BENCHMARK CALCULATIONS FOR ELECTRON COLLISIONS
WITH COMPLEX ATOMS AND IONS

Klaus Bartschat, Drake University

VAMDC-USA Workshop

Special Thanks to
Oleg Zatsarinny

and to

many AMO theorists who we work with;
many AMO experimentalists who we work with;
a growing number of plasma modellers who we work with;

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BENCHMARK CALCULATIONS FOR ELECTRON COLLISIONS WITH COMPLEX ATOMS AND IONS

OVERVIEW:

I. Introduction: Production and Assessment of Atomic Collision Data

II. Time-Independent Close-Coupling Method
   • Treatment of the Ionization Continuum via Pseudo-States
   • Treatment of Relativistic Effects
   • The B-Spline R-matrix (BSR) method

III. Selected Results
   • Structure: Energies, Oscillator Strengths, Polarizabilities
   • Elastic Scattering and Excitation
   • Ionization

IV. Uncertainty Estimates

V. Summary and Outlook
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We have many beautiful results for angle-differential parameters, but the focus here is on angle-integrated cross sections.
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I could also talk about broader aspects, such as ...
I. Production and Assessment of Atomic Collision Data

II. Computational Methods for electron (positron) collisions with atoms
   - Special-Purpose Methods: Polarized Orbital, Optical Model Potential
   - Distorted-Wave Methods: DWBA and RDW
   - Close-Coupling Methods: CCC, RMPS, IERM, TDCC, ECS, BSR

III. Illustrative Results
   - Electron-Impact Excitation: H, He, Be; Ne, Ar, Kr, Xe;
     I, Au, Hg; C, (+ maybe Fe+, Mo)
   - Electron-Impact Ionization: H, He, Ne, C

IV. Conclusions
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and even ...
ELECTRON COLLISIONS WITH ATOMS, IONS, and MOLECULES — EXPERIMENT, THEORY, and MODELING APPLICATIONS

OVERVIEW:

Preamble: A Few Words about Philip G. Burke

I. Production and Assessment of Atomic Collision Data

II. Experimental Methods
   • Total Cross Sections
   • Differential Cross Sections
   • Recent Developments (Magnetic Angle Changer, Reaction Microscope)

III. Computational Methods [for electron/positron collisions]
   • Special-Purpose Methods
   • Distorted-Wave Methods
   • The Close-Coupling Method: Recent Developments
     CCC, RMPS, IERM, TDCC, B-spline R-matrix (BSR)

IV. A Few Illustrative Results
   • Structure Calculations
   • Cross Sections for Electron-Impact Excitation (Atoms, Ions, Molecules)

V. GEC Application: What We Can Learn from Modeling a Ne Discharge

VI. A Closer Look at Ionization
   • Basic Idea of B-spline R-matrix with Pseudo-States (BSRMPS)
   • Example Results
   • Solution of the Excitation Mystery in e-Ne Collisions

VII. Conclusions and Outlook
OVERVIEW:

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But not in < 30 mins, so it's back to this.
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

Basic Question: WHO IS RIGHT? (And WHY ???)
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    - 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” (→ ???)
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  - **good (or bad ?) guesses**
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- Sometimes the results are (obviously) wrong or (more often) inconsistent!
Production and Assessment of Atomic Data

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  - **calculations** (Opacity Project, Iron Project, ...)
    - relatively cheap
    - almost any transition of interest is possible
    - often restricted to particular energy ranges:
      - high ($\rightarrow$ Born-type methods)
      - low ($\rightarrow$ close-coupling-type methods)
    - cross sections may peak at “intermediate energies” ($\rightarrow$ ???)
  - **good (or bad ?) guesses**

- Sometimes the results are (obviously) wrong or (more often) inconsistent!

