Accurate Transition Probabilities in Atoms from Large-scale Multiconfiguration Calculations

A tribute to Charlotte Froese Fischer

Jacek Bieroń, Tomas Brage, Gediminas Gaigalas,
Michel Godefroid, Per Jönsson

PhD students and Post Docs
Simon Verdebout, Cedric Nazé, Pavel Rynkun,
Jon Grumer, Jiguang Li

3 oktober 2012

Outline

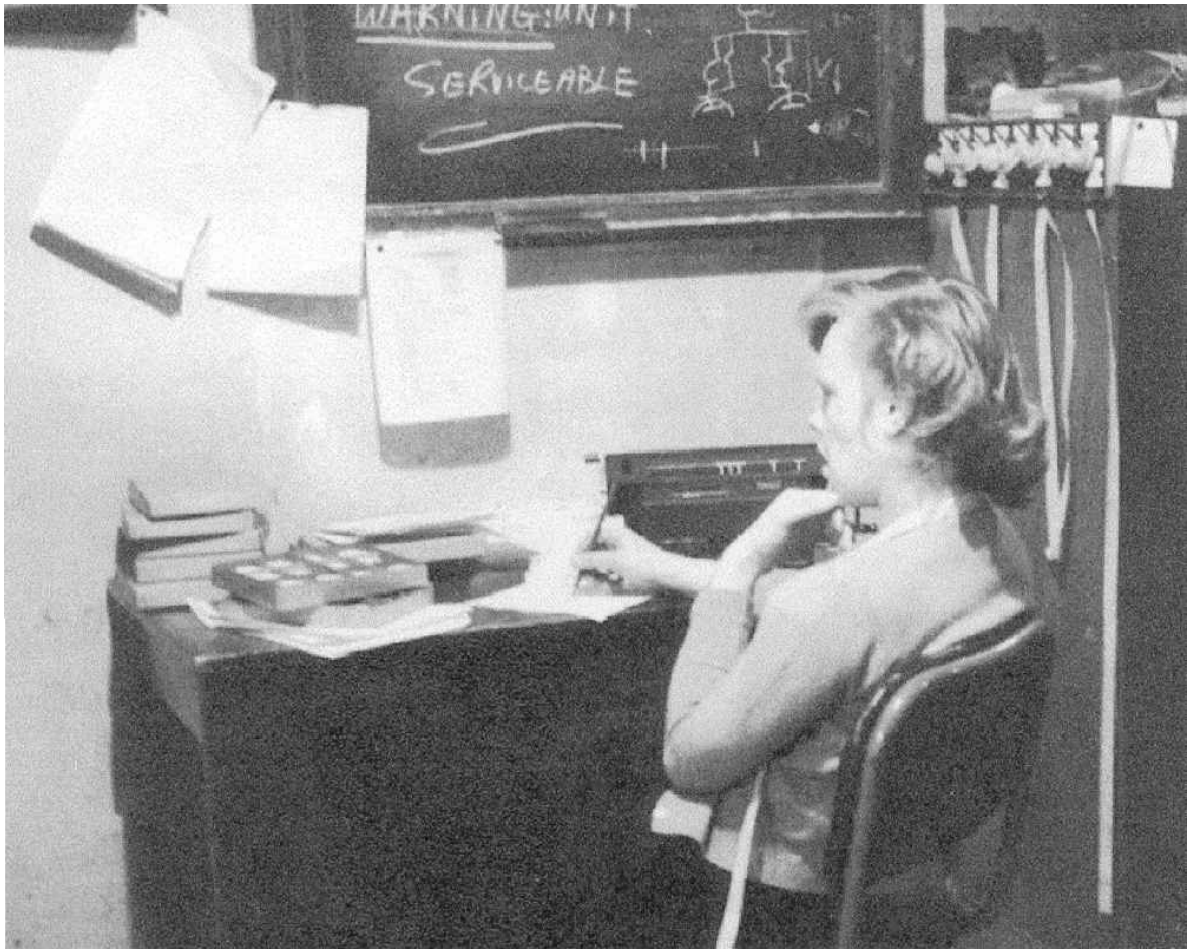
- Development of codes for atomic structure calculations with reference to the work of Charlotte Fischer
- Multiconfiguration methods
- Applications of the codes
- New developments

Computational atomic structure

The success of atomic structure calculations depends on the available computer software:

- Computational methods must constantly be improved
- New features should be added
- Adaptation to computer language
- Adaptation to computer systems
- Communication and sharing

Charlotte Froese Fischer at the Electronic Delay Storage Automatic Calculator (EDSAC)



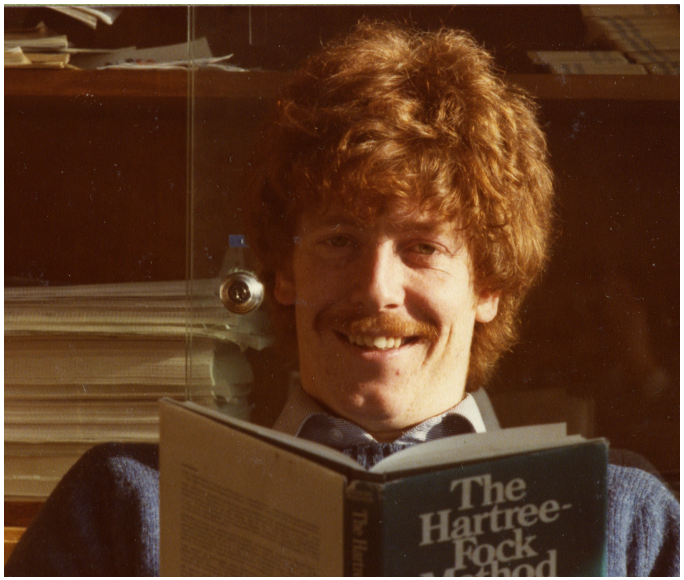
PhD in applied mathematics and computing in 1957 under the supervision of D. Hartree.

Impact through release of computer codes

A selection of atomic structure codes by Charlotte Fischer

- The MCHF atomic-structure code in 1969
- The MCHF atomic-structure package 1991
  – energies, relativistic corrections, transition rates, hfs, isotope shift, autoionization
- The GRASP92 code in 1996
- The ATSP2K, GRASP2K codes in 2007
  multiconfiguration codes for large scale computing
  – MPI, angular routines open f-shells, labels in LSJ-coupling, adapted for database

Impact by educating



C. Froese Fischer, The Hartree-Fock Method for Atoms: A Numerical Approach (Wiley 1977)

C. Froese Fischer et al. Computational Atomic Structure: An MCHF Approach (IoP 1997)

Impact by collaborating, sharing, and inspiring

Why atomic structure calculations?

