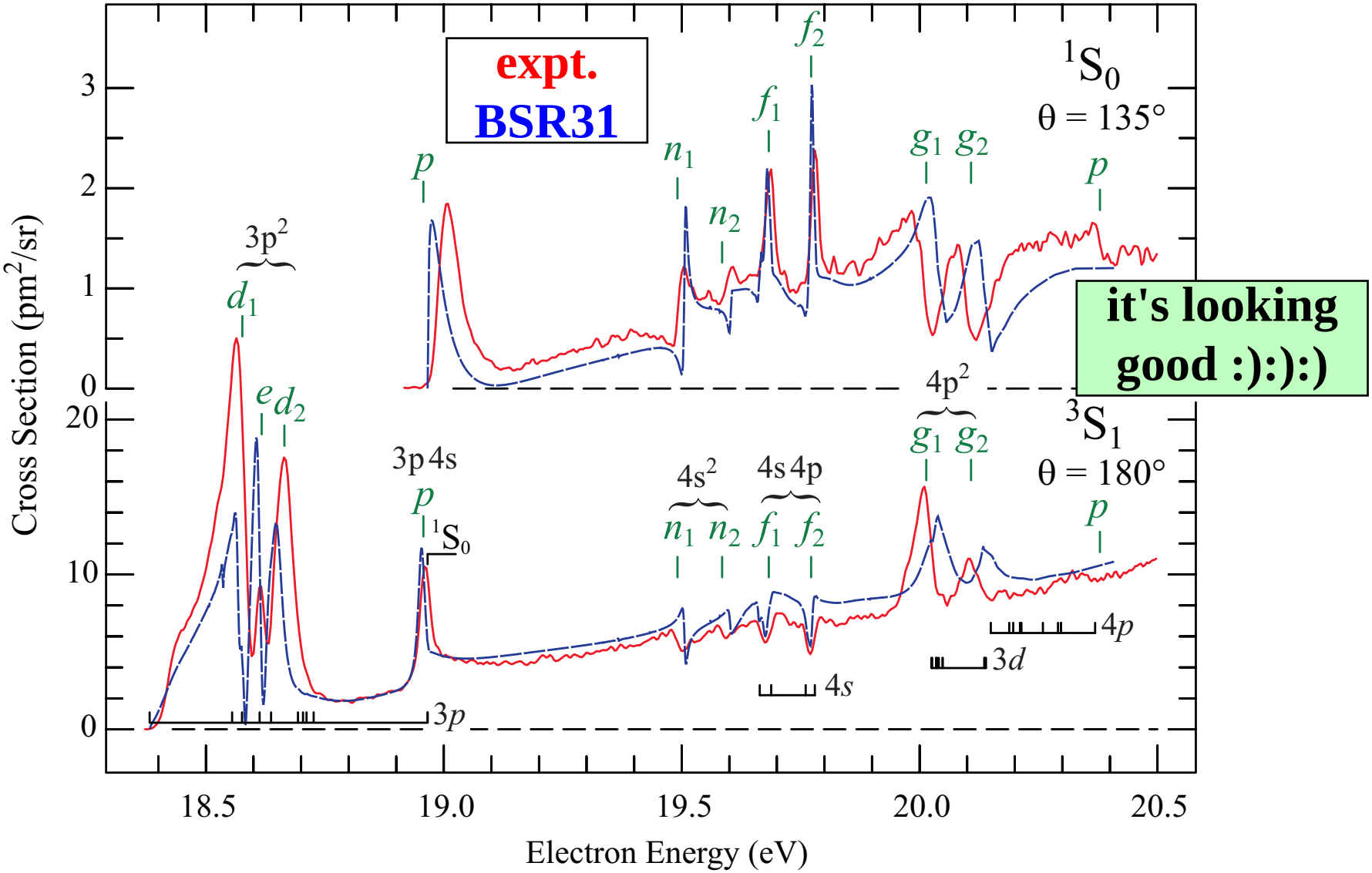
Metastable yield in e-Ne collisions

- 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



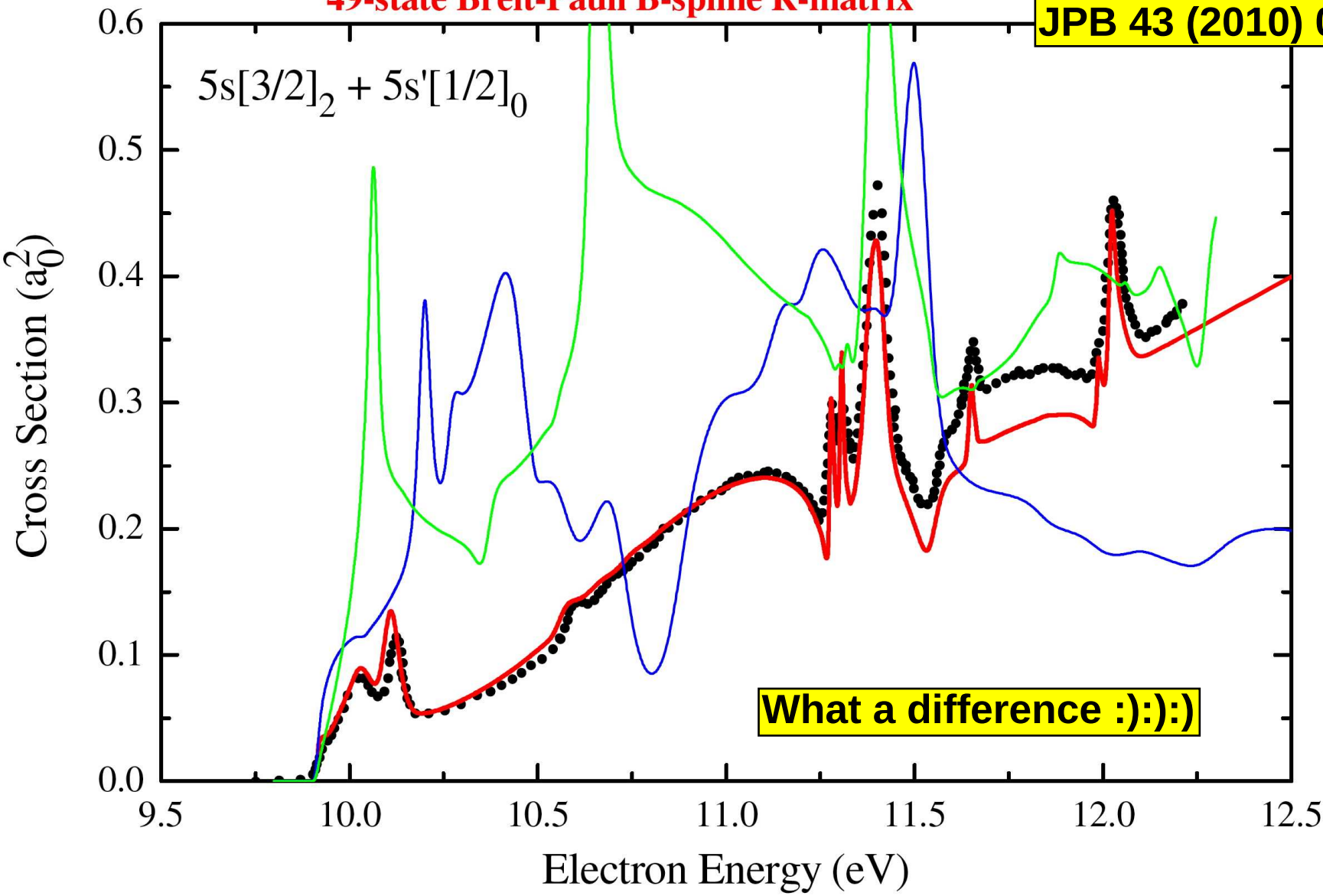
it's looking good :):):)

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.

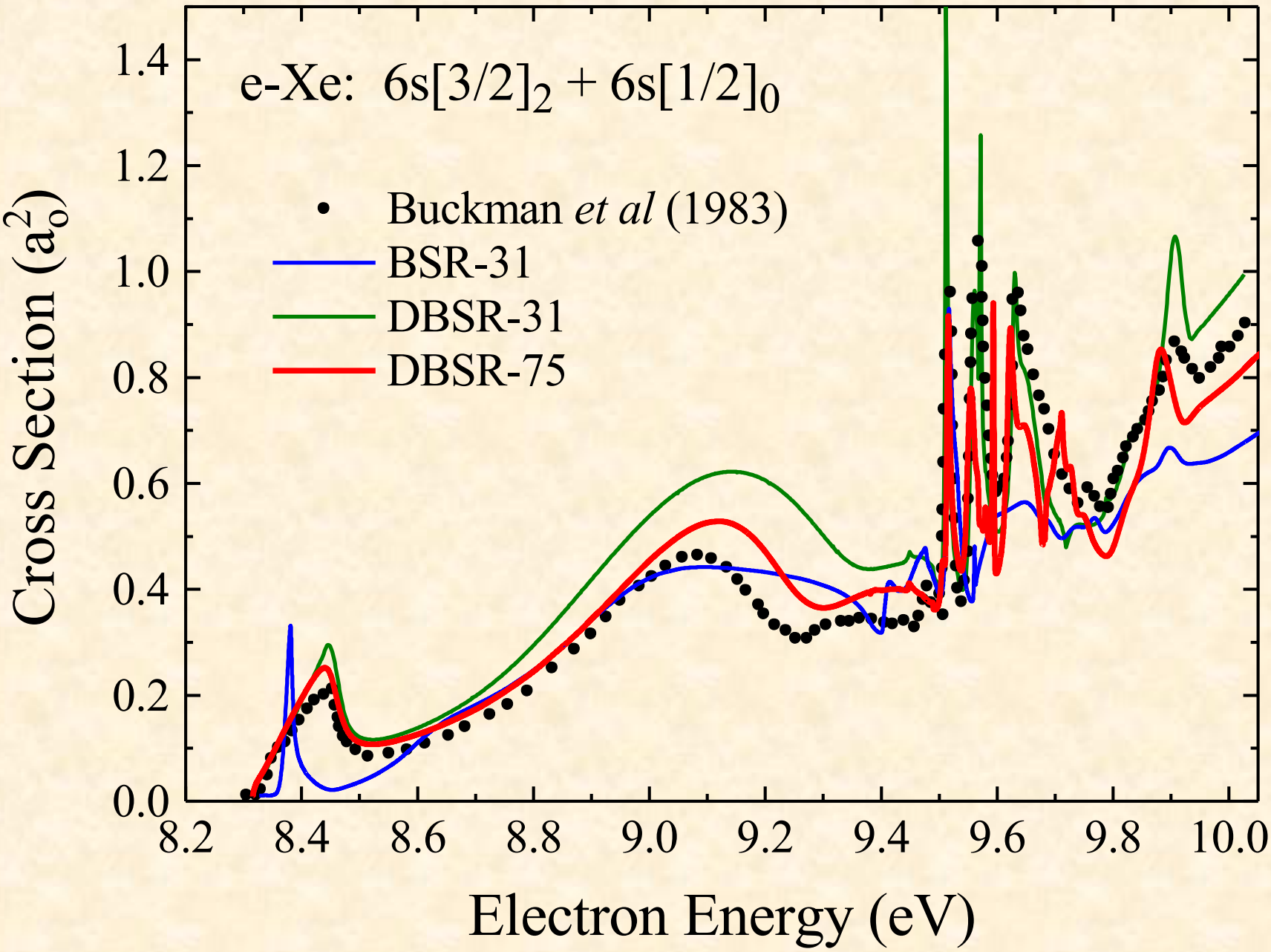
Metastable Excitation Function in Kr

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



DBSR versus BSR

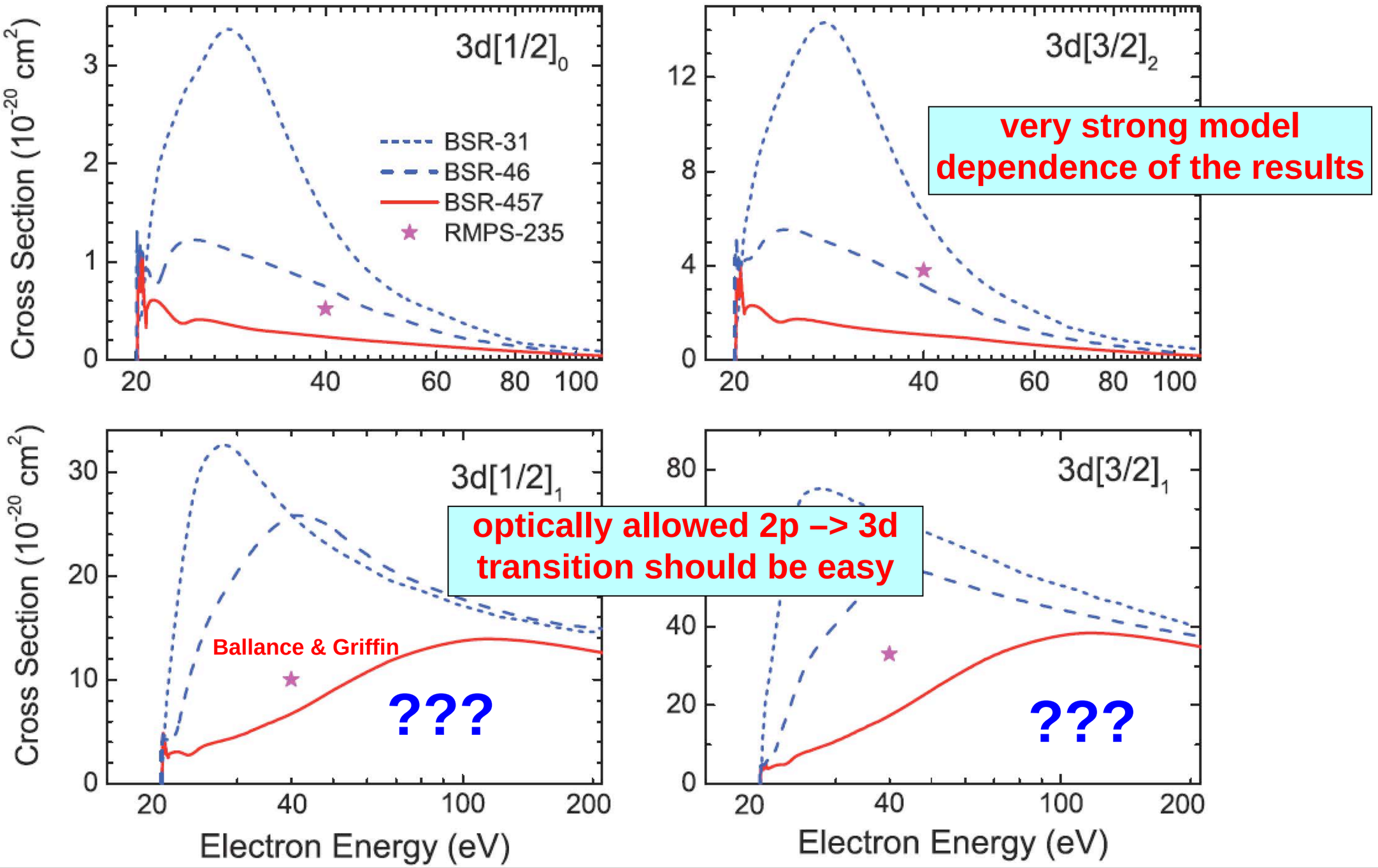


PHYSICAL REVIEW A **86**, 022717 (2012)

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.