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

**Consequence: Accuracy Assessment and Uncertainty Estimates for Theoretical Data are Important!**
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

\[ \Psi_{E}^{LS\pi}(r_1, \ldots, r_{N+1}) = A \sum_{i} \Phi_{i}^{LS\pi}(r_1, \ldots, r_{N}, \hat{r}) \frac{1}{r} F_{E,i}(r) \]

  - 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.
Time-Independent Close-Coupling

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

\[ \Psi_E^{LS\pi}(r_1, \ldots, r_{N+1}) = A \sum_i \Phi_i^{LS\pi}(r_1, \ldots, r_N, \hat{r}) \frac{1}{r} F_{E,i}(r) \]

- Target states \( \Phi_i \) diagonalize the \( N \)-electron target Hamiltonian according to

\[ \langle \Phi_i' | H_N^{T} | \Phi_i \rangle = E_i \delta_{i'i} \]

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

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

with the direct coupling potentials

\[ V_{ij}(r) = -\frac{Z}{r} \delta_{ij} + \sum_{k=1}^{N} \frac{1}{|r_k - r|} \langle \Phi_i | \Phi_j \rangle \]

and the exchange terms

\[ W_{ij} F_{E,j}(r) = \sum_{k=1}^{N} \frac{1}{|r_k - r|} \ (A - 1) \langle \Phi_i | \Phi_j F_{E,j} \rangle \]

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

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Inclusion of Relativistic Effects

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Benchmark Results for e-H Excitation

- Using a variational method, Schwartz solved the **low-energy elastic e–H scattering problem** with high accuracy in the early 1960’s.
- As seen in further benchmark work in the inelastic regime, **CCC, RMPS, and IERM predictions agree extremely well with each other, and also with the experimental data (dots on 2s, 2p) of Williams (1988).** [From Bartschat, Bray, Burke, and Scott, J. Phys. B 29 (1996) 5493.]

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**light quasi-one and quasi-two electron systems; theory looks very good :-)**
Total Cross Section and Spin Asymmetry in e-H Ionization


![Graph showing the total cross section in e-H ionization with energy in eV on the x-axis and cross section in $\pi a_0^2$ on the y-axis. The graph includes data points and curves for RMPS, CCC, and Shah et al. comparisons.]
In 1998, de Heer recommends 0.5 x (CCC+RMPS) for uncertainty of 10% — independent of experiment!
There are BIG discrepancies in excitation from the metastable! Who is right?
Electron Collisions with Laser Cooled and Trapped Metastable Helium Atoms: Total Scattering Cross Sections

L. J. Uhlmann, R. G. Dall, A. G. Truscott, M. D. Hoogerland, K. G. H. Baldwin, and S. J. Buckman

Bartschat [4] demonstrates that a total of four calculations, from an early eikonal approximation to several versions of the \textit{R}-matrix approach, and the CCC technique all give essentially the same result, which favors the lower excitation cross section. The present total cross section result, also shown in Fig. 4, should, by definition, be larger than any partial cross section that contributes to it. Thus our measurements also strongly favor the earlier Wisconsin result [18], which is smaller than the present total cross section, over the later one [19].
Inelastic electron scattering from light atomic species is of fundamental importance and has significant applications in fusion-plasma modeling. Therefore, it is of interest to apply advanced nonperturbative, close-coupling methods to the determination of electron-impact excitation for these atoms. Here we present the results of $R$ matrix with pseudostate (RMPS) calculations of electron-impact excitation cross sections through the $n = 4$ terms in Be, Be$^+$, Be$^{2+}$, and Be$^{3+}$. In order to determine the effects of coupling of the bound states to the target continuum in these species, we compare the RMPS results with those from standard $R$-matrix calculations. In addition, we have performed time-dependent close-coupling calculations for excitation from the ground and the metastable terms of Be$^+$ and the metastable term of Be$^{3+}$. In general, these results are found to agree with those from our RMPS calculations. The full set of data resulting from this work is now available on the Oak Ridge National Laboratory Controlled Fusion Atomic Data Center web site, and will be employed for collisional-radiative modeling of Be in magnetically confined plasmas.
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].
In 1998, de Heer recommends $0.5 \times (\text{CCC} + \text{RMPS})$ for uncertainty of 10% — independent of experiment!
Metastable Production in Electron Collisions with Heavy Noble Gases (status in 2002)