- Testing fundamental theories by systematic comparisons of atomic data obtained from:
  – theoretical models
  – experiments
- Assessing the reliability of theoretical and/or experimental values (realistic error bars?)
- Interpretation of spectroscopic data — energies, rates, hfs, isotope shifts, g_J values (talk by Gillian Nave))
- Atomic data production for astrophysics and plasma physics
- Interface with nuclear physics (talk by prof Nörtershäuser)

Variational multiconfiguration methods

MCHF, CI and MCDHF, RCI

- Expand wavefunction in basis functions (CSFs) $\Phi(\gamma_i JM_J)$

$$\Psi(\gamma JM_J) = \sum_i c_i \Phi(\gamma_i JM_J)$$

- CSFs are symmetry adapted and anti-symmetrized products of one-electron orbitals represented on a grid.
- The radial functions should be orthonormal
- Apply variational principle: equations for radial functions, eigenvalue problem for coefficients
- Solve the equations iteratively (self-consistent field)

Selection of CSF expansions

Success of a calculation depends on the CSF expansion

- Select a set of important CSFs (multireference)
- Generate CSFs by substituting orbitals in the multireference with orbitals in an active set according to some rule (correlation model)
- Increase active set systematically
- Monitor convergence of computed properties
- Vary the correlation model
- Expansions with around 1 000 000 CSFs possible
- Larger expansions can be run on a cluster

Strengths and weaknesses of variational methods

Strengths

- Flexible and versatile
- Any ion and state can (in principle) be computed
- Good at capturing close degeneracy and dynamic correlation
- Possible to estimate uncertainties

Weaknesses

- Sizes of the expansions grows very rapidly
- Difficult to capture core-core effects
- Energy focused

Unusual feature: biorthogonal transformation

PHYSICAL REVIEW E VOLUME 52, NUMBER 4 OCTOBER 1995

Transition probability calculations for atoms using nonorthogonal orbitals

Jeppe Olsen,[1] Michel R. Godefroid,[2] Per Jönsson,[3] Per Åke Malmqvist,[1] and Charlotte Froese Fischer[4]

Method to compute matrix elements $\langle \Psi_i | D | \Psi_f \rangle$ between separately optimized initial and final states wave functions.

- Problems with non-orthogonalities handled by fast transformation method
- Implemented in both ATSP2K and GRASP2K
- Separate optimization $\Rightarrow$ more accurate transition rates

Transition rates $1s^2 2s\ ^2S \rightarrow 1s^2 2p\ ^2P$ in Li I

All possible CSFs generated from the active set (CAS). $n = 3$ denotes active set $\{1s, 2s, 2p, 3s, 3p, 3d\}$ etc

Radiative data for $1s^2 2s\ ^2S \rightarrow 1s^2 2p\ ^2P^o$

n	ΔE (cm^{-1})	S_l	S_v	gf_l	gf_v
HF	14847.87	33.9474	35.1577	1.53107	1.58566
2	16336.91	33.7881	28.6945	1.67671	1.42394
3	15054.03	33.8075	32.7918	1.54593	1.49949
4	15000.35	33.2304	34.0001	1.51412	1.54920
5	14921.54	33.0870	33.0714	1.49967	1.49896
6	14908.90	33.0293	33.0234	1.49578	1.49552
7	14904.56	33.0150	33.0145	1.49470	1.49468
8	14903.13	33.0083	33.0024	1.49425	1.49399
9k	14902.55	33.0056	32.9954	1.49408	1.49361
10k	14902.22	33.0039	32.9974	1.49397	1.49367
11k	14902.05	33.0031	32.9994	1.49391	1.49374

Godefroid et al Physica Scripta T65 (1996) 70

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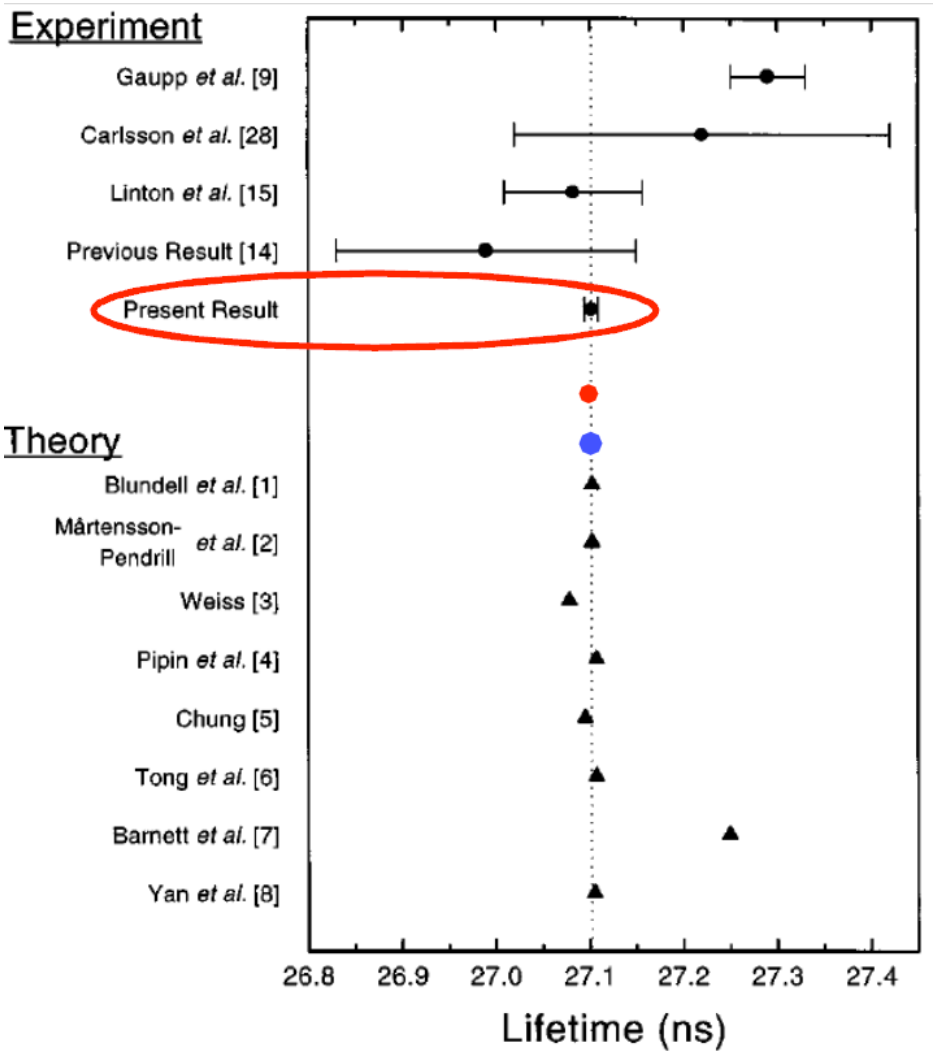