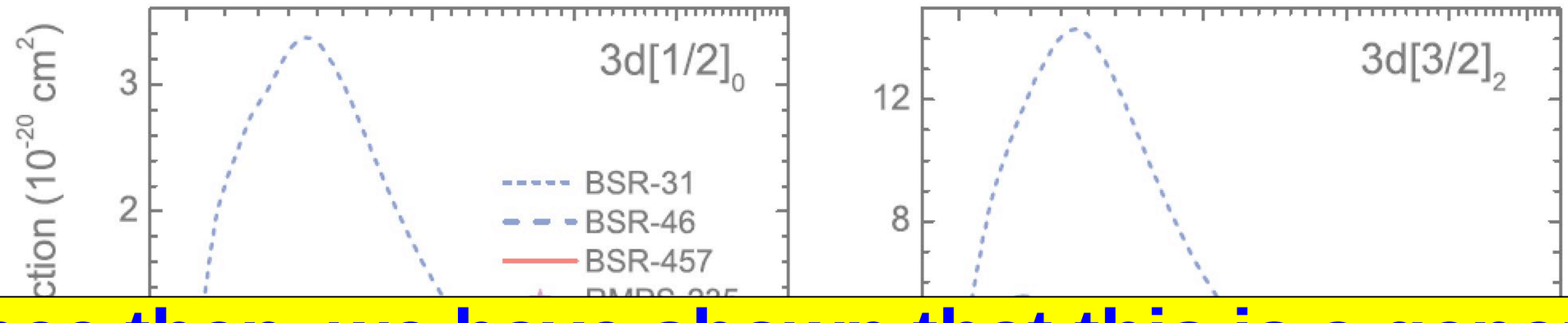
PHYSICAL REVIEW A **86**, 022717 (2012)

Electron-impact excitation of neon at intermediate energies

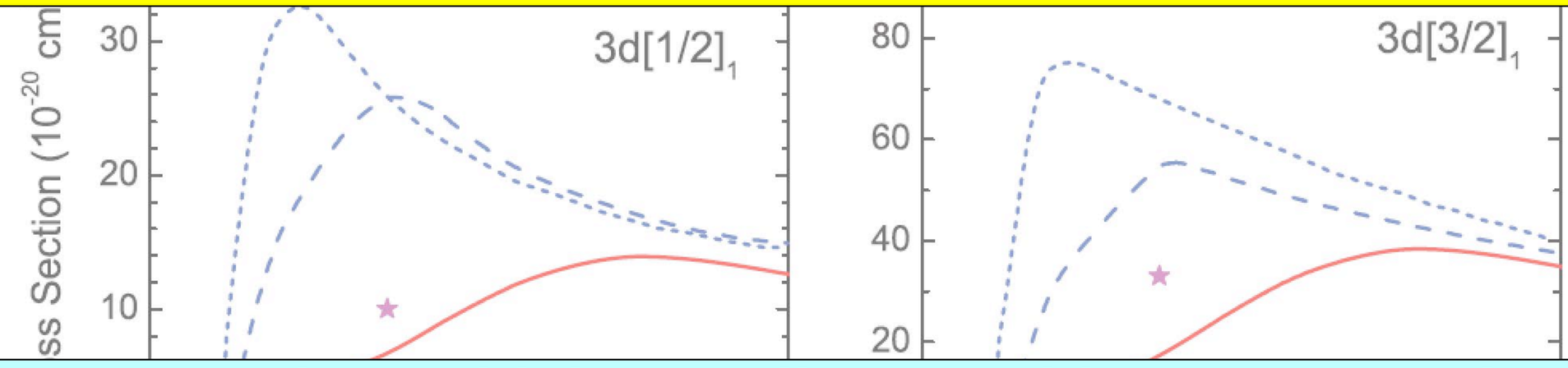
Oleg Zatsarinny and Klaus Bartschat

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:**

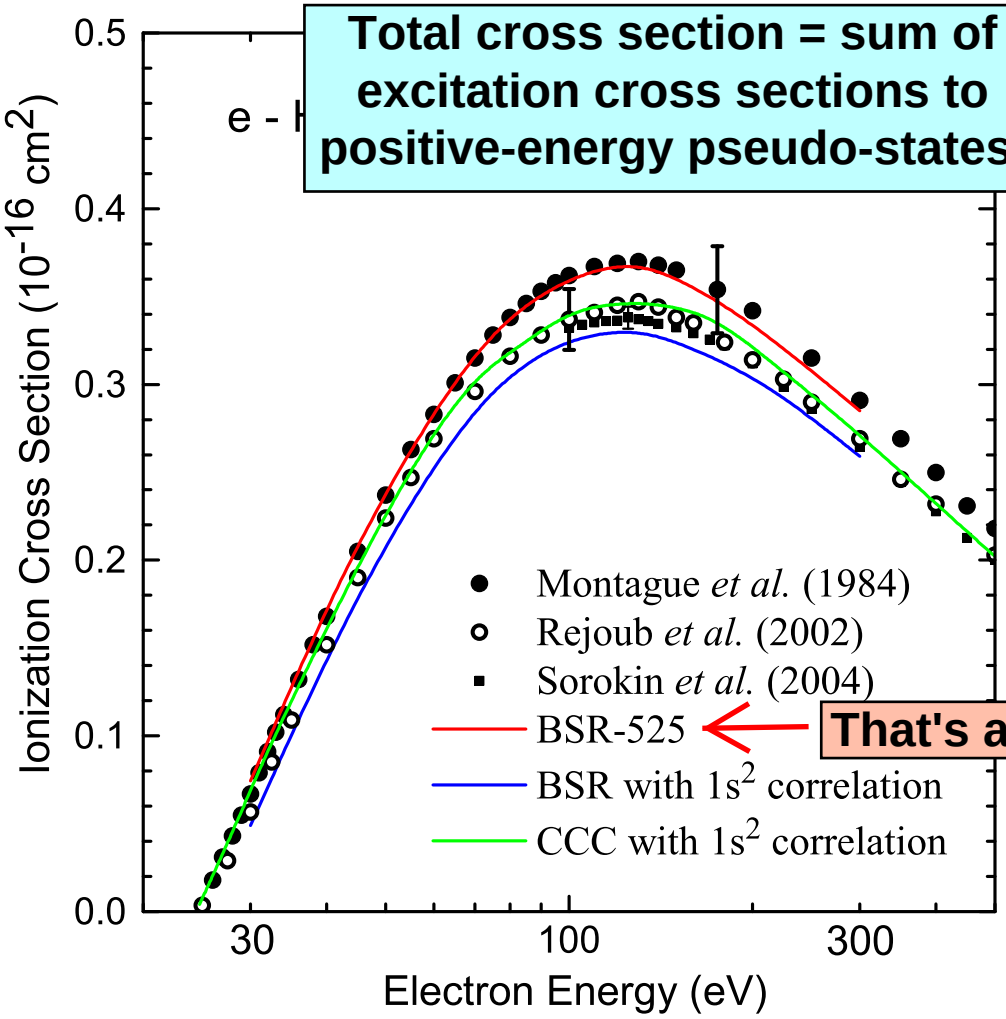
This direct projection is the essential idea – we'll see if it works.

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

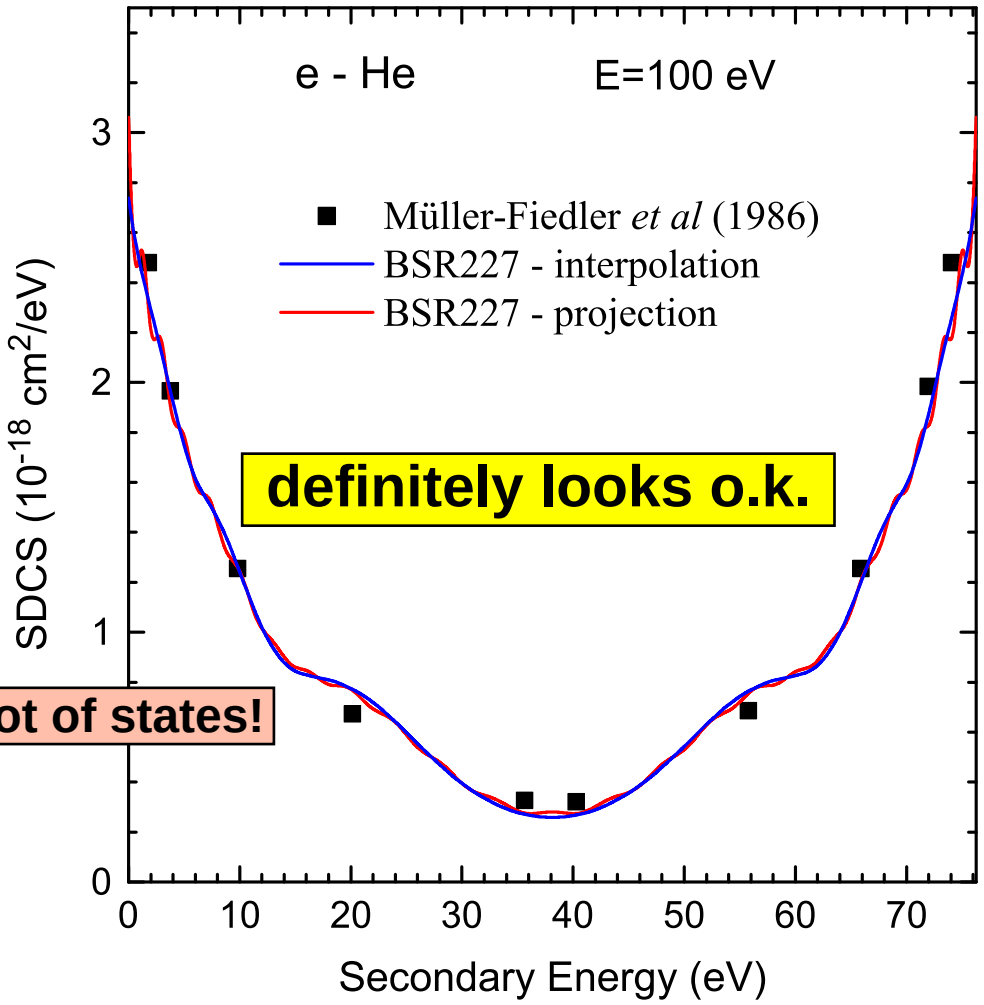
Some Checks: Ionization without Excitation (compare to CCC and TDCC)

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.

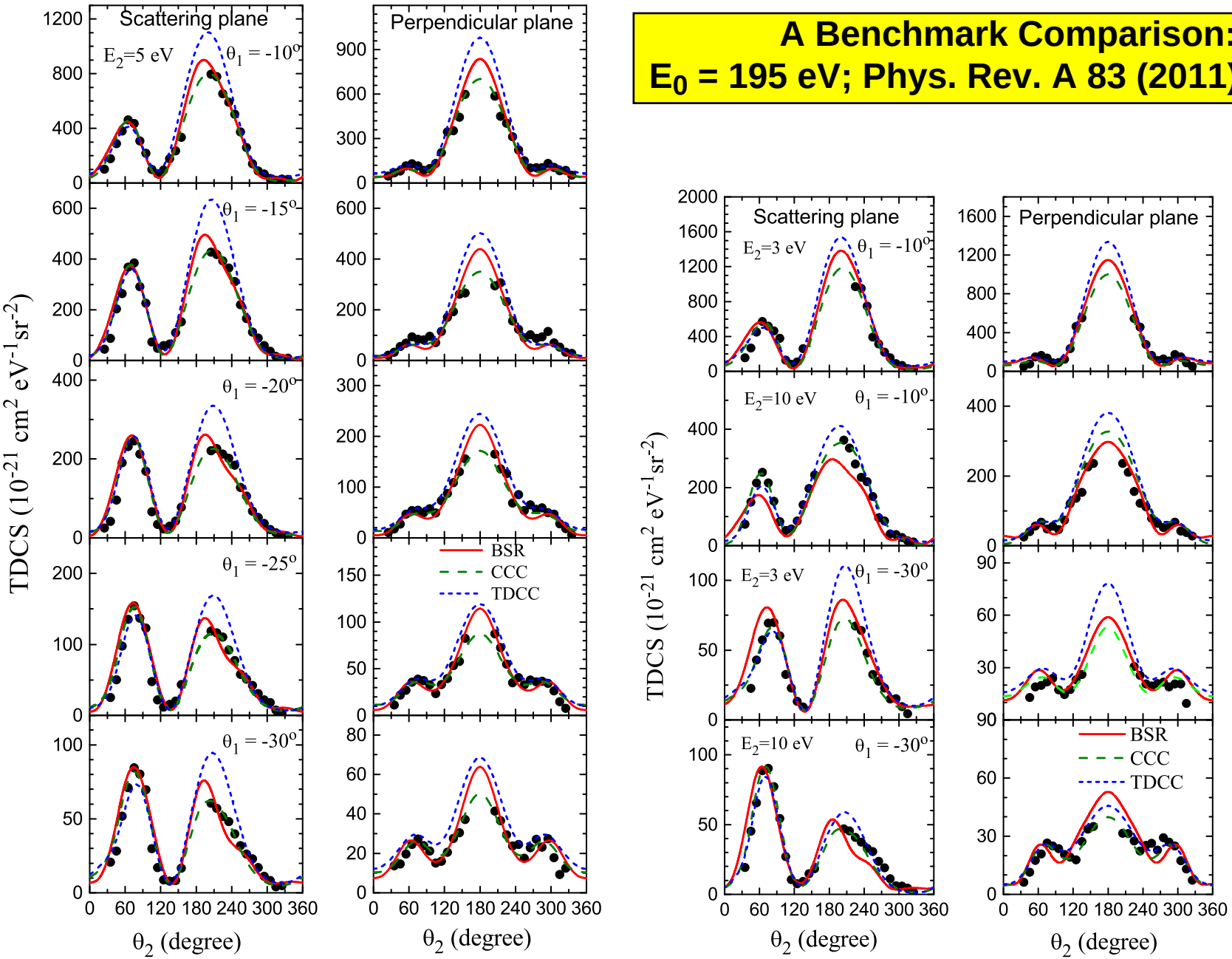
- **Including correlation in the ground state reduces the theoretical result.**
- **Interpolation yields smoother result, but direct projection is acceptable.**
- **DIRECT PROJECTION is NECESSARY for MULTI-CHANNEL cases!**