**Theory:** Breit-Pauli R-Matrix (Bartschat et al., 1999-2002)

**Experiment:** metastable count rate (Buckman et al., 1983)

Oops – not quite so good for more complex targets like the heavy noble gases :-(
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

- **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 50,000 and higher due to size of *B*-spline basis
  - Rescue: Excellent numerical properties of *B*-splines; use of (SCA)LAPACK *et al.*

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**Record:** 150,000 to do 50-100 times; 100 - 200 kSU

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**We also have to solve the problem outside the box for each energy (from 100’s to 1,000,000’s).**

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**O. Zatsarinny, CPC 174 (2006) 273**
BSR – General B-Spline R-Matrix Package

1. First implementation: Li photoionization (2000)
2. First presentation: ICPEAC XXX, Rosario, Argentina (2005)
5. RMPS extension/ionization e–He, Ne scattering (2011–2012)
### List of early calculations with the BSR code (rapidly growing)

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Authors</th>
<th>Journal</th>
<th>Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>$hv + Li$</td>
<td>Zatsarinny O and Froese Fischer C</td>
<td><em>J. Phys. B</em></td>
<td>2000</td>
</tr>
<tr>
<td>$hv + He^0$</td>
<td>Zatsarinny O, Gorczyca T W and Froese Fischer C</td>
<td><em>J. Phys. B</em></td>
<td>2002</td>
</tr>
<tr>
<td>$hv + B^0$</td>
<td>Zatsarinny O and Gorczyca T W</td>
<td>Abstracts of XXII ICPEAC</td>
<td>2003</td>
</tr>
<tr>
<td>$e + Ne$</td>
<td>Zatsarinny O and Bartschat K</td>
<td><em>J. Phys. B</em></td>
<td>2004</td>
</tr>
<tr>
<td>$e + Ar$</td>
<td>Zatsarinny O and Bartschat K</td>
<td><em>J. Phys. B</em></td>
<td>2004</td>
</tr>
<tr>
<td>$e + Zn$</td>
<td>Zatsarinny O and Bartschat K</td>
<td><em>Phys. Rev. A</em></td>
<td>2005</td>
</tr>
<tr>
<td>$e + Fe^+$</td>
<td>Zatsarinny O and Bartschat K</td>
<td><em>Phys. Rev. A</em></td>
<td>2005</td>
</tr>
<tr>
<td>$e + Kr$</td>
<td>Zatsarinny O and Bartschat K</td>
<td><em>J. Phys. B</em></td>
<td>2007</td>
</tr>
</tbody>
</table>

**at least 60 more since 2006**

**Topical Review:**

Our Apparatus — Supercomputers

- Lonestar (TACC)
- Kraken (NICS) (RIP since April 30, 2014)
- Stampede (TACC)

+ Gordon at the San Diego Supercomputer Center
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.
# Energy Levels in Heavy Noble Gases

**Table 1.** Binding energies (NIST [1]) and energy differences (computed–observed) in eV for some low-lying levels in Ne, Ar, Kr and Xe. The values in bold are average differences for the states in the respective configuration obtained when the core–valence correlation is omitted.