McAlexander et al Phys. Rev. A 54 (1996) R5

Transition rates $1s^2 2s^2\ ^1S \rightarrow 1s^2 2s2p\ ^1P$ in B II

VALENCE CORRELATION MCHF gf-VALUES IN B II

	$1s^2 2s^2\ ^1S$		$1s^2 2s2p\ ^1P^0$		$1s^2 2s^2\ ^1S \rightarrow 1s^2 2s2p\ ^1P^0$		
ACTIVE SET	E(a.u.)	Ncfg[a]	E(a.u.)	Ncfg[a]	gf_l	gf_v	ΔE (cm^{-1})
HF	−24.237575	1	−23.912873	1	1.44934	0.73292	71260
2s1p	−24.296082	2	−23.912873	1	1.06474	0.78927	84100
3s2p1d	−24.298330	7	−23.956320	6	1.03593	1.06883	75059
4s3p2d1f	−24.298647	16	−23.960103	17	1.02566	1.05692	74298
5s4p3d2f1g	−24.298767	30	−23.961101	36	1.02296	1.05715	74105
6s5p4d3f2g1h	−24.298826	50	−23.961448	65	1.02218	1.05690	74042
7s6p5d4f3g2h1i	−24.298852	77	−23.961607	106	1.02191	1.05683	74013
Experiment	...	...	...	...	...	...	73397

FULL CORRELATION MCHF gf-VALUES IN B II

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4s3p2d1f	−24.342409	460	−24.001844	713	1.01860	1.02582	74741
5s4p3d2f1g	−24.346046	1066	−24.008886	2300	1.00413	1.00375	73994
6s5p4d3f2g1h	−24.347410	2306	−24.011624	5211	1.00075	0.99978	73693
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Godefroid et al ApJ 450 (1997) 443

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Transition rates $1s^2 2s^2\ ^1S \rightarrow 1s^2 2s2p\ ^{1,3}P$ in Be sequence

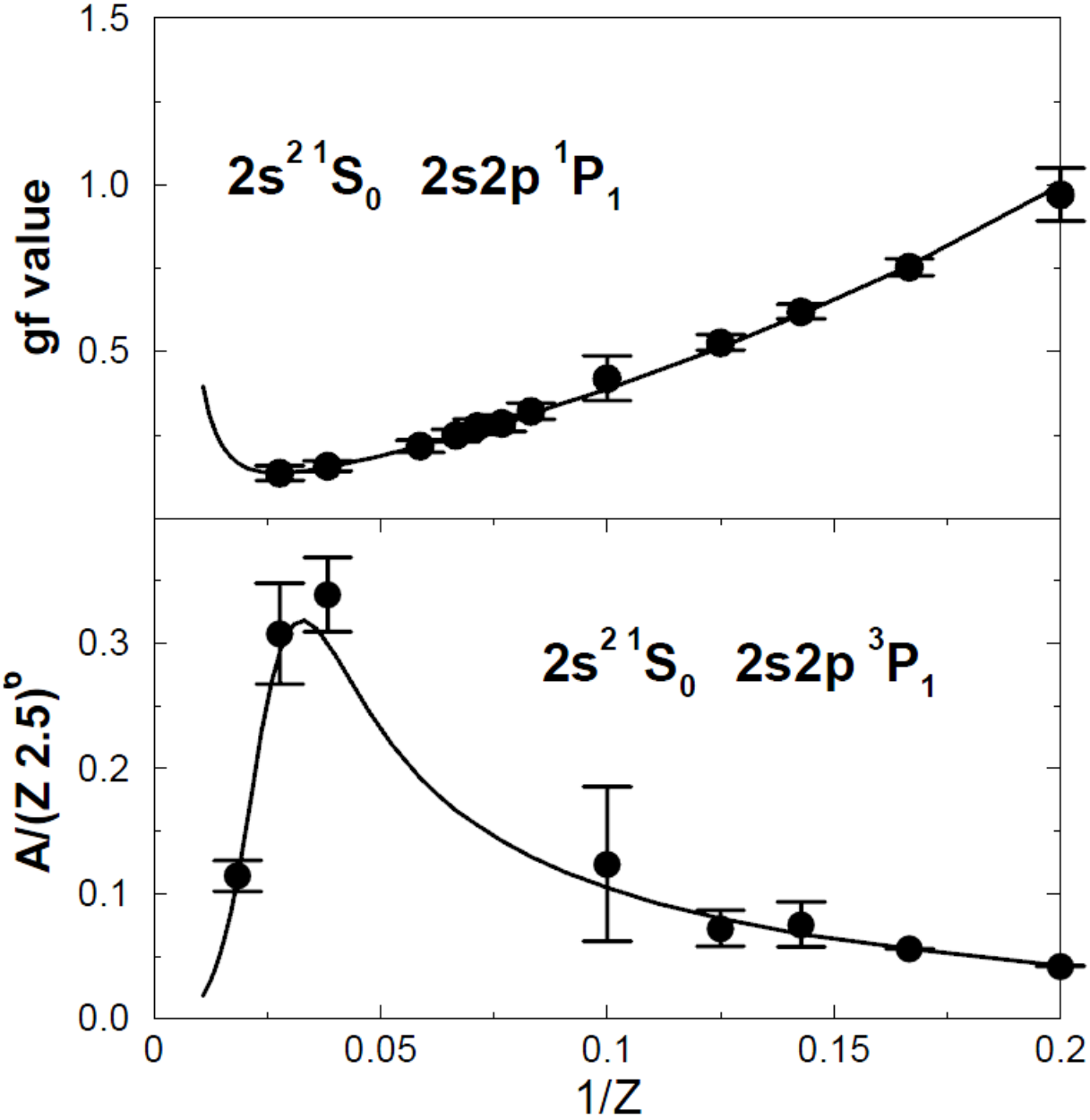
J. Phys. B: At. Mol. Opt. Phys. **31** (1998) 3497–3511. Printed in the UK PII: S0953-4075(98)92442-

On the status and perspectives of MCDF calculations and measurements of transition data in the Be isoelectronic sequence

P Jönsson†, C Froese Fischer‡ and E Träbert§

- Systematic calculations with increasing active set of orbitals
- Convergence monitored
- Comparison between computed and experimental transition rates for $2s^2\ ^1S_0 \rightarrow 2s2p\ ^{1,3}P_1$ in the Be-sequence

Comparing theory and experiment

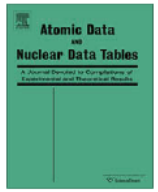


Spectrum calculations C II, N III, O IV

Contents lists available at ScienceDirect

Atomic Data and Nuclear Data Tables

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



Hyperfine structures, isotope shifts, and transition rates of C II, N III, and O IV from relativistic configuration interaction calculations