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

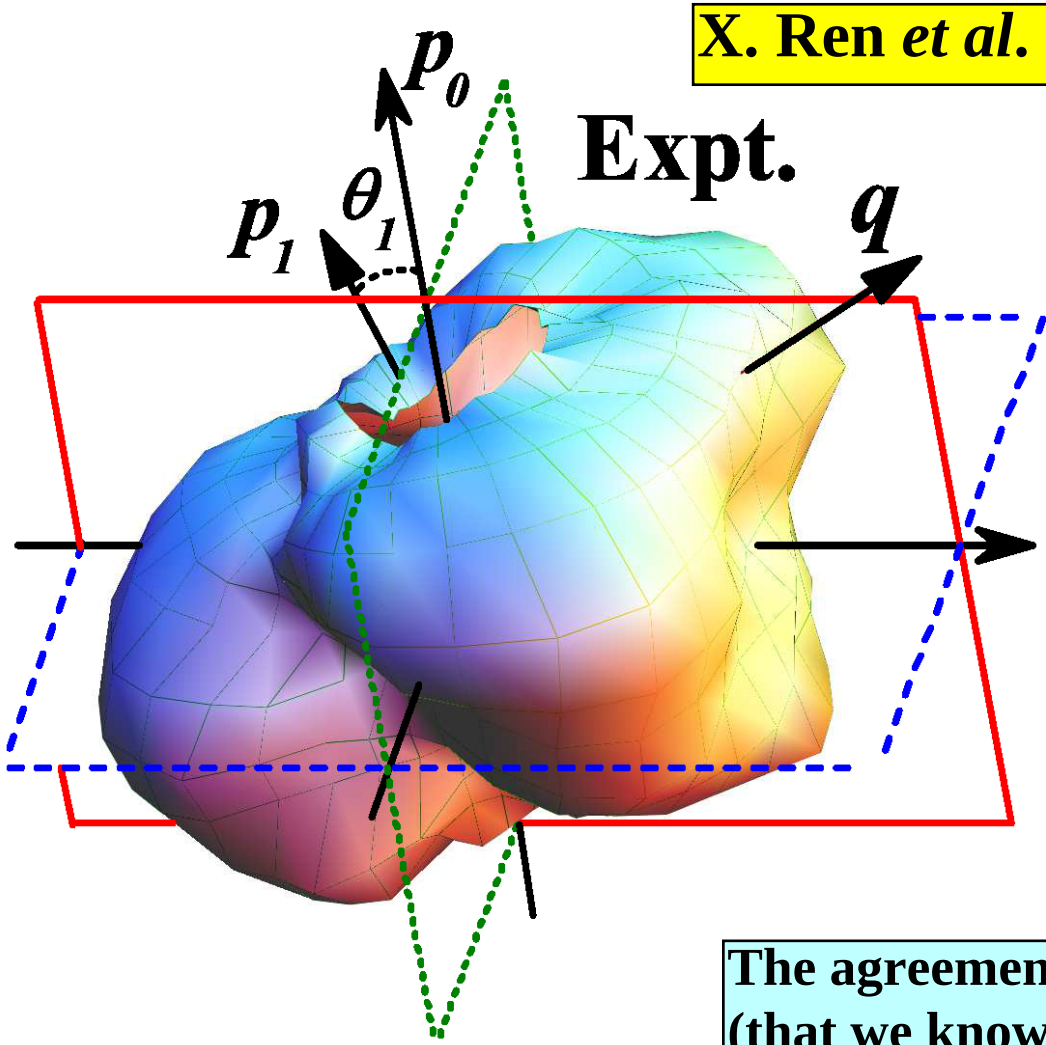


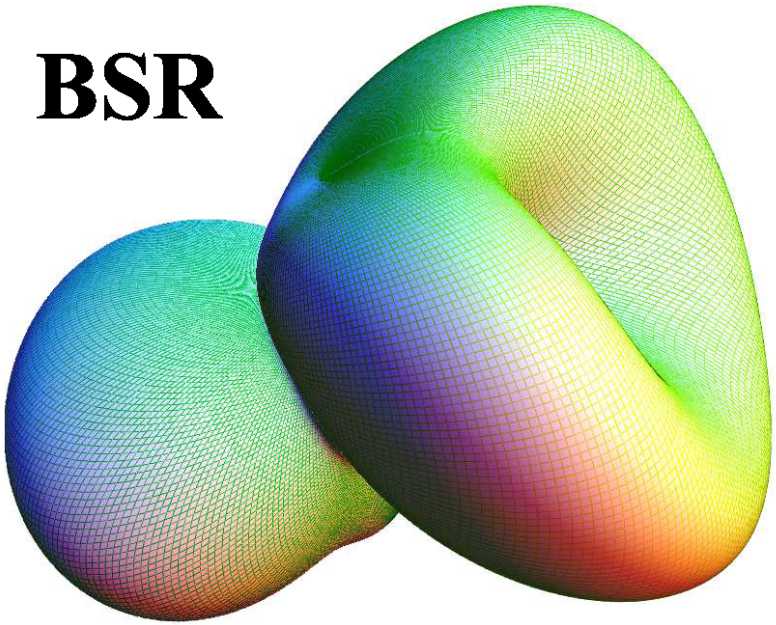
(e,2e) on Ar is a very l .. o .... n ..... g story. It includes the discovery of an error in the processing of the raw experimental data, which was found by the confidence gained in BSR predictions ...

(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

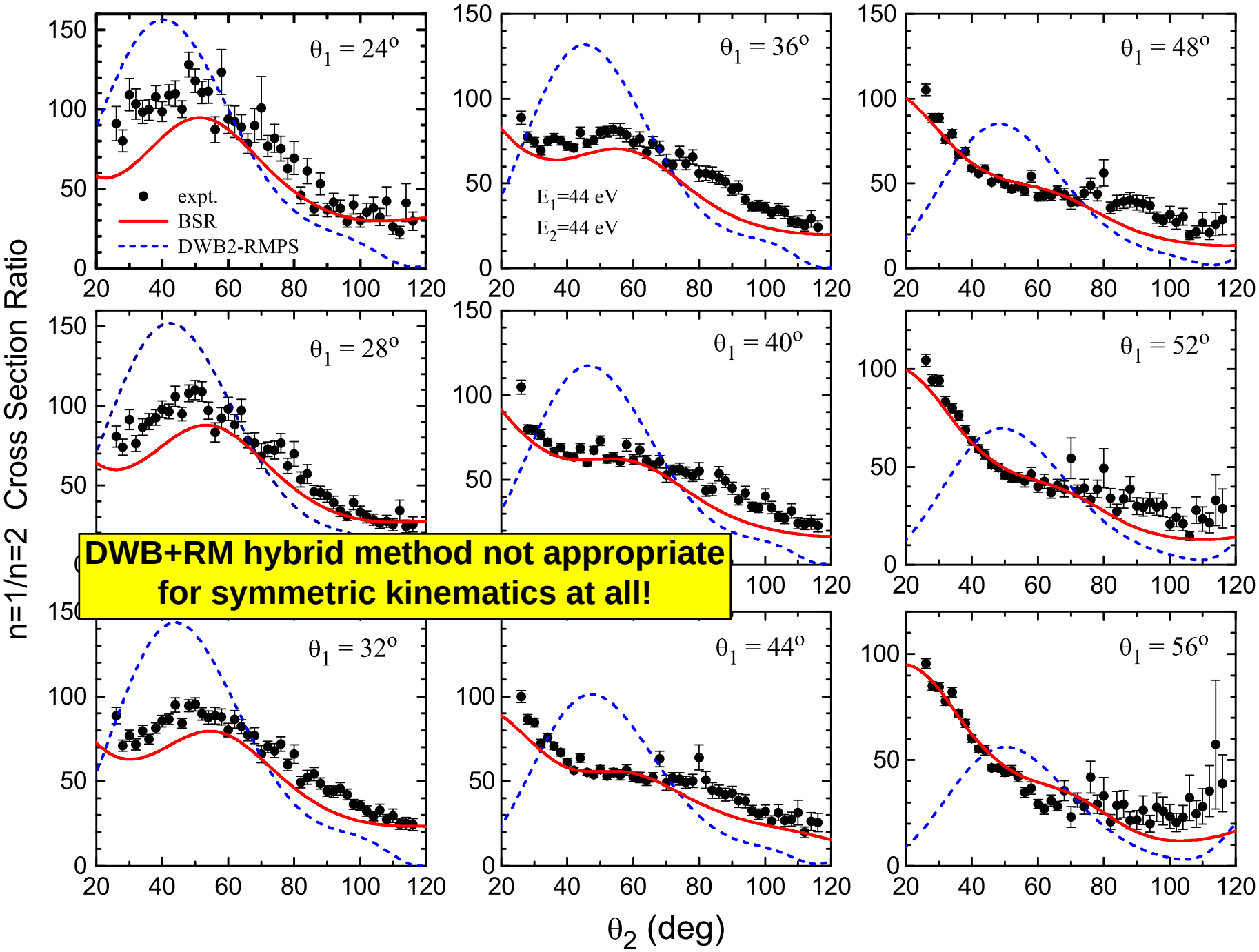
All Three Electrons Change Their Quantum State

(Movie by Allison Harris, Illinois State University)

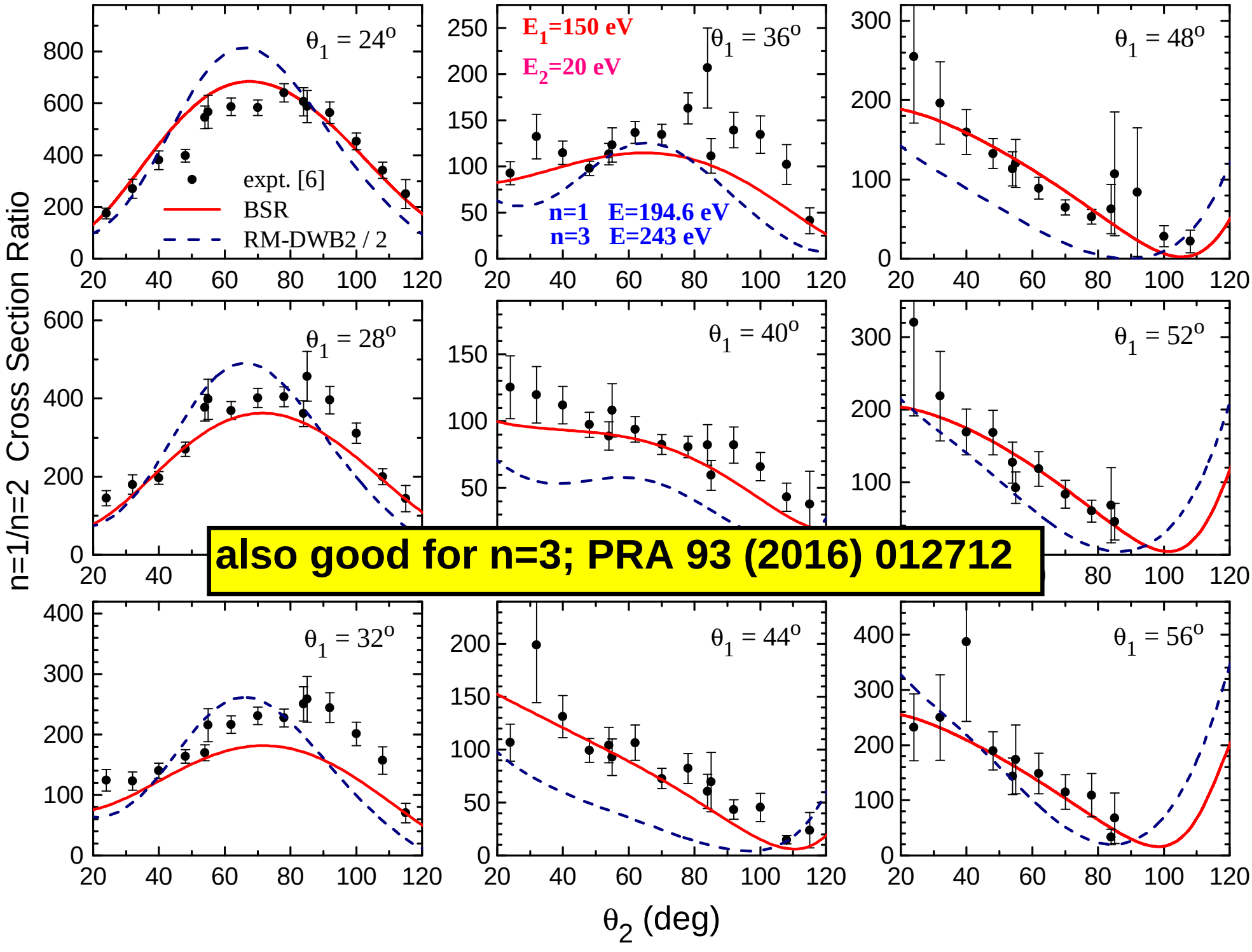
BSRMPS works great: PRL 107 (2011) 023203

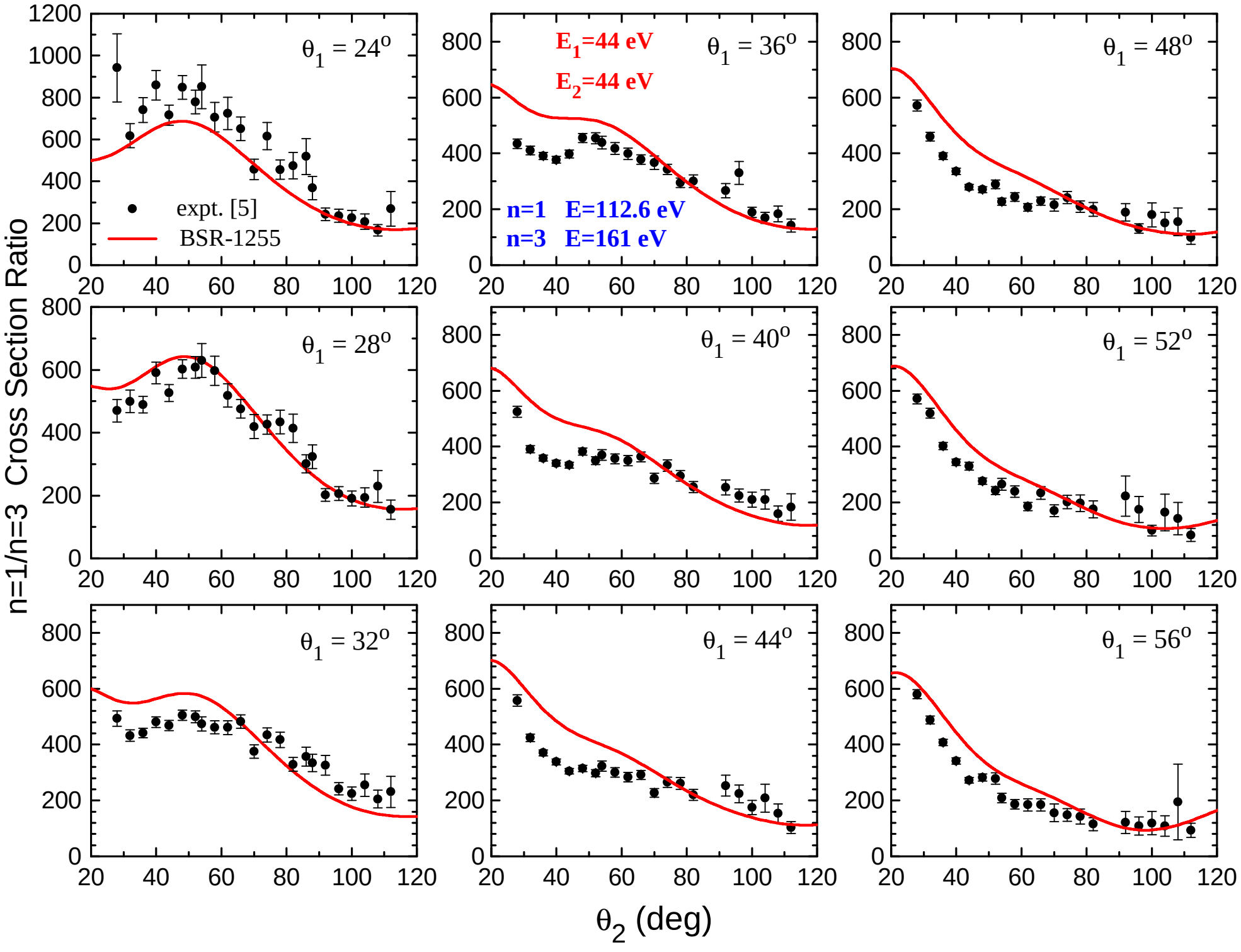
Triple-Differential Cross Section Ratio

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

PERSPECTIVE

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)

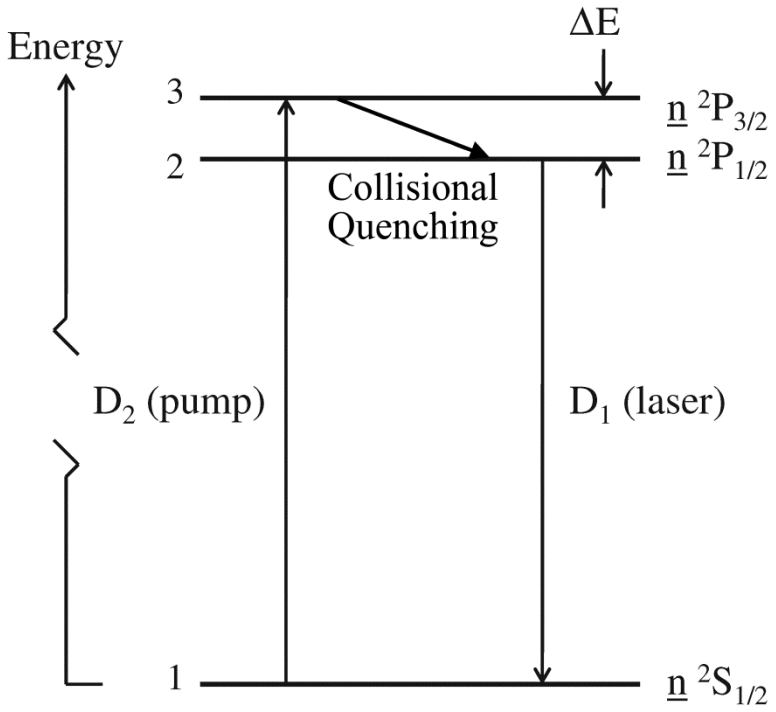
Electron collisions with atoms, ions, molecules, and surfaces are critically important to the understanding and modeling of low-temperature plasmas (LTPs), and so in the development of technologies based on LTPs. Recent progress in obtaining experimental benchmark data and the development of highly sophisticated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