<table>
<thead>
<tr>
<th></th>
<th>Ne</th>
<th>Ar</th>
<th>Kr</th>
<th>Xe</th>
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<tbody>
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<td></td>
<td>NIST</td>
<td>Diff.</td>
<td>NIST</td>
<td>Diff.</td>
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<tr>
<td>2p⁶</td>
<td>21.565</td>
<td>0.061</td>
<td>15.760</td>
<td>0.044</td>
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<tr>
<td>3s[3/2]₂</td>
<td>4.945</td>
<td>0.012</td>
<td>4s[3/2]₂</td>
<td>4.211</td>
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<td>3s[3/2]₁</td>
<td>4.894</td>
<td>0.015</td>
<td>4s[3/2]₁</td>
<td>4.136</td>
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<tr>
<td>3p[1/2]₁</td>
<td>3.183</td>
<td>0.007</td>
<td>4p[1/2]₁</td>
<td>2.853</td>
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<tr>
<td>3p[5/2]₃</td>
<td>3.009</td>
<td>0.009</td>
<td>4p[5/2]₃</td>
<td>2.684</td>
</tr>
<tr>
<td>3p[5/2]₂</td>
<td>2.989</td>
<td>0.007</td>
<td>4p[5/2]₂</td>
<td>2.665</td>
</tr>
<tr>
<td>3p[1/2]₀</td>
<td>2.853</td>
<td>0.008</td>
<td>4p[1/2]₀</td>
<td>2.487</td>
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<tr>
<td>3d[1/2]₀</td>
<td>1.540</td>
<td>0.004</td>
<td>3d[1/2]₀</td>
<td>1.915</td>
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<tr>
<td>3d[1/2]₁</td>
<td>1.538</td>
<td>0.004</td>
<td>3d[1/2]₁</td>
<td>1.896</td>
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<tr>
<td>3d[7/2]₃</td>
<td>1.530</td>
<td>0.006</td>
<td>3d[7/2]₄</td>
<td>1.780</td>
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<td>3d[3/2]₁</td>
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<td>1.524</td>
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<td>1.697</td>
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<td>3d[5/2]₂</td>
<td>1.516</td>
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<td>3d[5/2]₃</td>
<td>1.661</td>
</tr>
</tbody>
</table>
# Oscillator Strengths in Neon

OZatsarinney and K Bartschat

**Table 2.** Oscillator strengths for excitation from the ground state in Ne, as obtained in the length ($f_L$) and velocity ($f_V$) forms of the electric dipole operator.

<table>
<thead>
<tr>
<th>Upper level</th>
<th>$f_L$</th>
<th>$f_V$</th>
<th>Other theory</th>
<th>Experiment</th>
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<tr>
<td></td>
<td></td>
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<td>[10]</td>
<td>[13]</td>
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<tr>
<td>$3s[3/2]_1$</td>
<td>0.0118a</td>
<td>0.0116a</td>
<td>0.0109</td>
<td>0.0102</td>
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<tr>
<td></td>
<td>0.0163b</td>
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<td></td>
<td>0.161a</td>
<td>0.147a</td>
<td>0.144b</td>
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<td>$4s[3/2]_1$</td>
<td>0.0126</td>
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<td></td>
<td>0.0174</td>
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<td>0.0152</td>
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<td>$3d[1/2]_1$</td>
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<td>0.0146</td>
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<td>0.0130</td>
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<td>$3d[3/2]_1$</td>
<td>0.0194</td>
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<td></td>
<td>0.00718</td>
<td>0.00731</td>
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<td>0.00628</td>
<td>0.00640</td>
<td>0.0068</td>
<td>0.00727</td>
</tr>
<tr>
<td></td>
<td>0.00481</td>
<td>0.00490</td>
<td>0.0053</td>
<td>0.00502</td>
</tr>
<tr>
<td>$4d[1/2]_1 + 4d[3/2]_1$</td>
<td>0.00906</td>
<td>0.00895</td>
<td>0.0101</td>
<td></td>
</tr>
<tr>
<td>$4d'[3/2]_1$</td>
<td>0.00432</td>
<td>0.00427</td>
<td>0.00481</td>
<td>0.00439(22)</td>
</tr>
<tr>
<td>$6s[3/2]_1$</td>
<td>0.00325</td>
<td>0.00331</td>
<td>0.00371</td>
<td>0.00330(30)</td>
</tr>
<tr>
<td>$6s'[1/2]_1$</td>
<td>0.00168</td>
<td>0.00172</td>
<td>0.00203</td>
<td>0.00156(16)</td>
</tr>
<tr>
<td>$5d[1/2]_1 + 5d[3/2]_1$</td>
<td>0.00520</td>
<td>0.00510</td>
<td>0.00538</td>
<td>0.00543(54)</td>
</tr>
<tr>
<td>$5d'[3/2]_1$</td>
<td>0.00255</td>
<td>0.00249</td>
<td>0.00273</td>
<td>0.00229(23)</td>
</tr>
</tbody>
</table>

---

*a* Avgoustoglou and Beck [12]—relativistic MBPT.