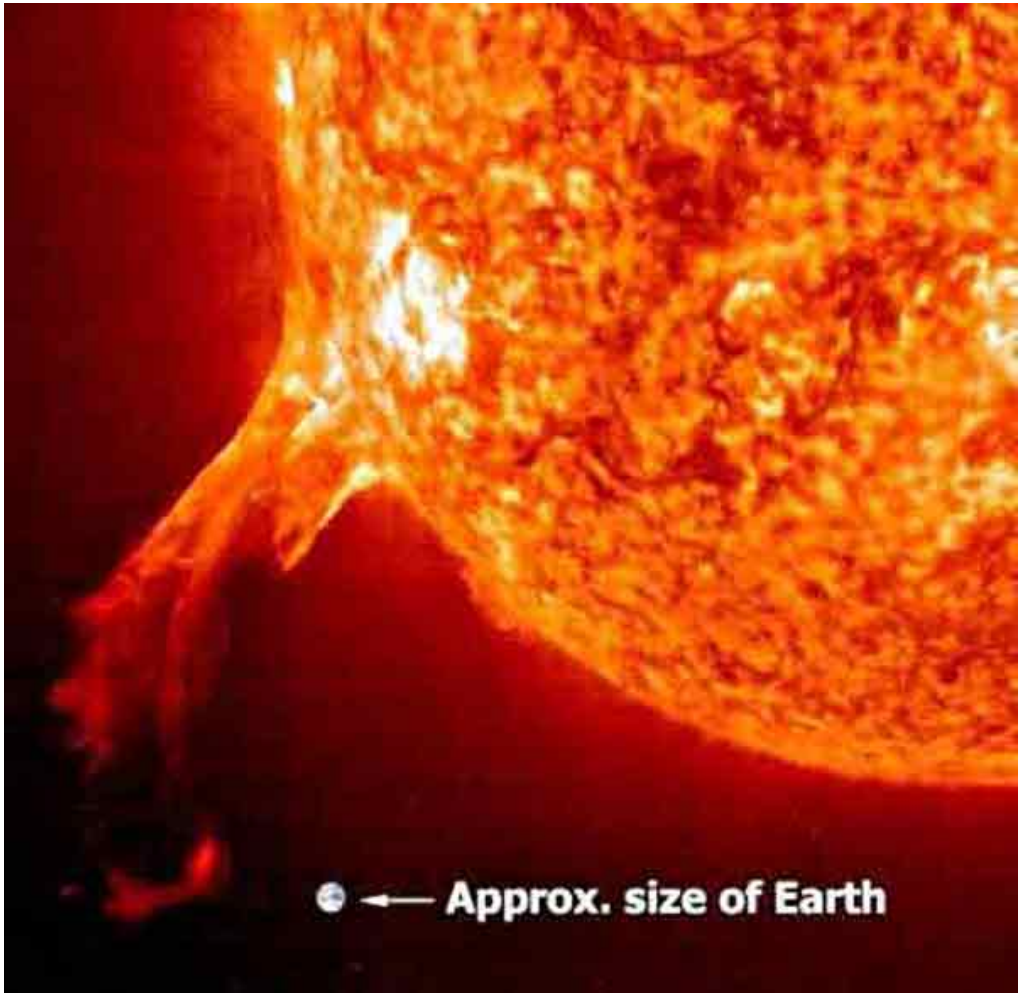
Per Jönsson [a,*], Jiguang Li [b], Gediminas Gaigalas [c,d], Chenzhong Dong [b,e]

- $2s^2 2p, 2s2p^2, 2p^3, 2s^2 3s, 2s^2 3p, 2s^2 3d, 2s2p3s$
- MR with SD substitutions to $n = 10$ and $l = 6$, between 800 000 and 1 000 000 CSFs
- Convergence with respect to the increasing active set
- Convergence with increasing MR
- Odd and even states separately optimized

O IV energies, comparison with experiment

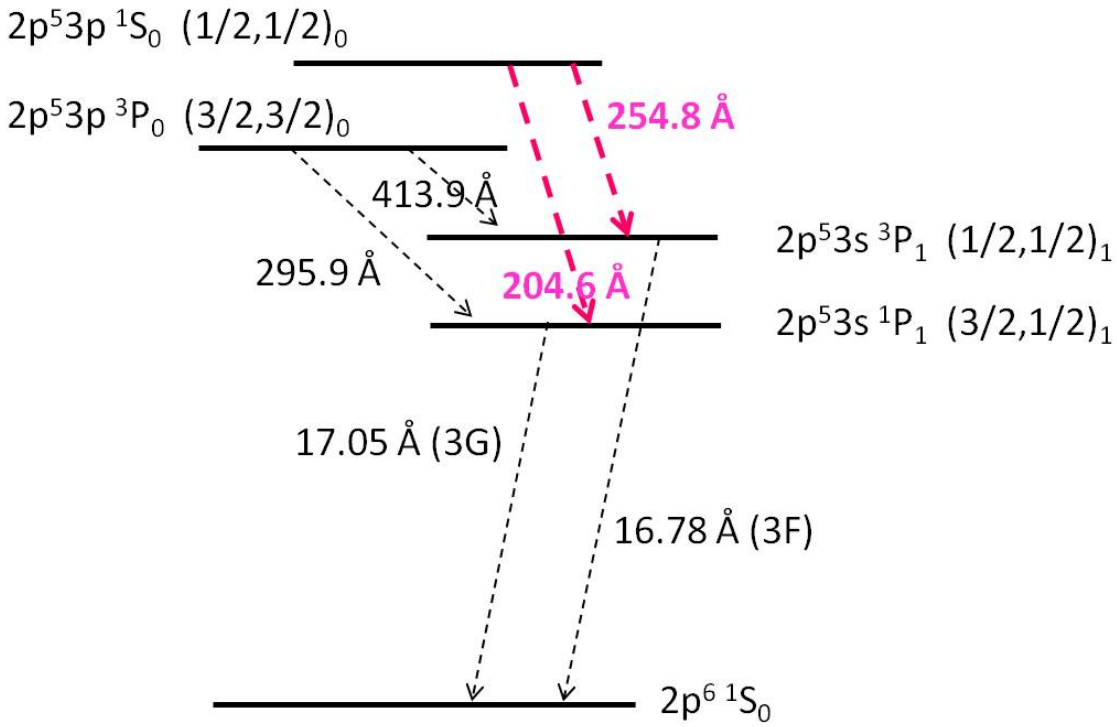
O IV						
Level	Level (cm^{-1})			Splitting (cm^{-1})		
	Theory	Obs.	Diff.	Theory	Obs.	Diff.
$2s^2 2p\ ^2P^o_{3/2}$	384.97	385.9	−0.9	385.0	385.9	−0.9
$2s2p^2\ ^4P_{1/2}$	71 309.65	71 439.8	−130.1			
$2s2p^2\ ^4P_{3/2}$	71 440.48	71 570.1	−129.6	130.8	130.3	0.5
$2s2p^2\ ^4P_{5/2}$	71 624.16	71 755.5	−131.3	314.5	315.7	−1.2
$2s2p^2\ ^2D_{5/2}$	127 193.45	126 936.3	257.1			
$2s2p^2\ ^2D_{3/2}$	127 206.92	126 950.2	256.7	13.5	13.9	−0.4
$2s2p^2\ ^2S_{1/2}$	164 790.37	164 366.4	424.0			
$2s2p^2\ ^2P_{1/2}$	180 856.34	180 480.8	375.5			
$2s2p^2\ ^2P_{3/2}$	181 098.83	180 724.2	374.6	242.5	243.4	−0.9
$2p^3\ ^4S^o_{3/2}$	231 509.54	231 537.5	−28.0			
$2p^3\ ^2D^o_{5/2}$	255 376.18	255 155.9	220.3			