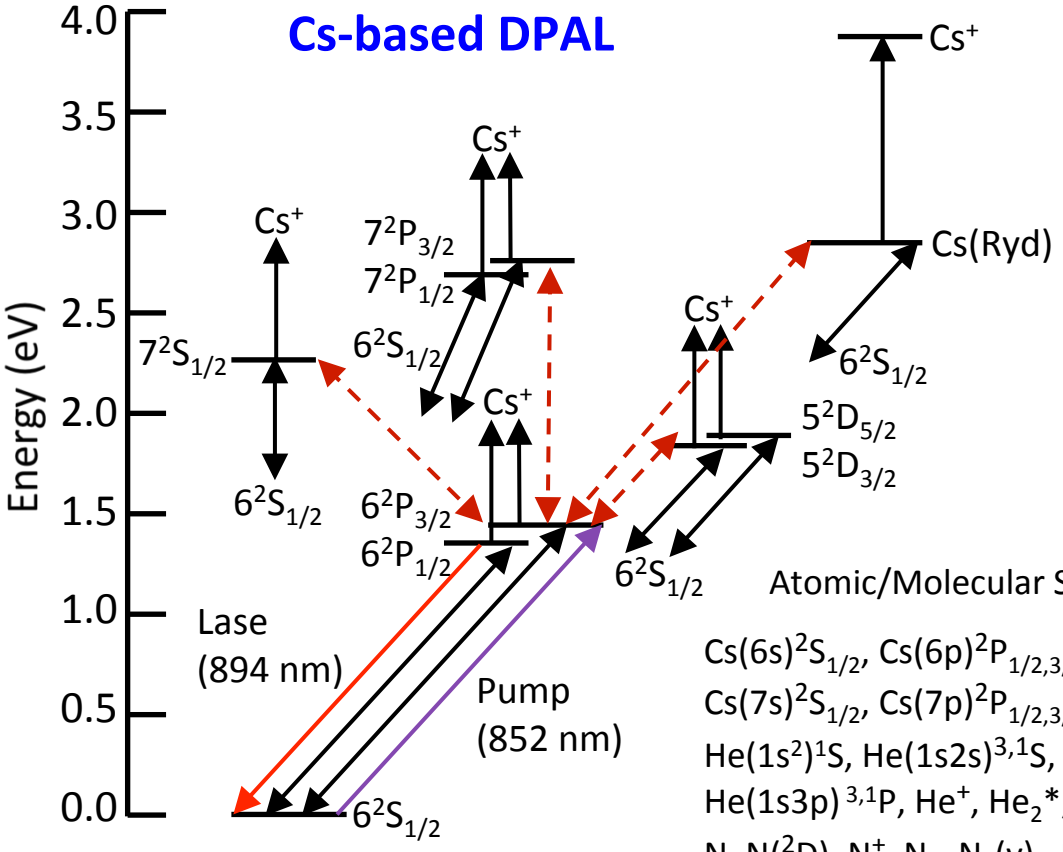
DIODE-PUMPED ALKALI LASERS (DPALs)

- **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.)

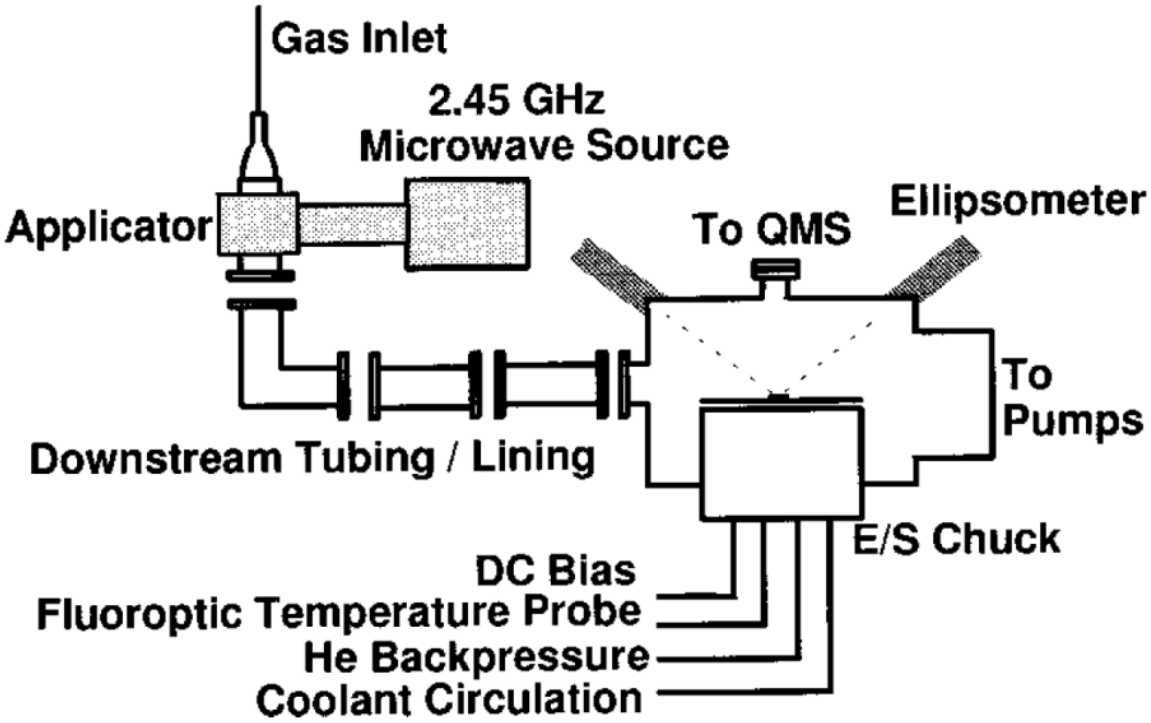


Atomic/Molecular Species in the Model

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

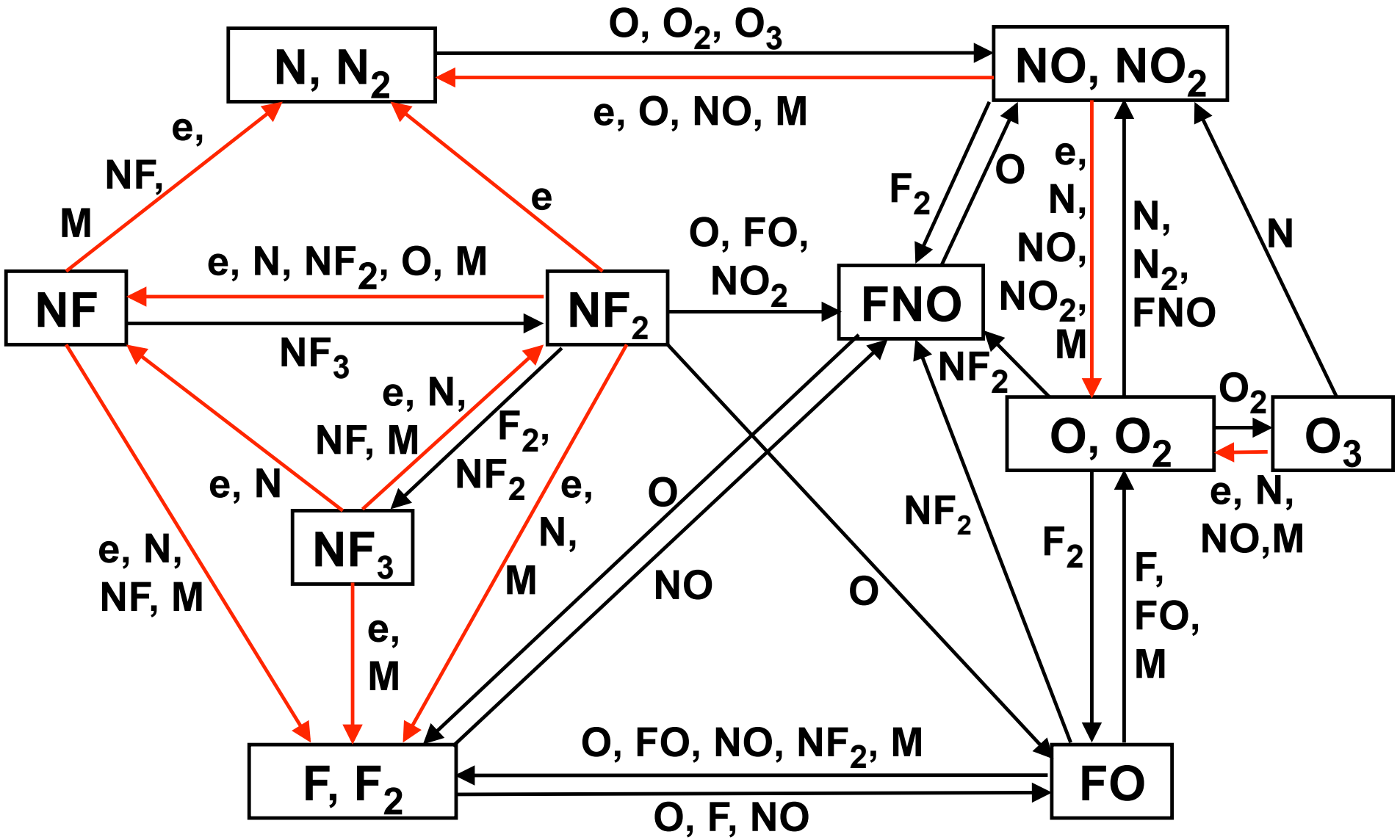


- Schematic of RPS.[1]

- 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"!

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

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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Received 18 March 2016, revised 15 June 2016
Accepted for publication 7 July 2016
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.

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.

CONTACT: O. Zatsarinny and K. Bartschat
Drake University
Des Moines, Iowa 50311, USA
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 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

Oleg Zatsarinny and Klaus Bartschat

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

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 !

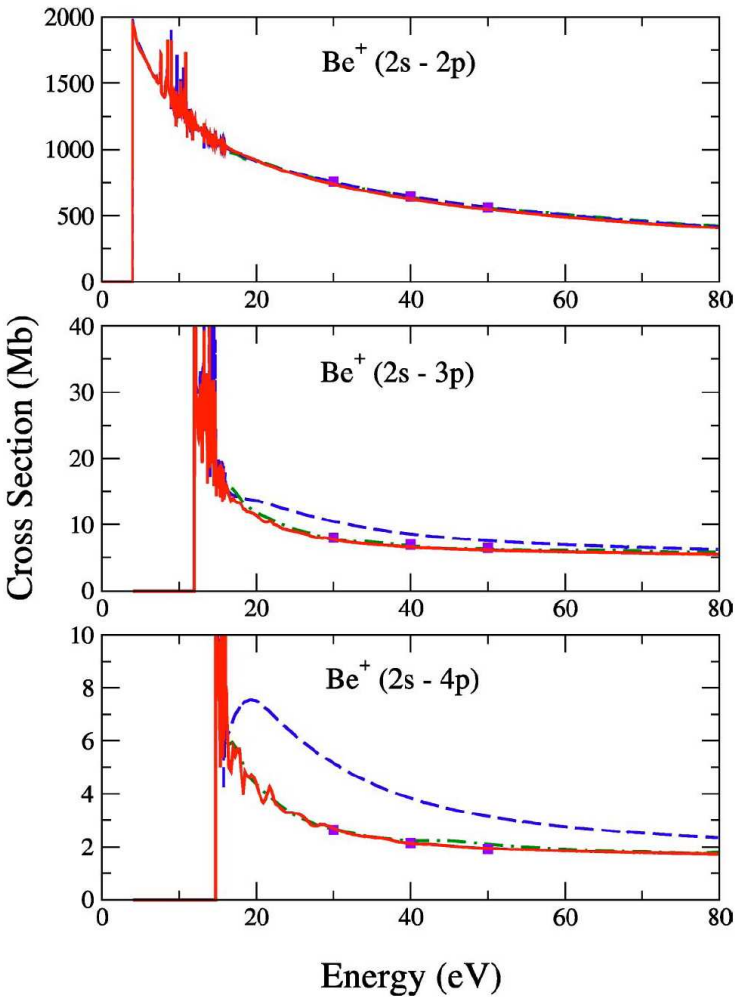

FIG. 4. Electron-impact excitation cross sections from the 2*s* ground term of Be^+ to the *np* excited terms. Dashed curves are from the present 14-term *R*-matrix calculation; solid curves are from the present 49-term RMPS calculation; solid squares are from the present TDCC calculation; dot-dashed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

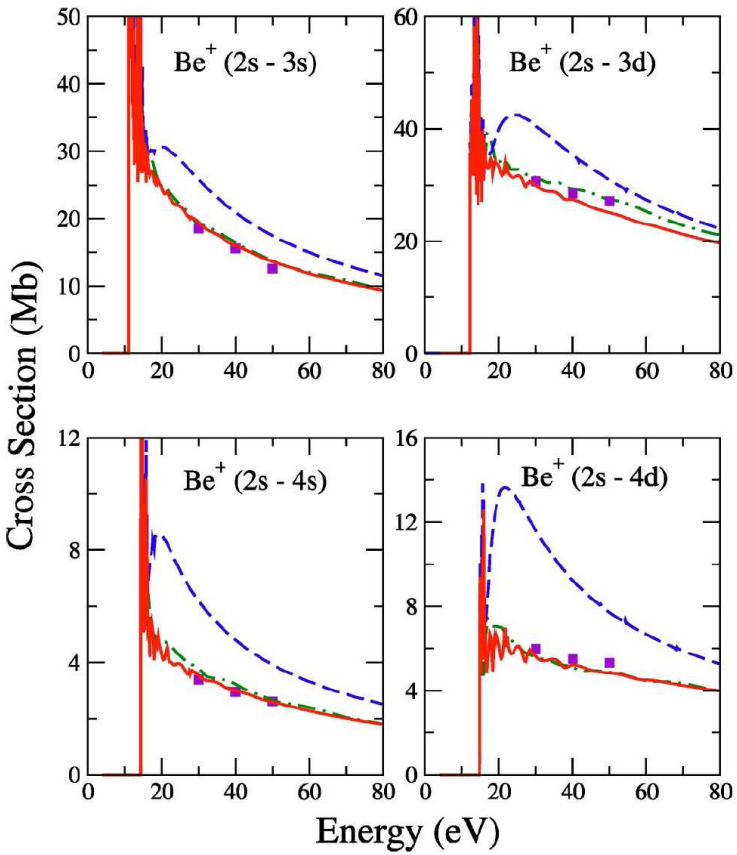

FIG. 5. Electron-impact excitation cross sections from the 2*s* ground term of Be^+ to the *ns* and *nd* excited terms. Dashed curves are from the present 14-term *R*-matrix calculation; solid curves are from the present 49-term RMPS calculation; solid squares are from the present TDCC calculation; dot-dashed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