*b* Dong *et al* [15]—MCDF calculations.
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 $n = 12$.

<table>
<thead>
<tr>
<th>Element</th>
<th>States</th>
<th>Transitions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ne</td>
<td>299</td>
<td>11300</td>
</tr>
<tr>
<td>Ar</td>
<td>359</td>
<td>19000</td>
</tr>
<tr>
<td>Kr</td>
<td>212</td>
<td>6450</td>
</tr>
<tr>
<td>Xe</td>
<td>125</td>
<td>2550</td>
</tr>
</tbody>
</table>

• All calculations are fully ab initio.

• The computer code BSR used in the present calculations and the results for Ar were recently published:

Using our semi-relativistic \( B \)-spline \( R \)-matrix (BSR) method [Zatsarinny and Bartschat, J. Phys. B 37, 2173 (2004)], we achieved unprecedented agreement with experiment for angle-integrated cross sections in \( e^-\text{Ne} \) collisions.
BSR calculations (experiment renormalized, within absolute uncertainty)

What a difference!
Full-Relativistic Version for Heavy Targets

DBSR Code – Dirac B-Spline R-Matrix

**Dirac–Coulomb–Breit Hamiltonian**

\[
H_{DCB} = \sum_i h_D(r_i) + \sum_{i<j} \left( \frac{1}{r_{ij}} + b_{ij} \right)
\]

\[
h_D = c \alpha \cdot p + \beta c^2 + V_{\text{nuc}}(r)
\]

\[
b_{ij}^0 = -\frac{1}{2r_{ij}} \left[ \alpha_i \cdot \alpha_j + \frac{(\alpha_i \cdot r_{ij})(\alpha_j \cdot r_{ij})}{r_{ij}^2} \right]
\]

**R-matrix basis functions**:

\[
\Psi^{\alpha JM}(x_1, \ldots, x_{N+1}) = A \sum_i \left[ \Phi_i^{\alpha_i, J, M_i}(x_1, \ldots, x_N) \cdot \phi_j(x_{N+1}) \right]^{JM} + \sum_i \chi_i^{JM}(x_1, \ldots, x_{N+1}) b_i^{JM}
\]

\[
\phi_{nkm}(r) = \frac{1}{r} \left( \frac{P_{nk}(r)\chi_{km}(\hat{r})}{iQ_{nk}(r)\chi_{-km}(\hat{r})} \right);
\]

\[
P(r) = \sum_i p_i B_i^{k_p}(r); \quad Q(r) = \sum_i q_i B_i^{k_q}(r) \quad k_p \neq k_q \quad !!!!
\]

- **Retain key feature**: both bound and continuum radial functions can be represented by non-orthogonal term-dependent radial orbitals.
- Target wave-functions – **GRASP2K** (Jönsson, He and Froese Fischer, CPC, 2007)

Spurious–states problem: fixed by Froese Fischer & Zatsarinny (CPC, 2009)
full-relativistic DBSR vs. semi-relativistic BSR for e-Xe

**e-Xe:** \(6s^{3/2}_2 + 6s^{1/2}_0\)

- Buckman *et al* (1983)

Cross Section \((a_0^2)\)

Electron Energy \((eV)\)
Let's use these data in a real plasma model! (Dirk Dodt's PhD Thesis)

\[ f(E, T_e) \]

EEDF

\[ n_i(r) \]

population densities

collisional - radiative model

\[ 150 \text{ cross sections} \]

many more details in the collisional-radiative model ...

\[ \varepsilon_{i j}(r) = \frac{h \nu_{i j}}{4 \pi} \Theta_{i j} A_{i j} n_i(r) \]

emission coefficient

Einstein's coefficients (radiation transport)

\[ L_{i j} = \int \frac{\varepsilon_{i j}(s, r_\perp)}{A_\perp(s)} \, ds \, dA_\perp \]

radiance

line of sight integration

\[ L_\lambda = \sum_{i j} L_{i j} f(\lambda - \lambda_{i j}) \]

spectral radiance

\[ I_i = L_\lambda \cdot \frac{I_{i,\text{calib}}}{L_{\lambda,\text{calib}}} \]

spectrometer pixels

intensity calibration

line profile (aparatus width)
Use of the Data in a Discharge Modelling Application