Flares, violent eruptions



Calculations for Fe XVII

Fe XVII 3p $^1S_0 \rightarrow$ 3s $^{1,3}P_1$



Compare poster of Prof Watanabe and talk by Prof Nakamura

Benchmark calculations for Fe XVII

A&A 508, 1517–1526 (2009)
DOI: 10.1051/0004-6361/200911729

Astronomy & Astrophysics

Benchmarking atomic data for astrophysics: Fe XVII EUV lines

G. Del Zanna[1] and Y. Ishikawa[2]

- Benchmark calculations for $n = 3$ provided by Del Zanna and Ishikawa, A & A 508 (2009) 1517
- Analysis and reinterpretation of energy levels
- Intensities based on R-matrix calculations by Loch et al J. Phys. B 39 (2006) 85

Calculations for Fe XVII

Jönsson et al ADNDT accepted (2012) (together with NIFS Japan)

- Systematic MCDHF and RCI calculations for all $2p^6$, $2p^5 3s$, $2p^5 3p$ and $2p^5 3d$ states.
- All states belonging to a configuration are optimized together
- The orbital set is systematically increased to $n = 7$ and $l = 6$
- Convergence monitored
- Final calculations for $2p^5 3d$ contains more than 700 000 CSFs
- Energies in perfect agreement with the ones given in Del Zanna and Ishikawa, A & A 508, 1517-1526 (2009)

Comparison with observed energies

Label		E_{calc} (cm^{-1})	E_{obs} (cm^{-1})	Diff
$2p^6$	$^1S_0$	0	0	0
$2p^5 3s$	$^3P^o_2$	5 849 108	5 849 490	−382
$2p^5 3s$	$^1P^o_1$	5 864 469	5 864 760	−291
$2p^5 3s$	$^3P^o_0$	5 951 003	5 951 478	−475
$2p^5 3s$	$^3P^o_1$	5 960 633	5 961 022	−389
$2p^5 3p$	$^3S_1$	6 093 573	6 093 568	5
$2p^5 3p$	$^3D_2$	6 121 769	6 121 756	13
$2p^5 3p$	$^3D_3$	6 134 794	6 134 815	−21
$2p^5 3p$	$^1P_1$	6 143 898	6 143 897	1
$2p^5 3p$	$^3P_2$	6 158 481	6 158 540	−59
$2p^5 3p$	$^3P_0$	6 202 542	6 202 620	−78
$2p^5 3p$	$^1S_0$	6 353 605	6 353 356	249
$2p^5 3d$	$^3P^o_0$	6 463 913	6 464 095	−182
$2p^5 3d$	$^3P^o_1$	6 471 519	6 471 233	286
$2p^5 3d$	$^3P^o_2$	6 486 166	6 486 440	−274

Summary Be – Ne-like sequences

- Errors in calculated energies typically a few hundred cm^{-1}
- Possible to spot line identifications that are wrong
- Transition data accurate enough to aid line identifications
- Transition rates
  - very good agreement between benchmark calculations for strong transitions
  - good agreement for weak (intercombination transitions)
  - for some lines there are large (unexplained) differences

Systematic calculations by Froese Fischer and Tachiev

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Atomic Data and Nuclear Data Tables 87 (2004) 1–184

Atomic Data AND Nuclear Data Tables

www.elsevier.com/locate/adt

Breit–Pauli energy levels, lifetimes, and transition probabilities for the beryllium-like to neon-like sequences☆