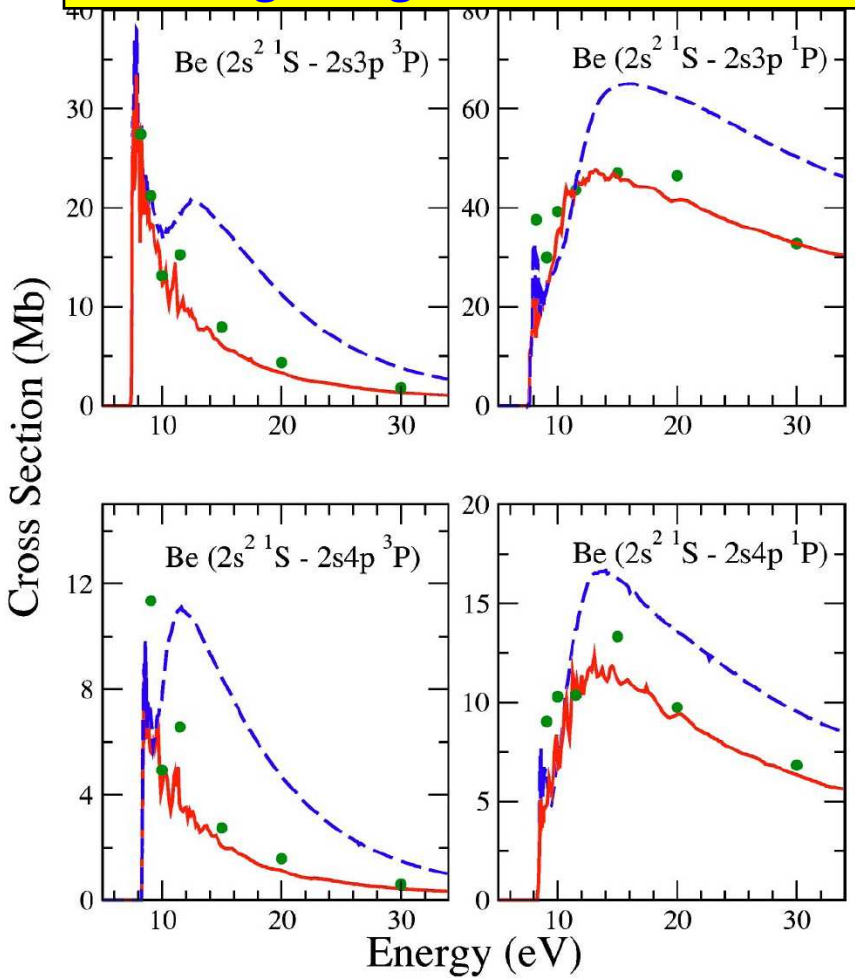

FIG. 2. Electron-impact excitation cross sections from the $2s^2\,{}^1S$ ground term of Be to the $2snp\,{}^3P$ and $2snp\,{}^1P$ excited terms for $n=3$ and 4. Dashed curves are from the present 29-term R-matrix calculation; solid curves are from the present 280-term RMPS calculation; solid circles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

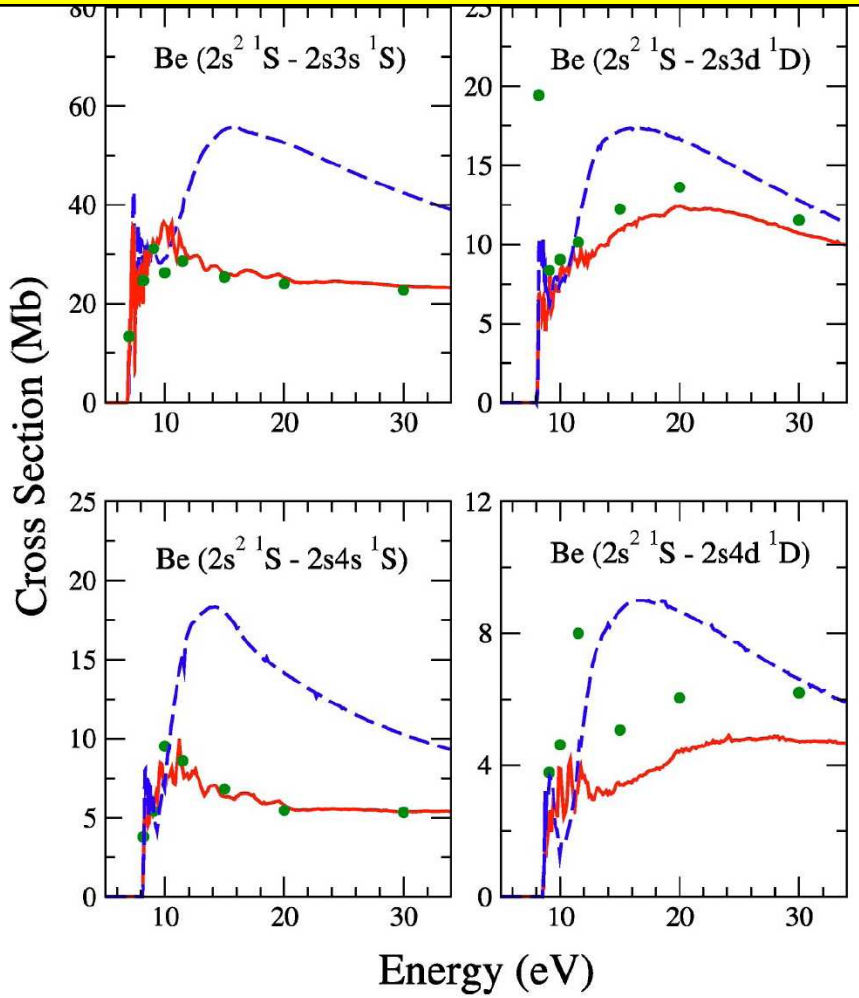

FIG. 3. Electron-impact excitation cross sections from the $2s^2\,{}^1S$ ground term of Be to the $2sns\,{}^1S$ and $2snd\,{}^1D$ excited terms. Dashed curves are from the present 29-term R-matrix calculation; solid curves are from the present 280-term RMPS calculation; solid circles are from CCC calculations 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.

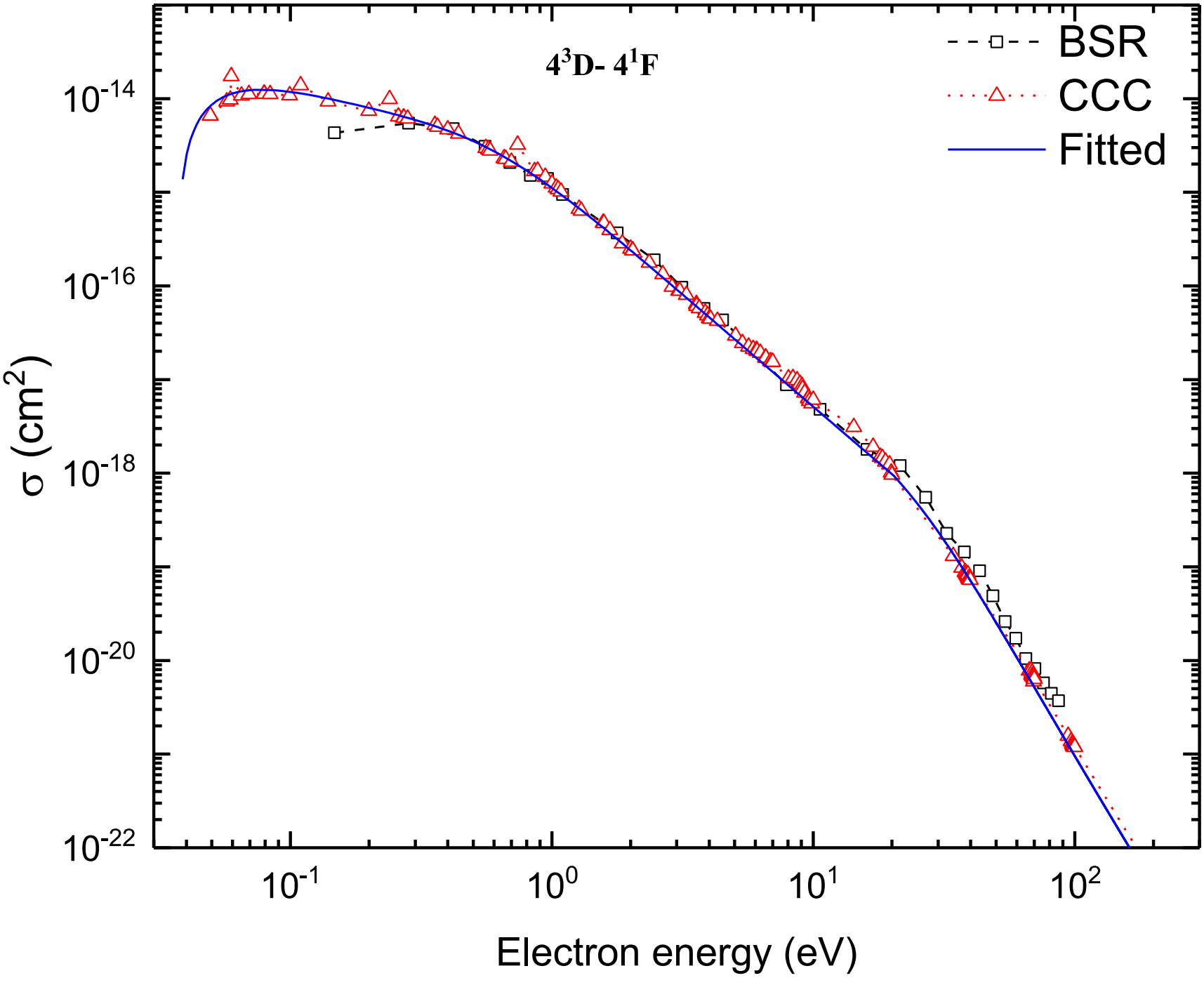

Fig. 4. Electron-impact excitation cross sections for the spin-forbidden ($4^3D \rightarrow 4^1F$) transition.

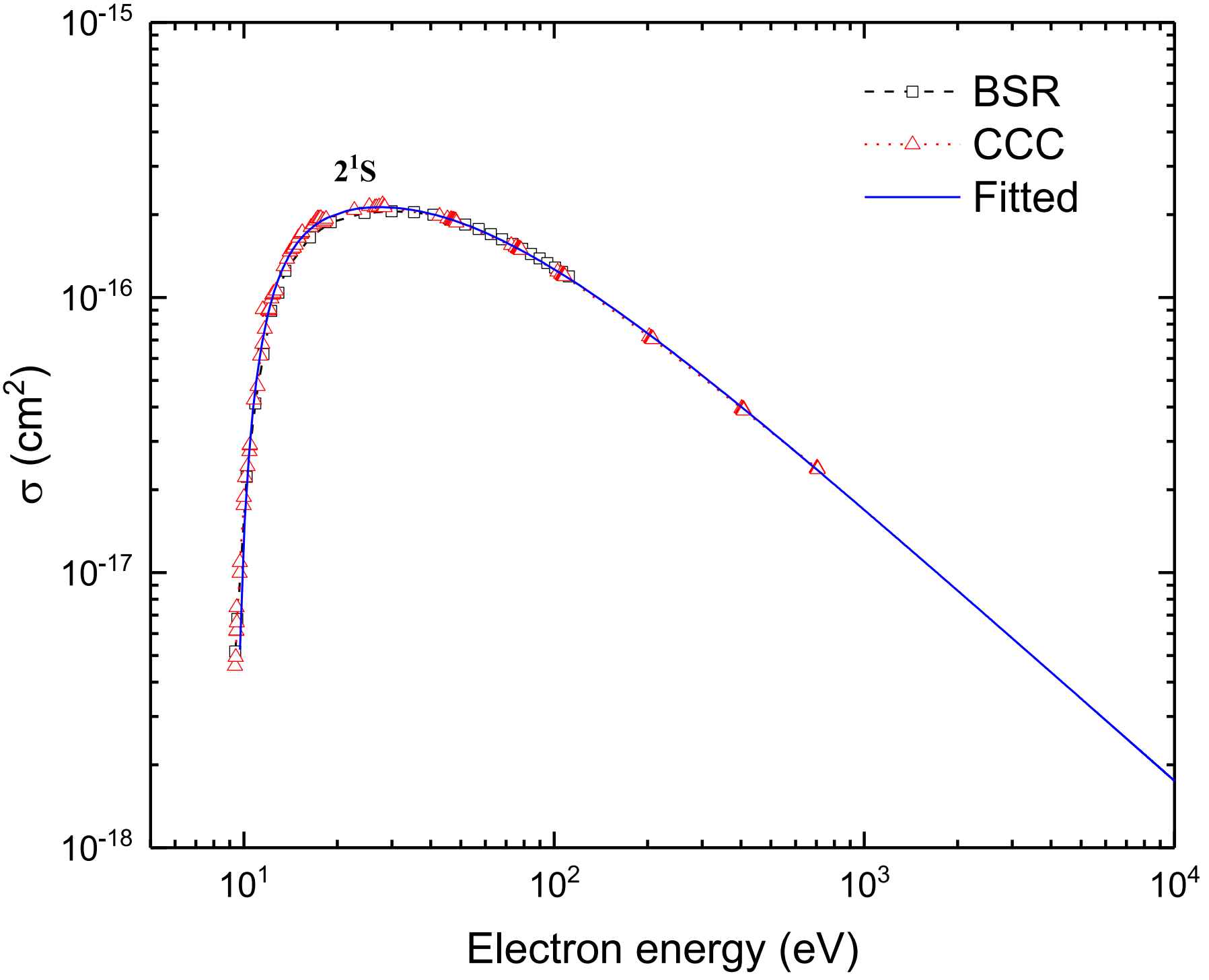

Fig. 6. Electron-impact ionization cross sections from the 2^1S state.

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

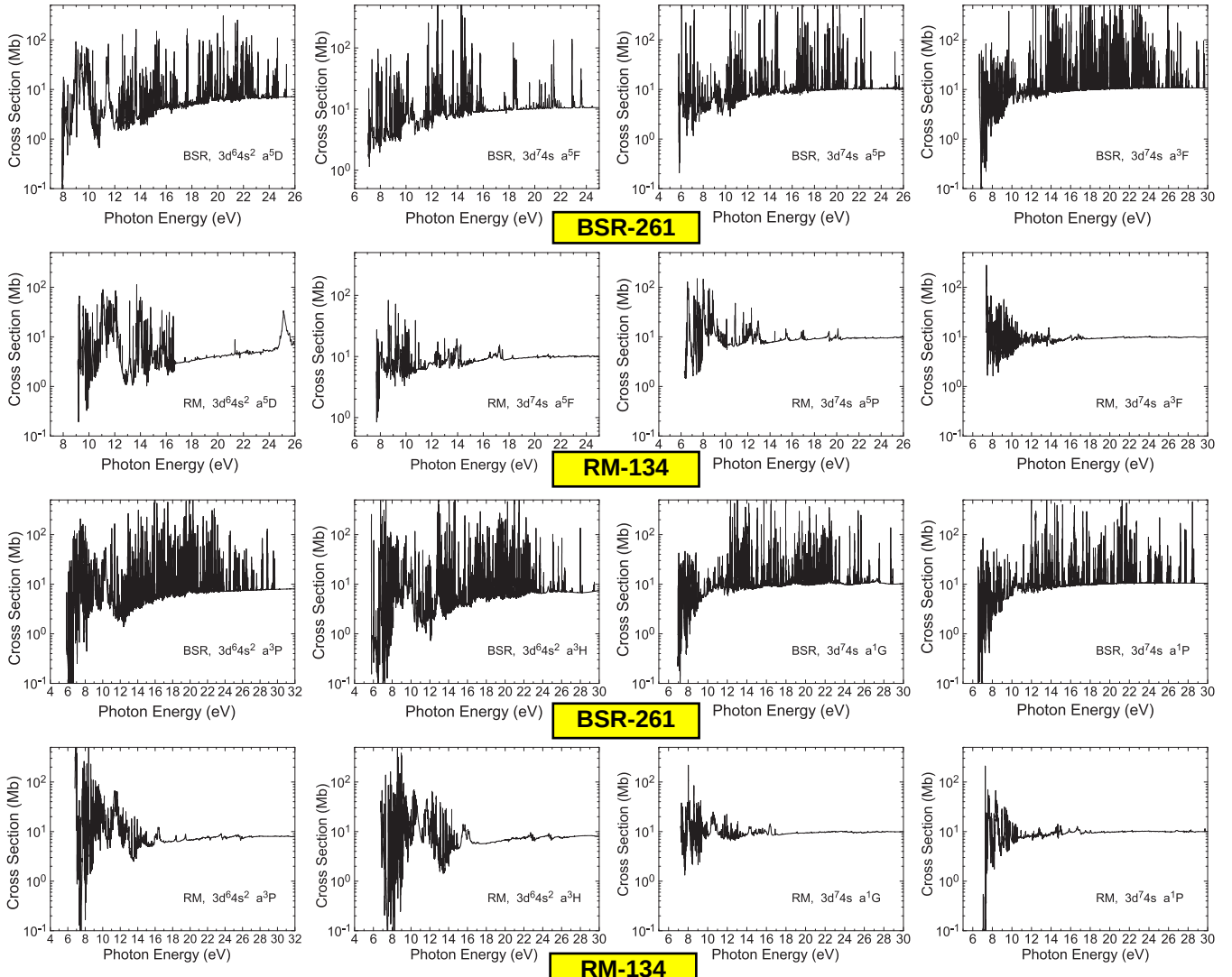

FIG. 1. Photoionization cross sections as a function of photon energy for a sample of low-lying even-parity states of Fe I. The present BSR-261 (BSR in the legend, first and third row) predictions are compared with the RM-134 (RM in the legend, second and fourth row) results of Bautista *et al.* [3].