Modeled Spectrum With “Reasonable Uncertainty in Atomic Data”
(at least 10% for large oscillator strengths, 10%–60% for cross sections)

D. Dodt, A. Dinklage, K. Bartschat, and O. Zatsarinny,
This is the real check:
- If theory and experiment are perfect, the "correction" factors are exactly 1.0
- If imperfect theory is consistent with imperfect experiment, the error bars cover 1.0

OOPS ?!?!?!
Results: Significant Correction Factors for a Few Transitions

Most significant corrections obtained from the measured spectral data. The corrections are given for cross sections of excitation from the ground state and the lowest 3s state.

<table>
<thead>
<tr>
<th>final state:</th>
<th>initial state:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>ground</td>
</tr>
<tr>
<td>$2p^5(2P_{3/2}^o),3d,^2[\frac{1}{2}]^o,,J = 1$</td>
<td>0.43$^{+0.3}_{-0.27}$</td>
</tr>
<tr>
<td>$2p^5(2P_{3/2}^o),3d,^2[\frac{3}{2}]^o,,J = 1$</td>
<td>0.27$^{+0.17}_{-0.14}$</td>
</tr>
<tr>
<td>$2p^5(2P_{1/2}^o),3d,^2[\frac{3}{2}]^o,,J = 1$</td>
<td>0.17$^{+0.15}_{-0.11}$</td>
</tr>
<tr>
<td>$2p^5(2P_{3/2}^o),3p,^2[\frac{1}{2}],,J = 1$</td>
<td>$1.3^{+0.2}_{-0.16}$</td>
</tr>
<tr>
<td>$2p^5(2P_{1/2}^o),3p,^2[\frac{1}{2}],,J = 0$</td>
<td>$0.66^{+0.28}_{-0.21}$</td>
</tr>
</tbody>
</table>

These factors mean that the input cross sections are most likely too large. => !?!?!?:-(- :-(

Explanation: The results for these transitions are very sensitive to the inclusion of continuum coupling! (already suggested in 2004 by Ballance and Griffin)
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)

Confirming the solution to the e-Ne excitation mystery:
Coupling to the continuum is very, very important.
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).
Total Cross Section for Electron Impact Excitation of Neon
Effect of Channel Coupling to Discrete and Continuum Spectrum

Electron Energy (eV) vs Cross Section ($10^{-18}$ cm$^2$) for different energy levels and theories.

- $3s[3/2]_2$
- $3s'[1/2]_0$
- $3s[3/2]_1$
- $3s'[1/2]_1$

Theoretical calculations are represented by solid lines, while experimental data are indicated by markers.

Theories and experimental data sources:
- Kato et al. (2011)
- Suzuki et al. (1994)
- Khakoo et al. (2002)
- Register et al. (1984)
- Phillips et al. (1985)
Effect of Channel Coupling to Discrete and Continuum Spectrum in Ar

Electron Energy (eV)

Cross Section ($10^{-18}$ cm$^{-2}$)

BSR-31
BSR-500

Chutjian & Cartwright (1981)

4s$[3/2]_1$

4s$'[1/2]_1$

4s$[3/2]_2$

4s$'[1/2]_0$
Effect of Channel Coupling to Discrete and Continuum Spectrum in Ar

Note the scatter in the experimental data, and the size of the error bars.
Electron Impact Excitation of Fluorine \((2p^5 \ ^2P)\)

- **BSR-690** - Gedeon et al. (2014)
- **BSR-39** - the same target states
- **RM-11** - Boliyan & Bhatia (1994)

**Total number of states** - 690
**Bound states** - 53
**Continuum pseudostates** - 637 \((l=0-3, L=0-5)\)
**Continuum energy cover** - 20 eV
**Number of channels** - 1727
**R-matrix radius** - 30 \(a_o\)
**Number of B-splines** - 68
**Hamiltonian matrix** - 100,000