Charlotte Froese Fischer* and Georgio Tachiev

ELSEVIER

Available online at www.sciencedirect.com
ScienceDirect

Atomic Data and Nuclear Data Tables 92 (2006) 607–812

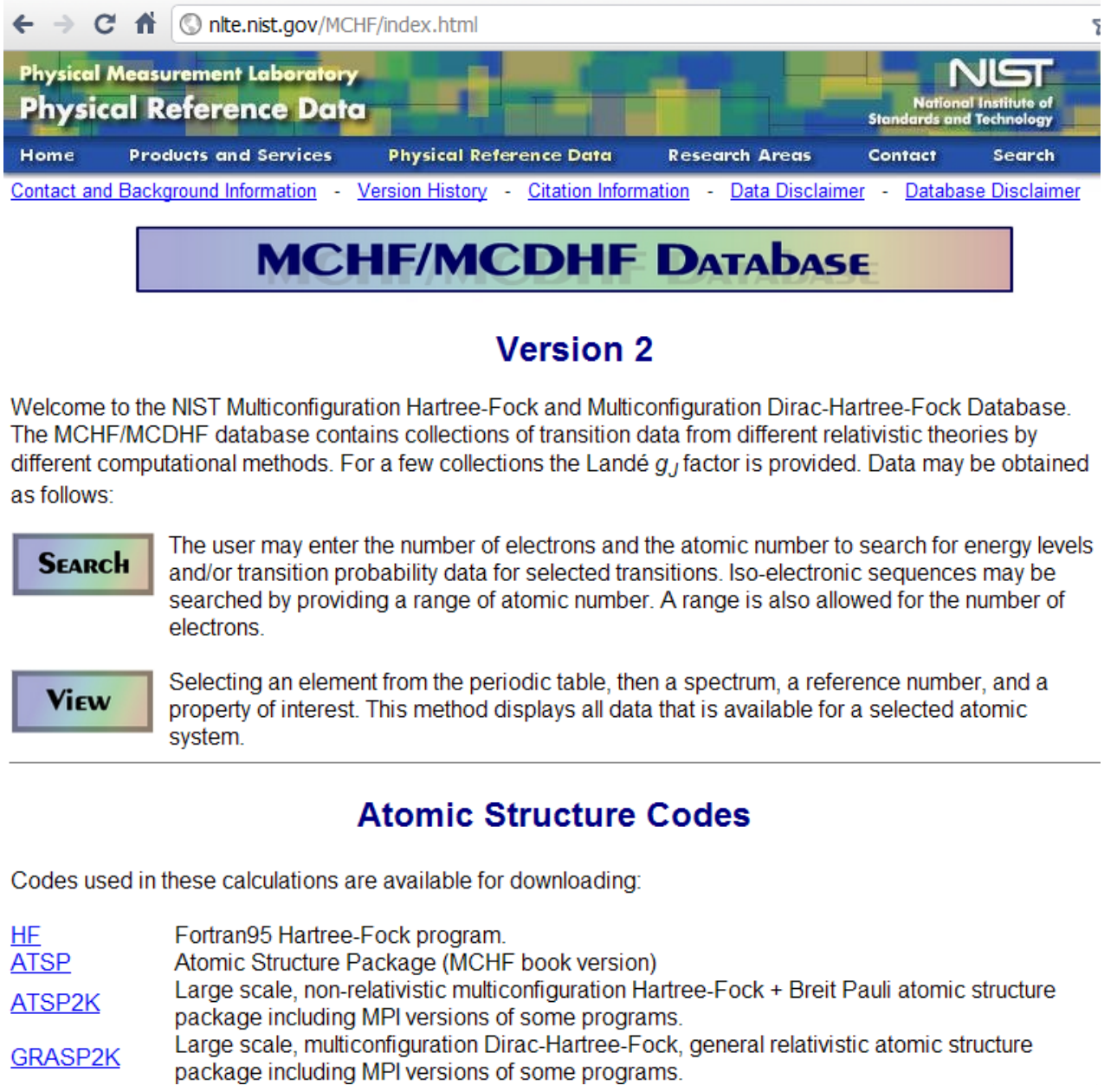
Atomic Data AND Nuclear Data Tables

www.elsevier.com/locate/adt

Relativistic energy levels, lifetimes, and transition probabilities for the sodium-like to argon-like sequences

Charlotte Froese Fischer *, Georgio Tachiev, Andrei Irimia

Froese Fischer and Tachiev atomic database at NIST



nlte.nist.gov/MCHF/index.html

Physical Measurement Laboratory
Physical Reference Data

NIST National Institute of Standards and Technology

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Contact and Background Information - Version History - Citation Information - Data Disclaimer - Database Disclaimer

MCHF/MCDHF Database

Version 2

Welcome to the NIST Multiconfiguration Hartree-Fock and Multiconfiguration Dirac-Hartree-Fock Database. The MCHF/MCDHF database contains collections of transition data from different relativistic theories by different computational methods. For a few collections the Landé g_J factor is provided. Data may be obtained as follows:

Search The user may enter the number of electrons and the atomic number to search for energy levels and/or transition probability data for selected transitions. Iso-electronic sequences may be searched by providing a range of atomic number. A range is also allowed for the number of electrons.

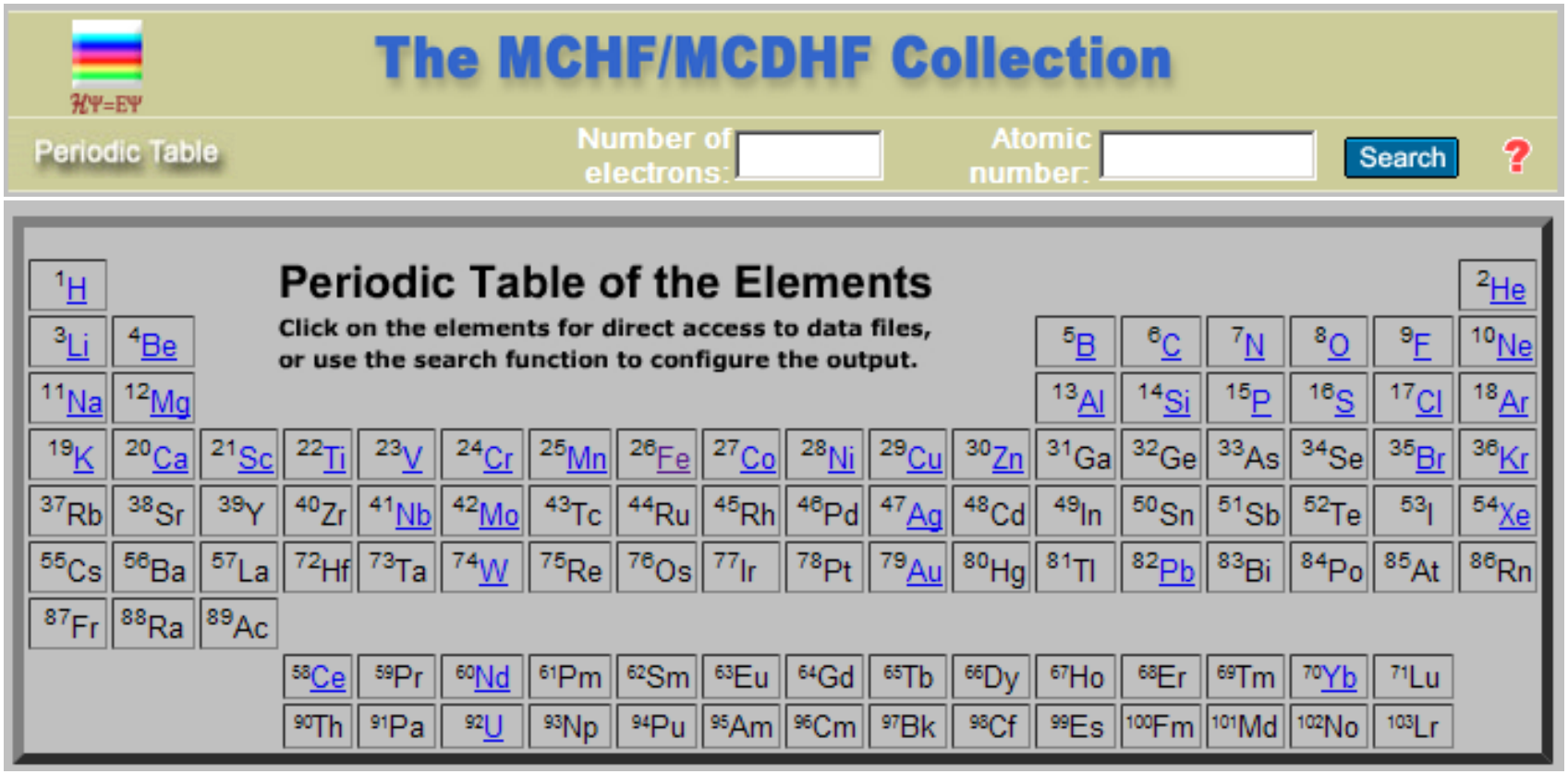
View Selecting an element from the periodic table, then a spectrum, a reference number, and a property of interest. This method displays all data that is available for a selected atomic system.

Atomic Structure Codes

Codes used in these calculations are available for downloading:

HF	Fortran95 Hartree-Fock program.
ATSP	Atomic Structure Package (MCHF book version)
ATSP2K	Large scale, non-relativistic multiconfiguration Hartree-Fock + Breit Pauli atomic structure package including MPI versions of some programs.
GRASP2K	Large scale, multiconfiguration Dirac-Hartree-Fock, general relativistic atomic structure package including MPI versions of some programs.