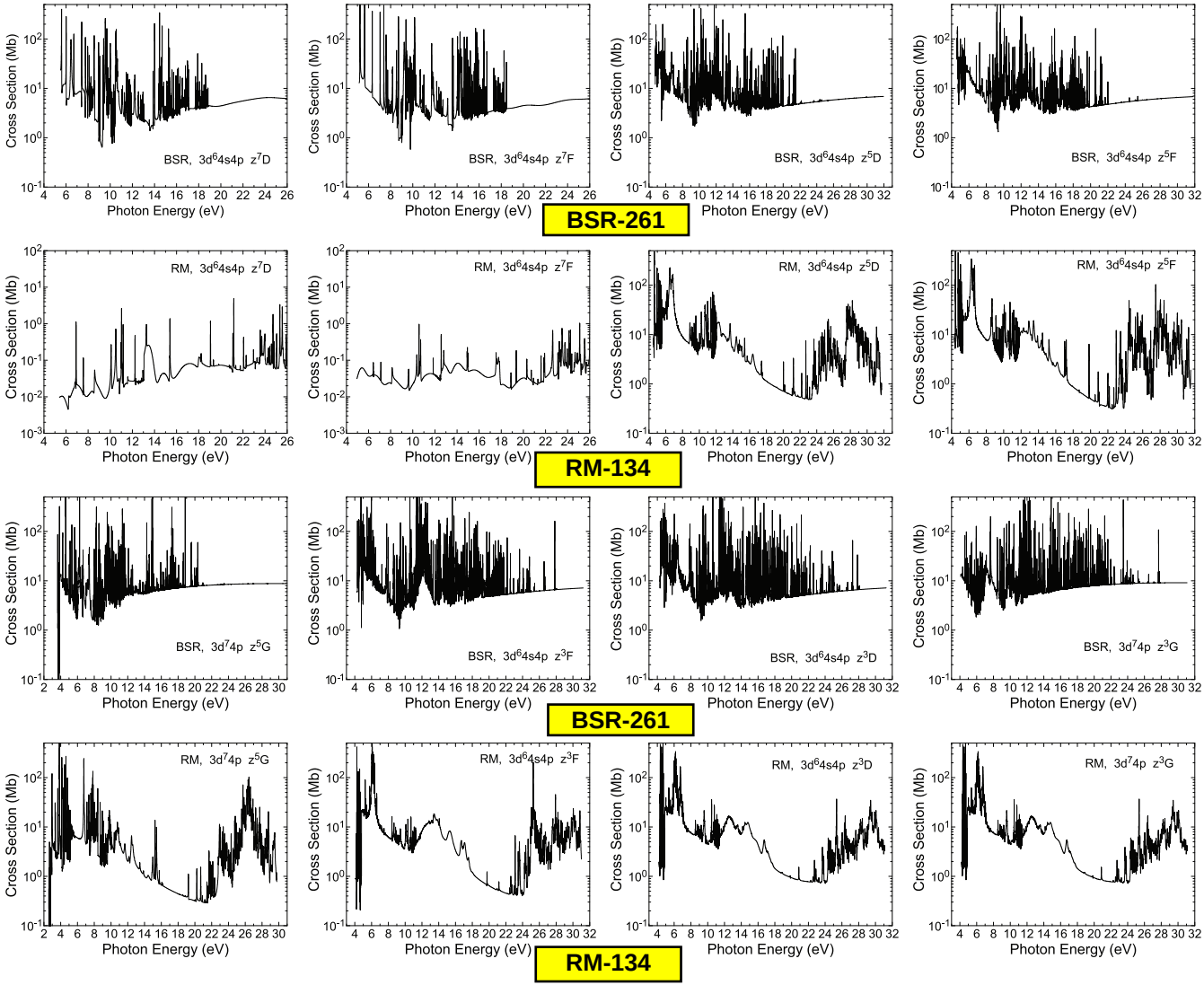

FIG. 4. Photoionization cross section for transitions from the first few odd-parity excited terms of Fe I. The present BSR-261 (BSR in the legend, first and third row) predictions are compared with the RM-134 (RM in the legend, second and fourth row) results of Bautista *et al.* [3].

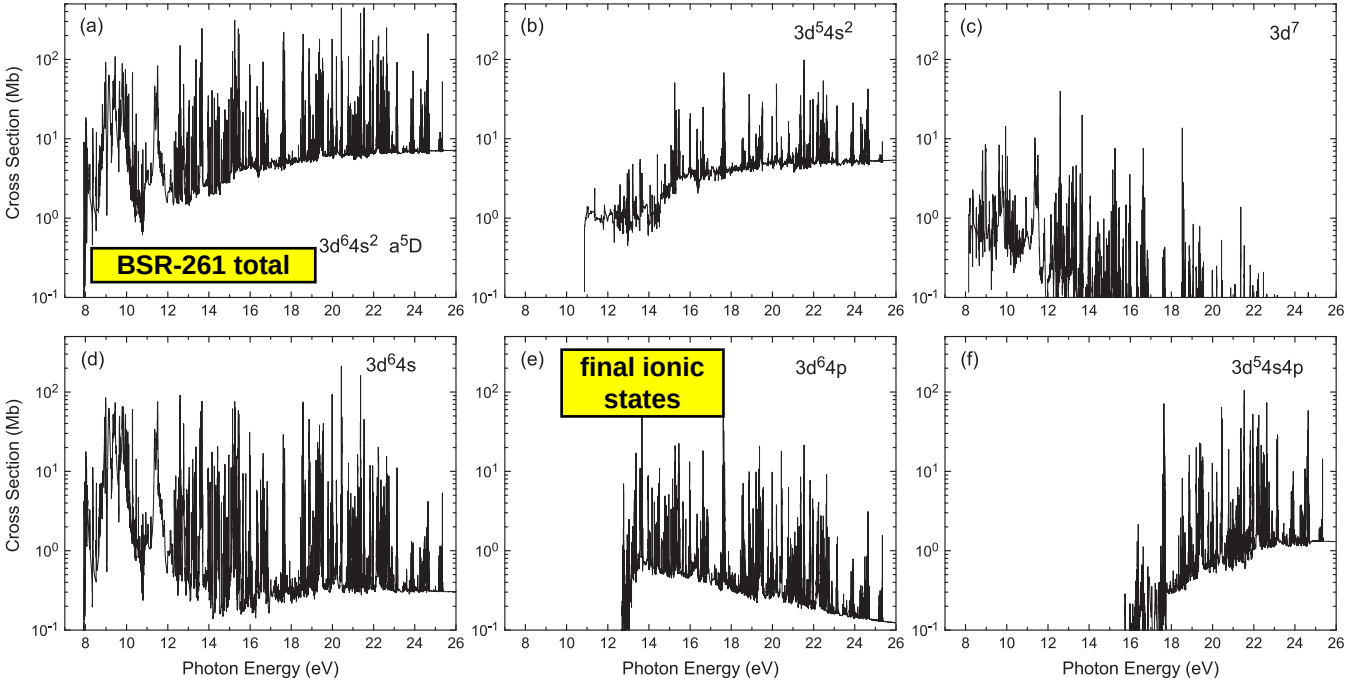

FIG. 2. Photoionization cross section of the $3d^6 4s^2\ ^5D$ ground state of Fe I (a), along with the contributions from different subsets (b)–(f) of final ionic configurations indicated in the legend.

Electron-impact excitations of Fe ions

(large-scale BSR calculations for astrophysical applications)

Fe VII $3p^6 3d^2$, $3p^5 3d^3$, $3p^6 3d4l$, $3p^5 3d^2 5s$, $3p^6 3d5p$

182 fine-structure levels

Fe VIII $3p^6 3d$, $3p^5 3d^2$, $3p^6 4l$, $3p^5 3d4s$, $3s3p^6 3d^2$, $3p^6 5l$

102 fine-structure levels

Fe IX $3p^6$, $3p^5 3d$, $3s3p^6 3d$, $3p^4 3d^2$, $3p^5 4l$, $3s3p^5 3d^2$, $3s3p^6 4l$, $3p^5 5s$

344 fine-structure levels

Fe II $3d^5 4s^2$, $3d^6 4s$, $3d^7$, $3d^6 4p$, $3d^5 4s4p$

261 LS terms, 716 fine-structure levels

- Direct Breit-Pauli (intermediate coupling) calculations
- More accurate target description
- Complete set of scattering and radiative parameters
  (rate coefficients and oscillator strengths between all levels)
- Extensive calculation of resonance structure (~20000 energy points)
- Do we get convergence?

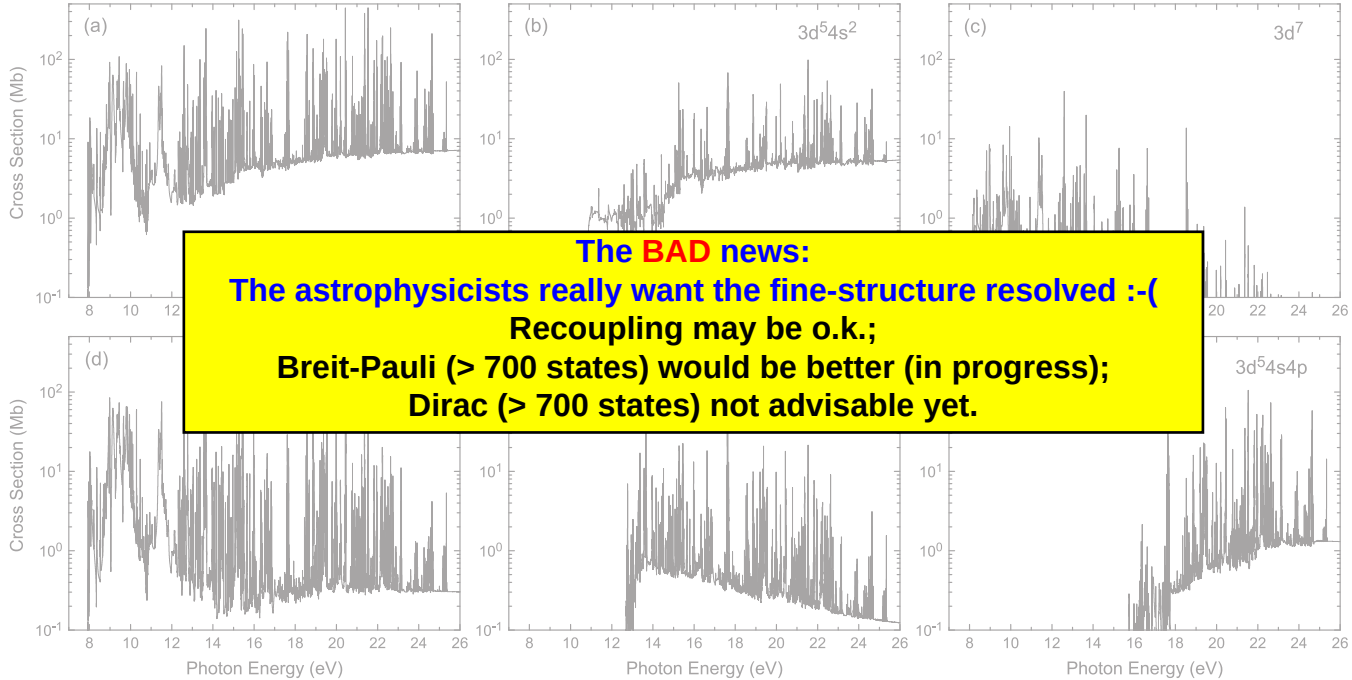

FIG. 2. Photoionization cross section of the $3d^6 4s^2\ ^5D$ ground state of Fe I (a), along with the contributions from different subsets (b)–(f) of final ionic configurations indicated in the legend.

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

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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.

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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

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A xenon collisional-radiative model applicable to electric propulsion devices: II. Kinetics of the 6*s*, 6*p*, and 5*d* states of atoms and ions in Hall thrusters

Xi-Ming Zhu[1,4], Yan-Fei Wang[1], Yang Wang[1,4], Da-Ren Yu[1], Oleg Zatsarinny[2], Klaus Bartschat[2], Tsanko Vaskov Tsankov[3] and Uwe Czarnetzki[3]

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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)

From electron scattering and weak-field ionization to ultrafast intense processes ...

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

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

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

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

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(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, nonorth The solution of the TDSE is the diagonalization of any la tion and ionization of Ne at ross sections for two-photon ionization is achieved.

This was an overkill – the box size is too large; we did not use the fact that in single ionization only one electron gets far away from the nucleus (–> RMT; Kathryn Hamilton)

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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

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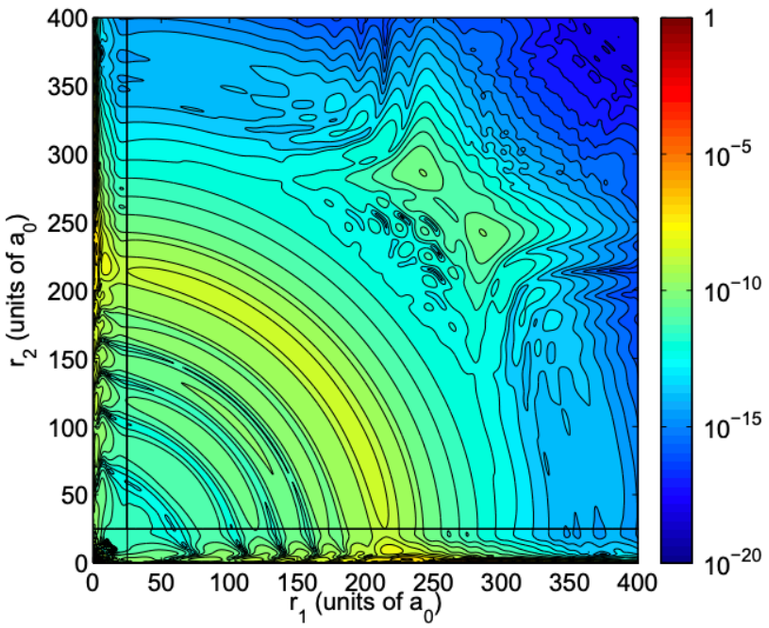
We even started double ionization, but got stuck at helium.

