Laboratoire Kastler Brossel
Physique quantique et applications

Perspectives for relativistic many-body and QED calculations for highly charged ions

Paul Indelicato

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EMMI ENS cnrs SORBONNE UNIVERSITÉ COLLÈGE DE FRANCE 1530

Outline

- Introduction: many body calculations in atoms and ions
- Exemple of applications to new high-precision experiments
  - few-electron uranium ions
  - medium-Z few electron ions
  - long-lived metastable states
- Conclusion and perspective

Many body effects

principles and exemples

MCDF method

$$\mathcal{H}^{\text{no pair}}\Psi_{\Pi,J,M}(\ldots,\boldsymbol{r}_i,\ldots) = E_{\Pi,J,M}\Psi_{\Pi,J,M}(\ldots,\boldsymbol{r}_i,\ldots),$$

$$\mathcal{H}^{\text{no pair}} = \sum_{i=1}^{N}\mathcal{H}_D(r_i) + \sum_{i<j}\mathcal{V}(|\boldsymbol{r}_i - \boldsymbol{r}_j|), \quad \mathcal{V}(|r_i - r_j|) = \Lambda^{++}V_{ij}\Lambda^{++},$$

$$\left|\Psi_{\Pi,J,M}\right\rangle = \sum_{\nu=1}^{n} c_\nu |\nu,\ \Pi,\ J,\ M\rangle.$$

c_ν obtained by diagonalisation of Hamiltonian matrix

$$|\nu,\ \Pi,\ J,\ M\rangle = \sum_{i=1}^{N_\nu} d_i \begin{vmatrix} \psi_1^i(r_1) & \cdots & \psi_m^i(r_1) \\ \vdots & \ddots & \vdots \\ \psi_1^i(r_m) & \cdots & \psi_m^i(r_m) \end{vmatrix}.$$

d_i obtained by diagonalisation of J^2 and J_z

MCDF method

$$E_{\Pi,J,M} = \frac{\langle \Psi_{\Pi,J,M} | \mathcal{H}^{\text{no pair}} | \Psi_{\Pi,J,M} \rangle}{\langle \Psi_{\Pi,J,M} | \Psi_{\Pi,J,M} \rangle}$$

$$\begin{pmatrix} V^i_{\mathrm{DF}}(r) & -\frac{d}{dr} + \frac{\kappa_i}{r} \\ \frac{d}{dr} + \frac{\kappa_i}{r} & V^i_{\mathrm{DF}}(r) - 2mc \end{pmatrix} \begin{pmatrix} P_i(r) \\ Q_i(r) \end{pmatrix}$$

$$= \alpha\lambda_{i,i} \begin{pmatrix} P_i(r) \\ Q_i(r) \end{pmatrix} + \begin{pmatrix} X^i_P(r) \\ X^i_Q(r) \end{pmatrix} + \sum_{j \neq i} \lambda_{j,i} \begin{pmatrix} P_j(r) \\ Q_j(r) \end{pmatrix}$$

Minimize

↓

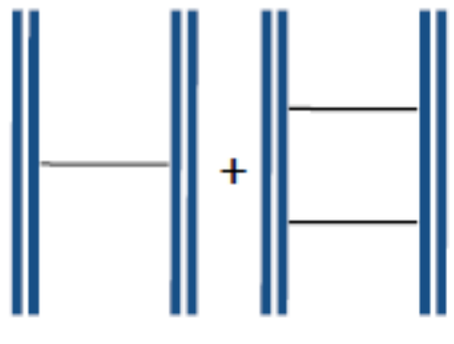
Inhomogeneous Dirac equation

MCDF method

- Build the energy expression with all one-electron and F, G, R integrals
- add the magnetic and retardation integrals
- Diagonalize the hamiltonian matrix
- solve each differential equation in turn up to all have reached some predefined accuracy (10^{-4} to 10^{-6})
- Diagonalize again and start an iterative solving cycle several times
- Check the energy numerical accuracy by evaluating it with two different expressions that **give the same value only if wavefunction and energy are well converged**