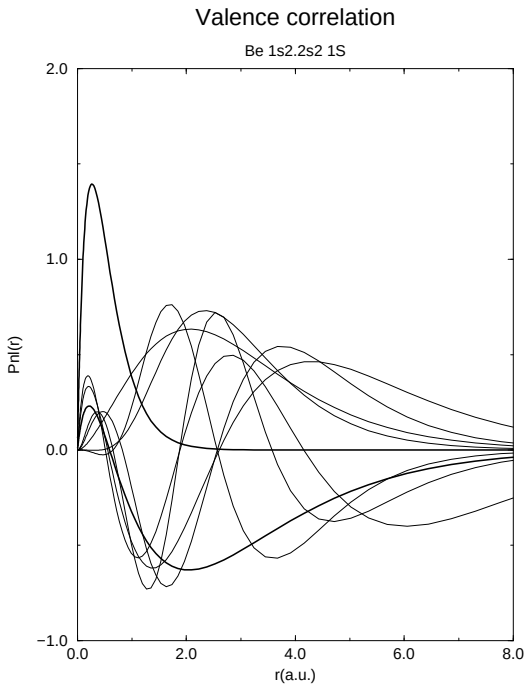
Elements in the database

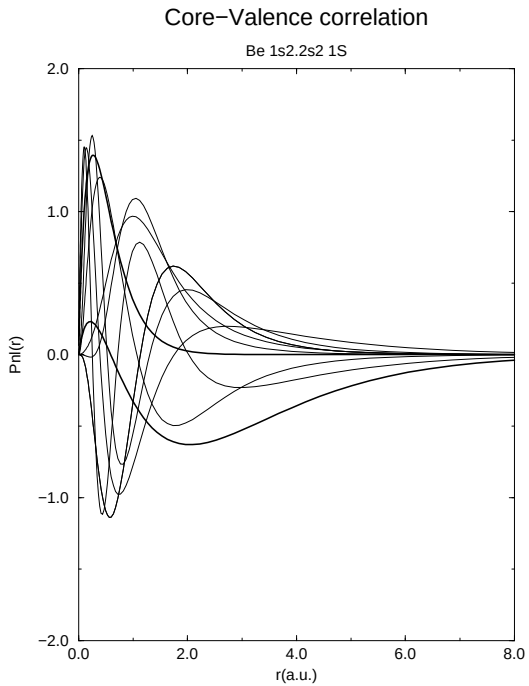


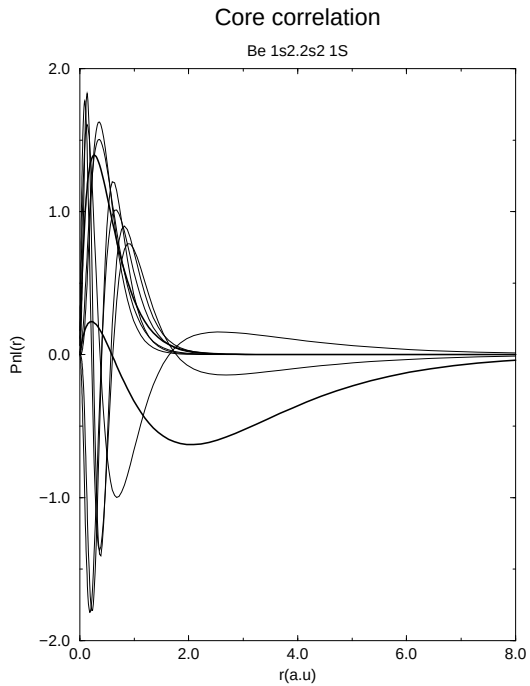
Correction of wave function: few electron system

Few electron system $1s^2 2s^2\ ^1S$. The CSF expansion grows comparatively slowly with respect to the increasing active set of orbitals

$$\left.\begin{array}{l} 1s^2 nln'l'\ ^1S \\ 1snl2sn'l'\ ^1S \\ nln'l'2s^2\ ^1S \end{array}\right\} \quad nl, n'l' \in \text{ active set}$$







Correction of wave function: many-electron system

Many-electron system $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2\ ^1S$. The CSF expansion grows unmanageably fast (scaling wall)

$$\left.\begin{array}{l} 1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} nln'l'\ ^1S \\ 1s^2 2s^2 2p^6 3s^2 3p^6 3d^9 nl4sn'l'\ ^1S \\ 1s^2 2s^2 2p^6 3s^2 3p^6 3d^8 nln'l'4s^2\ ^1S \\ 1s^2 2s^2 2p^6 3s^2 3p^5 nl3d^9 n'l'4s^2\ ^1S \\ .... \\ nln'l'2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2\ ^1S \end{array}\right\} \quad nl, n'l' \in \text{ active set}$$

New code development

Verdebout et al J. Phys B 43 (2010) 074017 (Poster 16b)

- Perform *separate* MCHF calculations for each expansion
- Remove main CSF and renormalize $\Rightarrow$ partitioned correlation function (PCF) built on an optimally located orbital basis
- Expand the wave function in a basis consisting of the CSFs in the MR and the PCFs
- Construct the Hamiltonian matrix and solve eigenvalue problem (low dimensional) to get expansion coefficients

Before very time consuming to construct the Hamiltonian matrix elements between PCFs due to non-orthogonalities. New fast biorthogonal transformation technique key to the method

Results for $1s^2 2s^2\ ^1S$ in Be

Tabell: Calculations based on PCFs. The energies are compared with CAS-MCHF results based on a single orthonormal orbital set.

$n \leqslant$	$E_{8\times 8}$	$E_{CAS-MCHF}$
4	−14.660 679 48	−14.661 403 17
5	−14.665 553 46	−14.664 839 93
6	−14.666 582 83	−14.666 067 32
7	−14.666 905 87	−14.666 541 14
8	−14.667 047 86	−14.666 857 41
9	−14.667 122 76	−14.667 012 75
10	−14.667 168 08	−14.667 114 20

- CAS-MCHF 650 000 CSFs, days on a super computer cluster
- Totally 600 CSFs used for the PCFs. Calculation takes minutes.

PCF expansion method

- Break down an unmanageably large MCHF run to a number of smaller MCHF runs for the PCFs (divide and conquer)
- The PCFs are built on optimally located radial orbital sets
- Possible to include correlation deeper down in core
- Better convergence properties
- Transition energies can be computed to spectroscopic precision?
- Great prospects for hfs and isotope shifs
- Interesting applications to continuum problems

Problems

Variational freedom lost since expansion coefficients of the CSFs in the PCFs are fixed from the separate MCHF calculations.