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)

THE R MATRIX WITH TIME DEPENDENCE METHOD



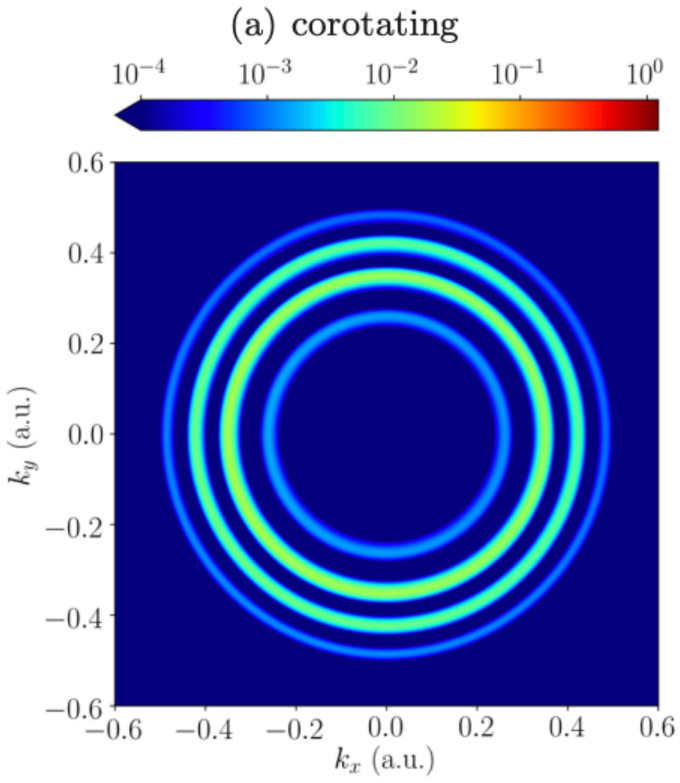
UK-AMOR › RMT › rmt › **Details**

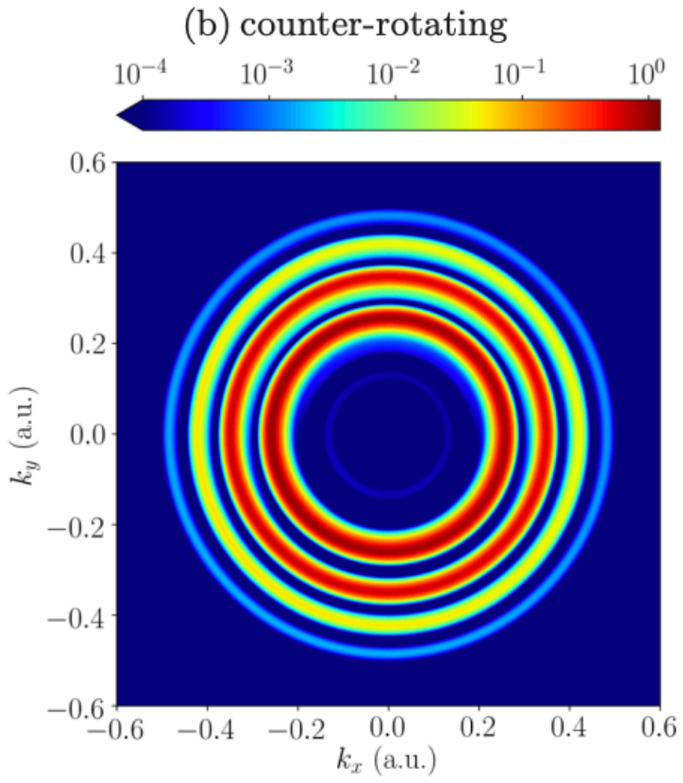
rmt

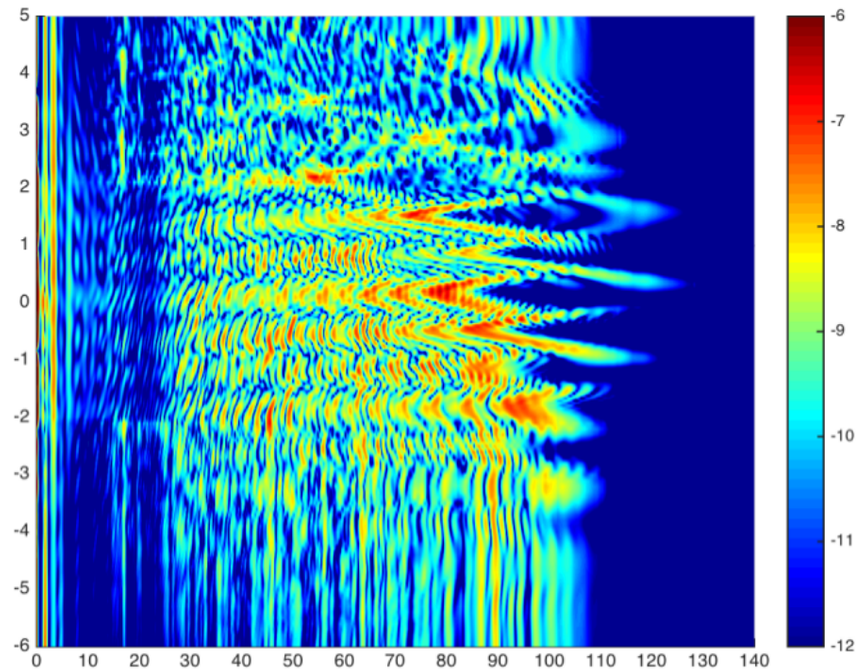
Project ID: 8383626

743 Commits **17** Branches **0** Tags **477.3 MB** Files

RMT codes for atoms and molecules in intense, arbitrarily polarised light fields







THE RMT METHOD

Goal:

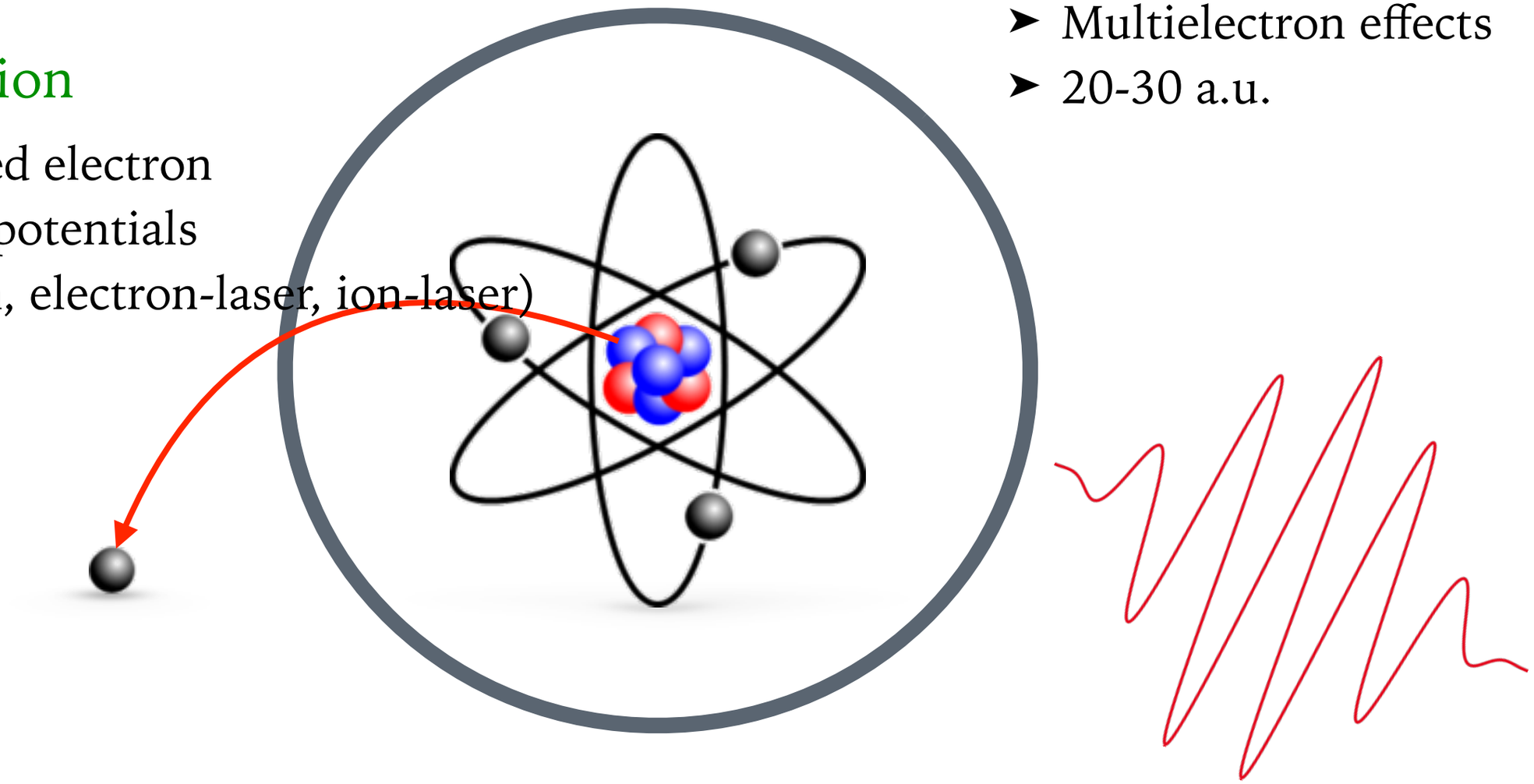
Solve the T.D.S.E. → Time-dependent Wavefunction → Observables

Inner Region

- N+1 electrons
- Multielectron effects
- 20-30 a.u.

Outer Region

- Single ejected electron
- Long range potentials
- (electron-ion, electron-laser, ion-laser)



L. Moore et al. “The RMT method for many-electron atomic systems in intense short-pulse laser light”, *Journal of Modern Optics*, **58:13** , 1132-1140 (2011)

THE RMT METHOD

Goal:

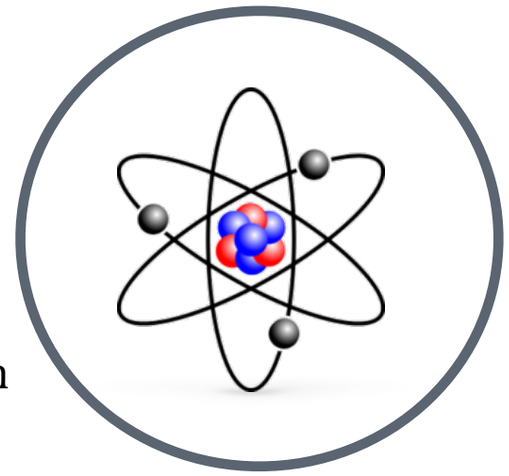
Solve the T.D.S.E. → Time-dependent Wavefunction → Observables

Inner Region

- N+1 electrons
- Multielectron effects
- 20-30 a.u.

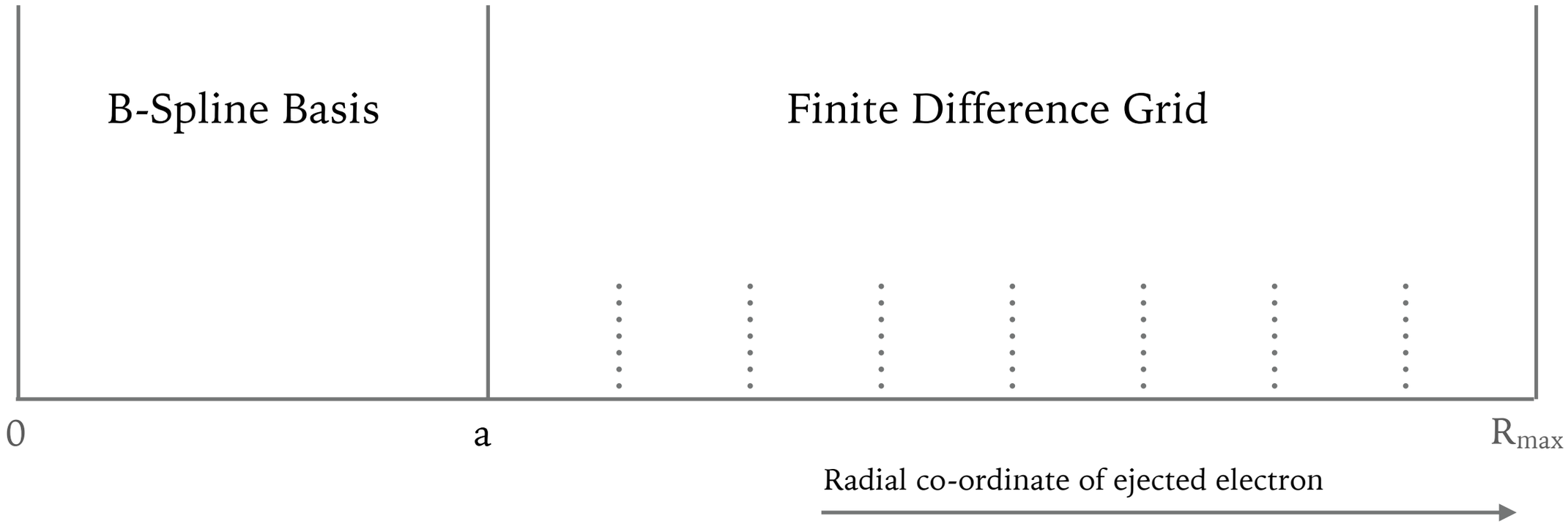
Outer Region

- Single ejected electron
- Long range potentials
- (electron-ion, electron-laser, ion-laser)



Inner Region

Outer Region



L. Moore et al. “The RMT method for many-electron atomic systems in intense short-pulse laser light”, *Journal of Modern Optics*, **58:13** , 1132-1140 (2011)

KEY EQUATIONS

Outer Region

$$\Psi(\mathbf{X}_{N+1}, t) = \sum_{p=1}^{n_p} \bar{\Phi}_p(\mathbf{X}_N; \hat{r}_{N+1}\sigma_{N+1}) r_{N+1}^{-1} F_p(r_{N+1}, t) \qquad r_{N+1} \geq a$$

Channel functions

Radial wave function of ejected electron

$$i\frac{\partial}{\partial t}F_p(r,t) = H_{ti_p}(r)F_p(r,t) + \sum_{p'} [(W_E)_{pp'}(r) + (W_D)_{pp'}(t) + (W_P)_{pp'}(r,t)]F_{p'}$$

Electron-ion **Ion-laser** **Electron-laser**

KEY EQUATIONS

Inner Region

$$\Psi_I(\mathbf{X}_{N+1}, t) = \sum_k \psi_k(\mathbf{X}_{N+1}) C_k(t)$$

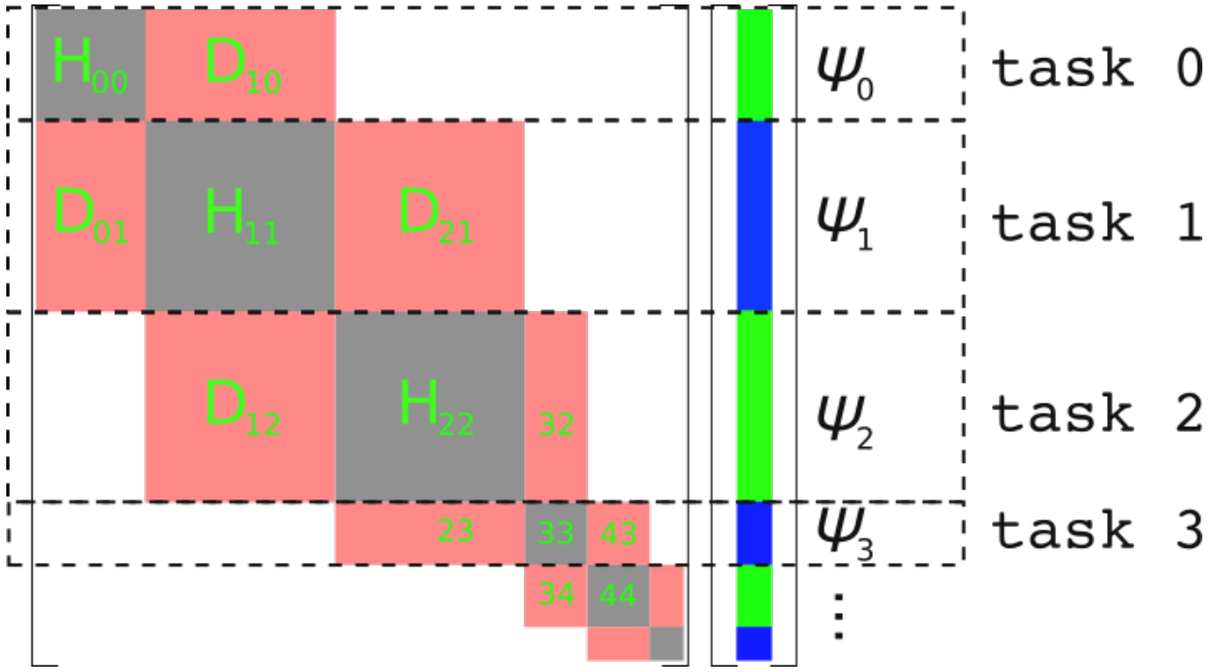
Eigenstates of Field-free Hamiltonian

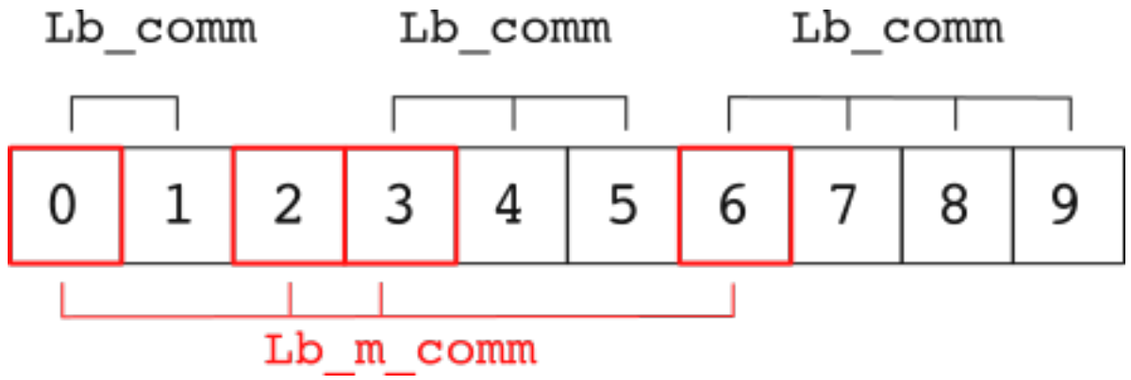
Time-dependent Coefficients

$$\frac{d}{dt} C_k(t) = -i \sum_{k'} H_{I_{kk'}}(t) C_{k'}(t) + \frac{i}{2} \sum_p \omega_{pk} \frac{\partial F_{pk}(r,t)}{\partial r}\bigg|_{r=a}$$