**Dipole transitions:**
- Crucial dependence on continuum pseudostates
- to lesser extent on target description
- \(2p^5\) excitation is most problematic
Electron Impact Excitation of Fluorine ($2p^5\,^2P$)

Non-dipole transitions:
- Crucial dependence on continuum pseudostates for all transitions
- Target description is very important
Electron Impact Excitation of Carbon (2p² 3P)

Total number of states — 696
Bound states — 51
Continuum pseudostates — 645
(1 = 0–3)
Continuum energy range — 30 eV
Number of channels — 1543
R-matrix radius — 30 a₀
Number of B-splines — 83
Hamiltonian matrix — 120,000

Crucial dependence on both the target description and continuum pseudostates

Message:
First check your target, then the convergence!
Elastic Scattering from Nitrogen

Cross Section (10^{-16} cm^2) vs. Electron Energy (eV)

- Tuned to position of the $2p^4\,^3P$ resonance at 62 meV (Mazeau et al. 1978).
- To get this position from \textit{ab initio} calculations seems almost impossible. Experiment is crucial!
Electron Impact Excitation of **Nitrogen** \( (2p^3 4S) \)

- 2p–2p; converged
- target continuum important
- experiment: ???
- estimated uncertainty: 10 %
Ionization in the Close-Coupling Formalism

- Recall: We are interested in the ionization process

  \[ e_0(k_0, \mu_0) + A(L_0, M_0; S_0, M_{S_0}) \rightarrow e_1(k_1, \mu_1) + e_2(k_2, \mu_2) + A^+(L_f, M_f; S_f, M_{S_f}) \]

- We need the ionization amplitude

  \[ f(L_0, M_0, S_0; k_0 \rightarrow L_f, M_f, S_f; k_1, k_2) \]
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We need the ionization amplitude

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We employ the \textit{B}-spline \textit{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:

\[ f(L_0, M_0, S_0; k_0 \rightarrow L_f, M_f, S_f; k_1, k_2) = \sum_p \langle \psi^k_{f_2} \Phi(L_p, S_p) \rangle f(L_0, M_0, S_0; k_0 \rightarrow L_p, M_p, S_p; k_{1p}) \]

This is the essential idea – we are still working on the details.
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!
Benchmark calculation of total cross sections for ionization–excitation of helium

Oleg Zatsarinny\textsuperscript{1} and Klaus Bartschat\textsuperscript{1,2}

\textsuperscript{1} Department of Physics and Astronomy, Drake University, Des Moines, IA 50311, USA
\textsuperscript{2} ITAMP, Harvard-Smithsonian Center for Astrophysics, Cambridge, MA 02138, USA

E-mail: oleg.zatsarinny@drake.edu and klaus.bartschat@drake.edu

Received 16 January 2014, revised 5 February 2014
Accepted for publication 6 February 2014
Published 4 March 2014

Abstract
Main Result

e + He(1s²) - He⁺(2p) + 2e

BSR (2 methods)
Ionization of Complex Targets

**Ionization Cross Sections (10^{-17} \text{ cm}^2)**

- \( e + \text{C} \rightarrow \text{C}^+ + 2e \) \((2p^2)^3\text{P}\)
- \( e + \text{N} \rightarrow \text{N}^+ + 2e \) \((2p^3)^4\text{S}^0\)
- \( e + \text{F} \rightarrow \text{F}^+ + 2e \)
- \( e^- + \text{Ne} \rightarrow 2e^- + \text{Ne}^+ \)

**Electron Energy (eV)**

- \( 0 \) to \( 200 \)
- \( 0 \) to \( 140 \)
- \( 20 \) to \( 120 \)
- \( 0 \) to \( 200 \)

**Comparisons with Experiments and Theoretical Predictions**

- Experiments, BSR-690, BEB (^3\text{P}:^1\text{D}:^1\text{S} - 9:5:1)
- BSR-679, Ballance et al. (2009), RMPS-347
- Pindzola et al. (2000), TDCC
- Rejoub et al. (2002)

**Sources**

- Krishnakumar & Strivastava (1988)
- Pindzola et al. (2000), TDCC
- Ballance et al. (2009), RMPS-347
- BSR-679
These results (and more) are now in the LXCAT database: http://fr.lxcat.net/home/

Excellent results in modeling of low-temperature Ne and Ar plasmas (Pitchford et al., J. Phys. D (2013)).
This is what happens when the data are not in the database (and often also if they are!)