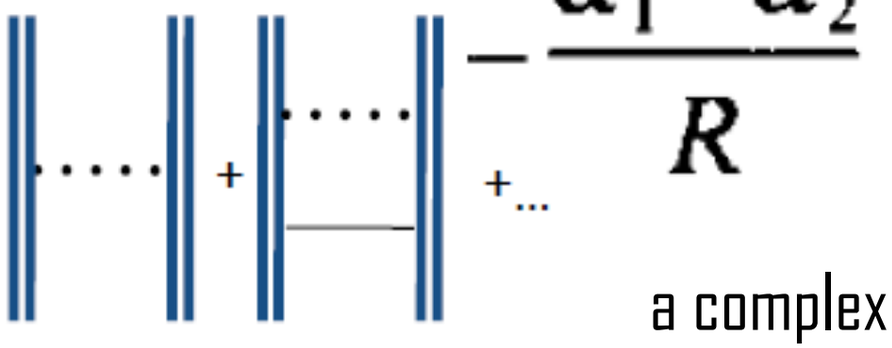
Electron-electron interaction

$$\frac{1}{R} - \frac{\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2}{R}\cos\omega R + (\boldsymbol{\alpha}_1 \cdot \boldsymbol{\partial}_1)(\boldsymbol{\alpha}_2 \cdot \boldsymbol{\partial}_2)\left(\frac{\cos\omega R - 1}{\omega^2 R}\right)$$



$$\frac{1}{R}$$

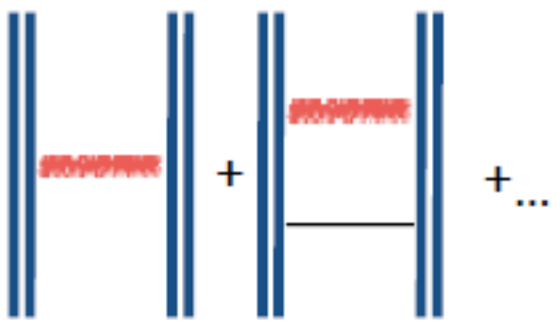
Coulomb: definition of the wave function



$$-\frac{\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2}{R}$$

Magnetic interaction (ω=0): perturbation or average potential in differential equation

a complex operator involving exponential functions of the one electron Hamiltonian.

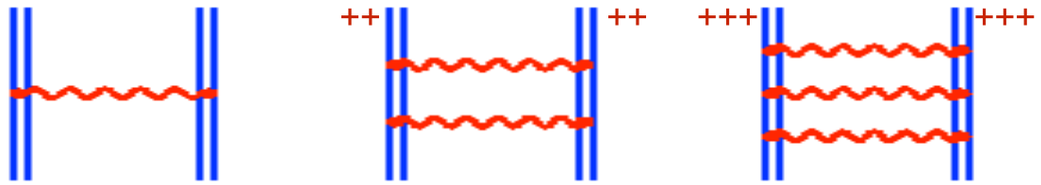


$$-\frac{\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2}{R}(\cos\omega R - 1) + (\boldsymbol{\alpha}_1 \cdot \boldsymbol{\partial}_1)(\boldsymbol{\alpha}_2 \cdot \boldsymbol{\partial}_2)\left(\frac{\cos\omega R - 1}{\omega^2 R}\right)$$

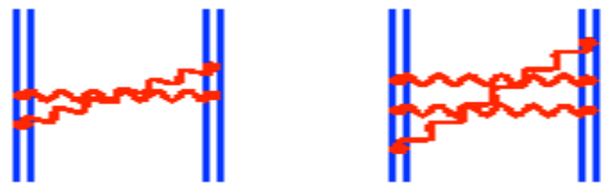
Retardation: the rest with $\omega = E_a - E_b$

many-body effects in few (≥3)-electron ions

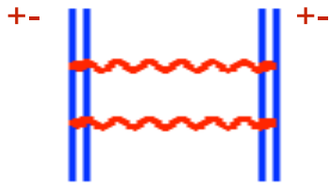
RMBPT or MCDF or RCI (1/Z expansion!)