Can be solved by so called deconstraining (see poster 16b)

Summary

- Atomic structure calculations require efficient codes
- Current programs ATSP2K and GRASP2K allows many systems and properties to be calculated very accurately
- New methodology based on PCFs allows the high accuracy for few electron systems to be carried over to many-electron systems?

Thank you

Thank you Charlotte for your support and encouragement and also for being such a good colleague and friend!

Challenges of hfs

IOP PUBLISHING JOURNAL OF PHYSICS B: ATOMIC, MOLECULAR AND OPTICAL PHYSICS

J. Phys. B: At. Mol. Opt. Phys. **40** (2007) 2417–2433 doi:10.1088/0953-4075/40/12/017

Spectral properties of In II from MCDHF calculations

Per Jönsson[1] and Martin Andersson[2]

- 24 even parity states up to $5s7d\ ^1D_2$ and 20 odd parity states up to $5s5f\ ^1F^o_3$.
- MR with SD substitutions to three layers of correlation orbitals. Valence and core-valence effects included and at most one excitation from the $4d$ core shell. S substitutions from all core shells.
- Odd and even states separately optimized

Hyperfine structures in In II

Level	A	B	A_{exp}	B_{exp}	g_J	g_{LSJ}
$5s5p\,^3P^o_1$	6832	−407	6949 ± 24	−420	1.4982	1.5011
$5s5p\,^3P^o_2$	5014	737	5088 ± 27	629	1.5011	1.5011
$5s5p\,^1P^o_1$	−229	546			1.0028	1.0000
$5s6s\,^3S_1$	11 758	0.2	12049 ± 12	0	2.0021	2.0023
$5s5d\,^1D_2$	521	611	549 ± 21	570	1.0090	1.0000
$5s5d\,^3D_1$	−4845	23.2			0.5042	0.4988
$5s5d\,^3D_2$	1778	339	1865 ± 30	−600	1.1673	1.1670
$5s5d\,^3D_3$	3340	94.9	3388 ± 60	−60	1.3341	1.3341

- Very large differences for B factors belonging to closely spaced states
- Hyperfine structure can not be described by A and B factors!
- Off-diagonal effects important

Hyperfine structures in Ga II

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS B: ATOMIC, MOLECULAR AND OPTICAL PHYSICS

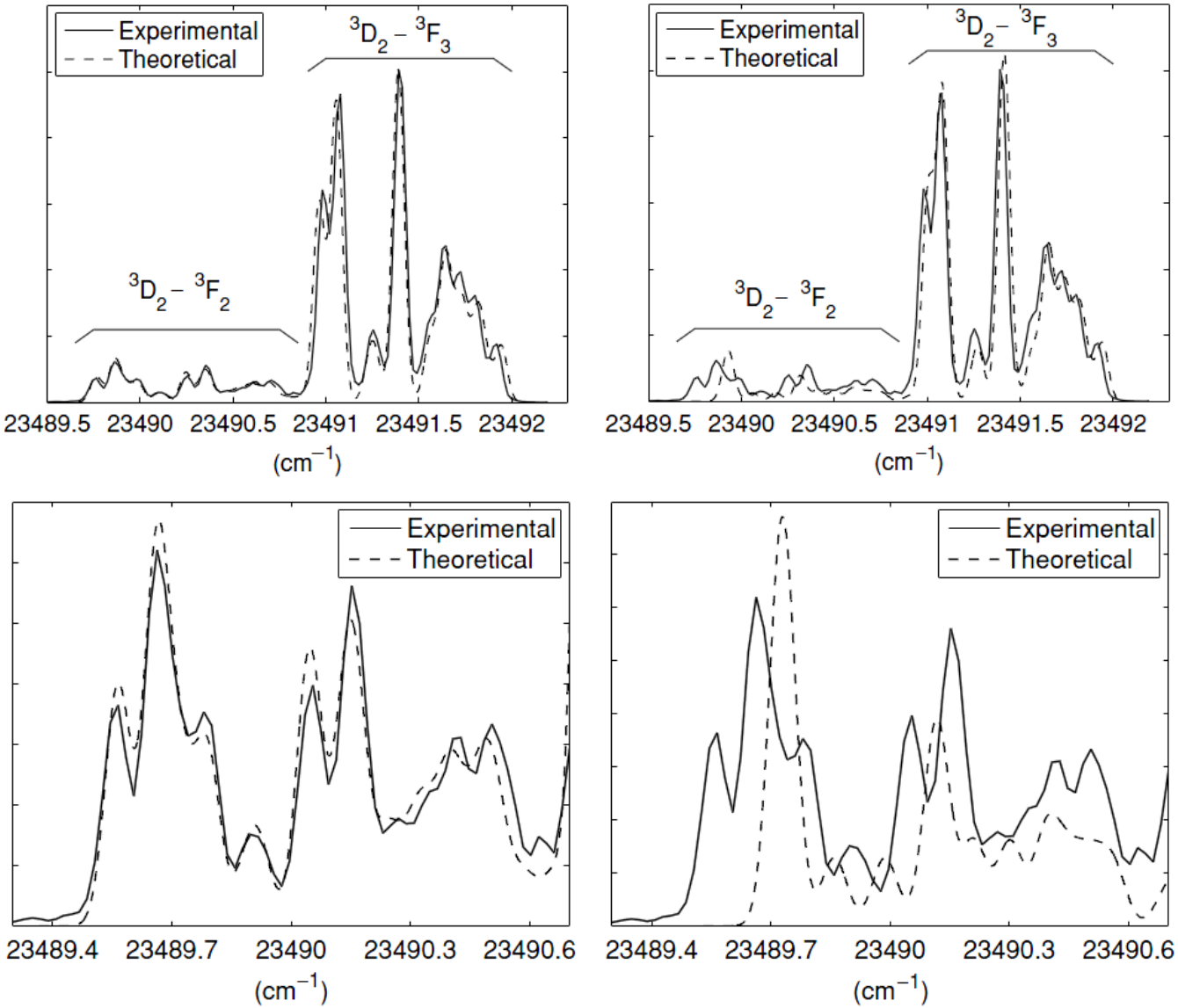
J. Phys. B: At. Mol. Opt. Phys. **39** (2006) 4239–4247 doi:10.1088/0953-4075/39/20/021

Hyperfine induced interference effects in the $4s4d\,^3D_2$–$4s4f\,^3F_{2,3}$ transitions in Ga II

Martin Andersson[1], Per Jönsson[1,2] and Hans Sabel[3]

- In closely spaced fine structure levels off-diagonal hfs interaction leads to redistribution of radiation
- Spectral lines changes dramatically
- Theoretical support needed to interpret spectra

FTS spectra of hfs transitions



Conclusions

- Traditional A and B hyperfine factors meaningless in many cases. Should not be used by astronomers
- Experiment or computation should supply astronomers with position and rates for all hyperfine transitions

Thank you

Thank you Charlotte for your support and encouragement and also for being such a good colleague and friend!