We are currently working on nitrogen discharges (actually dry air discharges, produced out of a mixture of N2-O2). Although the majority of dissociation happens for oxygen, we can also have up to 5% N2 dissociation, meaning that our nitrogen system is actually a mixture of N2+N.

But for N, there is little information available (to my knowledge). We would need at least the e+N momentum transfer cross section.

So, I wonder. Do you know of more recent references calculating/measuring the elastic differential cross section of N atoms (from which we could derive the corresponding momentum transfer)?

Would you be interested in doing such calculations?

Oleg Zatsarinny: Oct. 9, 2014: 12:44 (CDT)

Attached is archive of our last results for the e-N problem. It includes also the momentum transfer cross sections you are interested in (mt files, look in "read_me" for explanations)

Luis Alves: Oct. 9, 2014: 2:56 p.m. (CDT)

In one word: WOW! This is really just what I was looking for... and much more (since includes also excitation and ionization from ground state).
This year I won't attend the GEC, so I'm e-mailing you the following question / request.

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How accurate are theoretical results? --> PART 2

Joint Workshop with IAEA on Uncertainty Assessment for Atomic and Molecular Data

July 7-9, 2014

at ITAMP, Cambridge MA, USA

Organizers
James Babb (ITAMP)
Klaus Bartschat (Drake University)
Bastiaan J. Braams (IAEA)
H. Chung (IAEA)
David Schultz (University of North Texas)
Jonathan Tennyson (University College London)

The workshop will bring together experts working on electron collisions with atoms, ions, and molecules, heavy-particle collisions, and electronic structure of atoms and molecules (with structure viewed here as a prerequisite for collision calculations). The primary goals are to come up with reasonable uncertainty estimates for calculations using the various methods of collision physics: perturbative, nonperturbative, time-independent, time-dependent, semi-classical, etc. Generally, the workshop focus will be on theoretical atomic and molecular data relevant to fusion and astrophysical plasmas, where modeling codes mostly use theoretical atomic and molecular data for which assessments of accuracy are necessary. There will also be data users at the meeting, as well as those who manage databases.
Conclusions and Outlook

- Advanced close-coupling methods (CCC, RMPS, TDCC) have achieved a breakthrough in calculations of electron-impact excitation and ionization of simple target systems — provided the change in quantum state of ONE target electron dominates the process.

- The success of these methods to describe the most detailed (sometimes even “complete”) experiments has resulted in great confidence among application modelers in the predictions from these methods.
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- For complex targets, the BSR method with non-orthononal orbitals has achieved a breakthrough in the description of near-threshold phenomena. The major advantages are:
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  - reduced pseudo-resonance problems

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  - a highly accurate target description
  - reduced pseudo-resonance problems

- Relativistic RMPS calculations are very extensive, but they can be performed on massively parallel computing platforms.

- Applications to correlated processes, complex atomic targets, and even the simplest molecules present major computational challenges.

- We are in an excellent position and ready to face these challenges.
Impact of XSEDE

• The availability of supercomputing resources through XSEDE, together with a lot of algorithm development, has made it possible to:
  • tackle problems that were classified as essentially hopeless a few years ago;
  • drive many calculations to convergence and, in some cases, cast reasonable doubt on the “infallibility of experiment”;
  • provide extensive and truly useful datasets to the modelling community;
  • study atomic collision processes in real time (not in this talk).

Note: These calculations are not cheap! CPU time alone for production runs is at least $10,000 for one “real problem” (e.g. e-Ne) and grows quickly with complexity.

Finally: In spite (or because?) of these costs, the community should agree on benchmark studies to further assess the accuracy of theoretical predictions.

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