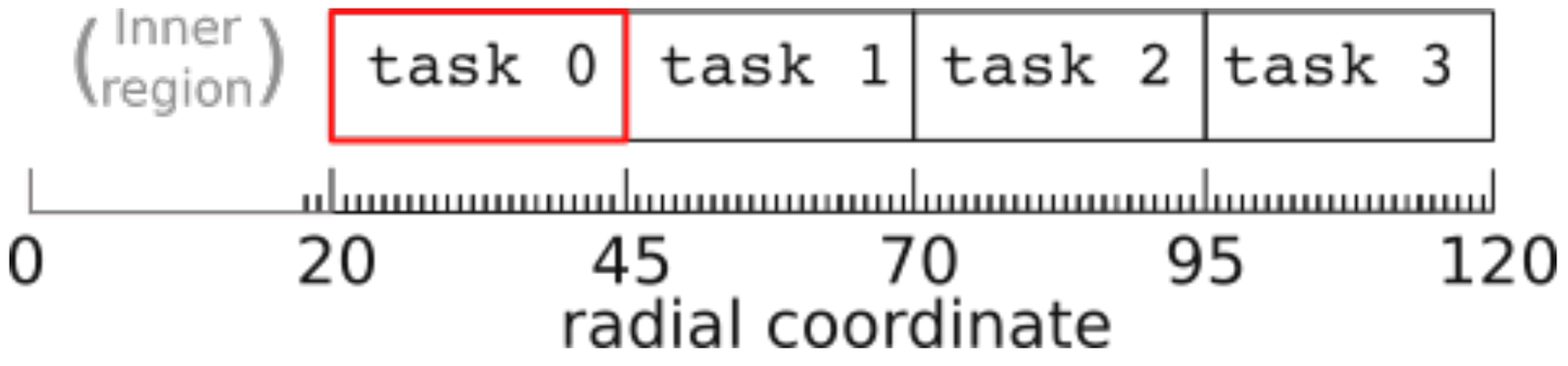
Surface Amplitudes

PARALLELISATION





Inner Region



Outer Region

RECENT DEVELOPMENTS

Limitations:

Linearly Polarised Light

Non-relativistic Targets

Atomic / Ionic Systems

RECENT DEVELOPMENTS

Limitations:

~~Linearly Polarised Light~~

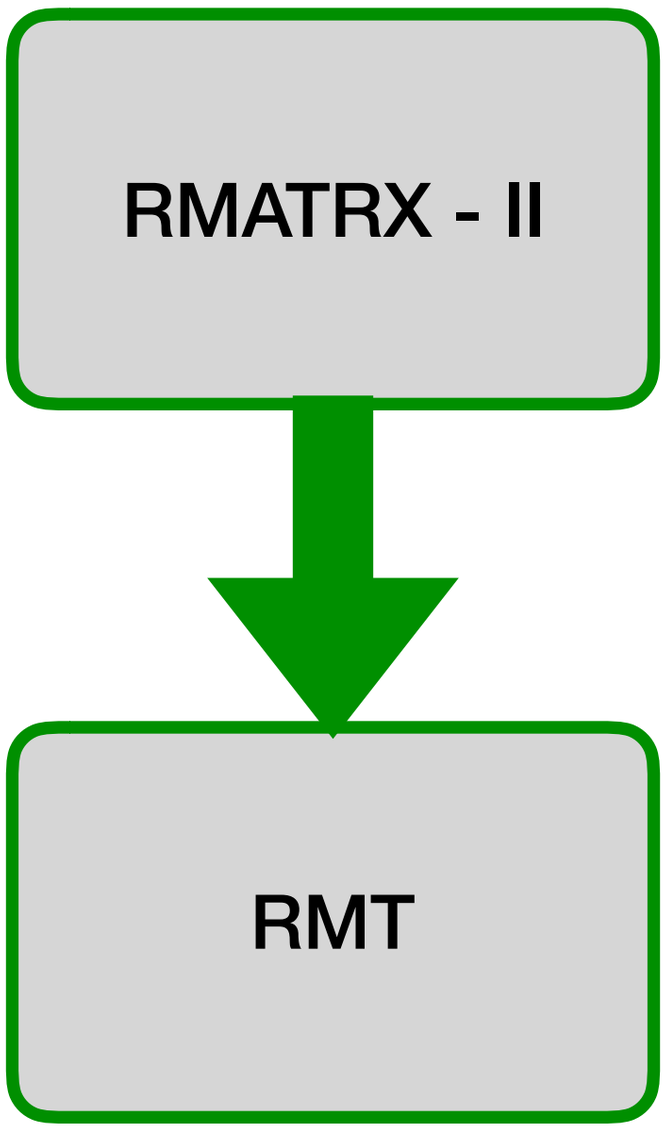
~~Non-relativistic Targets~~

~~Atomic / Ionic Systems~~

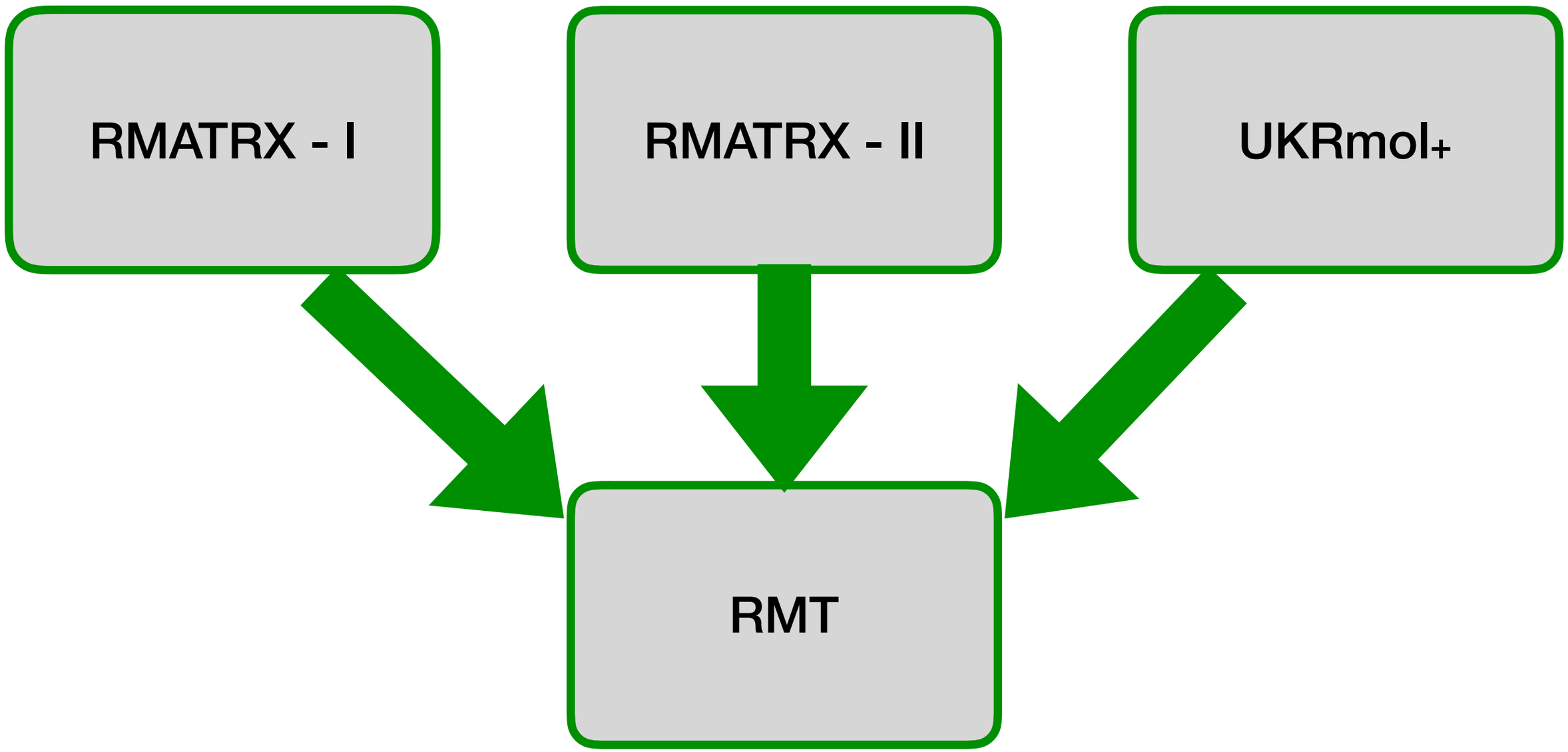
Computer Physics Communications 107062

RMT: R-matrix with time-dependence. Solving the semi-relativistic, time-dependent Schrödinger equation for general, multi-electron atoms and molecules in intense, ultrashort, arbitrarily polarized laser pulses

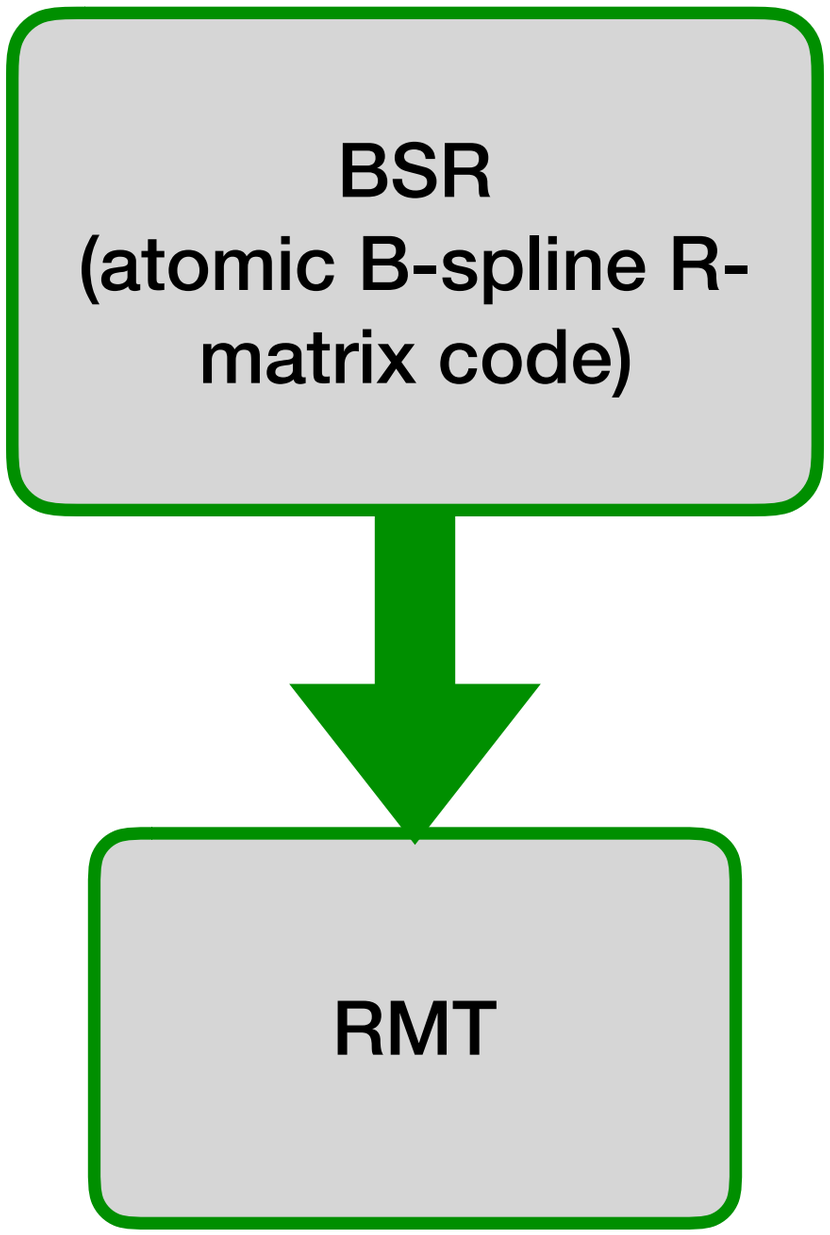
RMT INPUTS



RMT INPUTS



RMT INPUTS



Oleg Zatsarinny “BSR: B-spline atomic R-matrix codes”, *Computer Physics Communications*, **174**, 273-356 (2006).

INPUTS

H

D*

- `dipole_format_id` (INTEGER, 2) defines which version of the R-matrix codes has been used to generate the input data. The default is the R-matrix II codes (2). For relativistic calculations, R-matrix I (1) will be used. For molecular calculations, this parameter is ignored.
- `coupling_id` (INTEGER, 1) defines which coupling scheme to use. The default is LS coupling (1); jK coupling (2) can also be employed. For molecular calculations, this parameter is ignored.

H, D* similar format to RMATRX I

Splinedata — **Knot array, number of splines, order of splines etc**

knot.dat

Splinewaves — **Radial continuum functions**

APPLICATIONS

Time-dependent Dynamics of Complex atoms in Ultrashort light fields

- Multielectron atoms - Argon, Xenon
- Autoionisation
- Spin-orbit dynamics
- Electron Correlation effects

Summary and Outlook

- **The B-Spline R-Matrix (BSR) approach is an alternative implementation to the standard R-Matrix (RM) package developed in Belfast.**
- **Distinctive BSR features include the possibility to use sets of non-orthogonal orbitals and B-splines, which may speed up convergence and improve the numerics, particularly for complex collision systems.**
- **Apart from numerical details, the results from BSR, RM, and CCC should be the same, provided**
  - **the same quality of target description is used;**
  - **the same level of accounting for relativistic effects** is chosen; and
  - **the close-coupling expansion is driven to convergence** by including a sufficient number of pseudo-states to account for coupling to the high-lying Rydberg states and the ionization continuum.
- **The method can be used for**
  - **structure calculations** (frozen-core, box-based close-coupling)
  - **electron collisions**
  - **weak-field photoionization**
  - **short-pulse intense photo-induced processes** (work in progress)

Thank You for Your Attention!