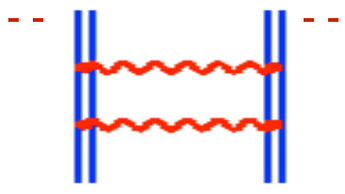
not included
in any calculation



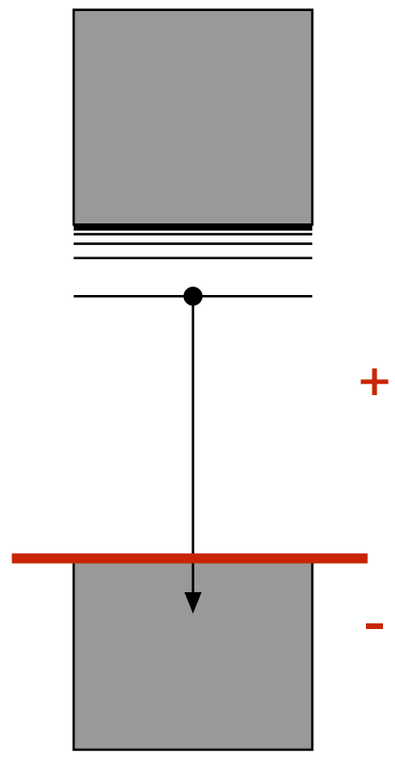
not included
in any calculation



not included
in any calculation



+ means remove below



Challenges:

- numerical convergence of very non-linear differential equation system
- evaluation of higher-order effects (three-body for example)
  - include double and triple excitations
  - include all single excitation
  - How to take into account high-order retardation? (value of ω, numerical instabilities)
  - Brillouin single excitations to get correct fine structure at low-Z…
  - Huge number of Coulomb and Breit integral for cases with many open shells with d, f, g orbitals

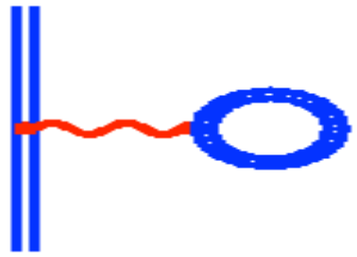
One electron BSQED corrections

QED, nuclear size corrections…

one electron QED at order α

Self Energy

$\frac{\alpha}{\pi}$



Vacuum Polarization

H-like "One Photon" order (α/π)

Many calculations, very accurate down to Z=1

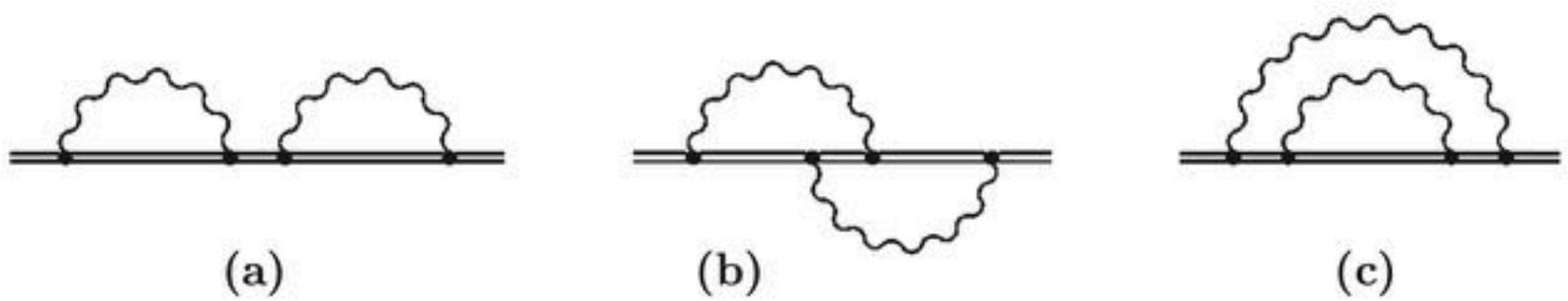
$$\Delta E_{SE} = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3}F(Z\alpha). \qquad \frac{\alpha}{\pi} = 2.3 \times 10^{-3}$$

$$E_{NR} = \frac{(Z\alpha)^2}{n^2}$$

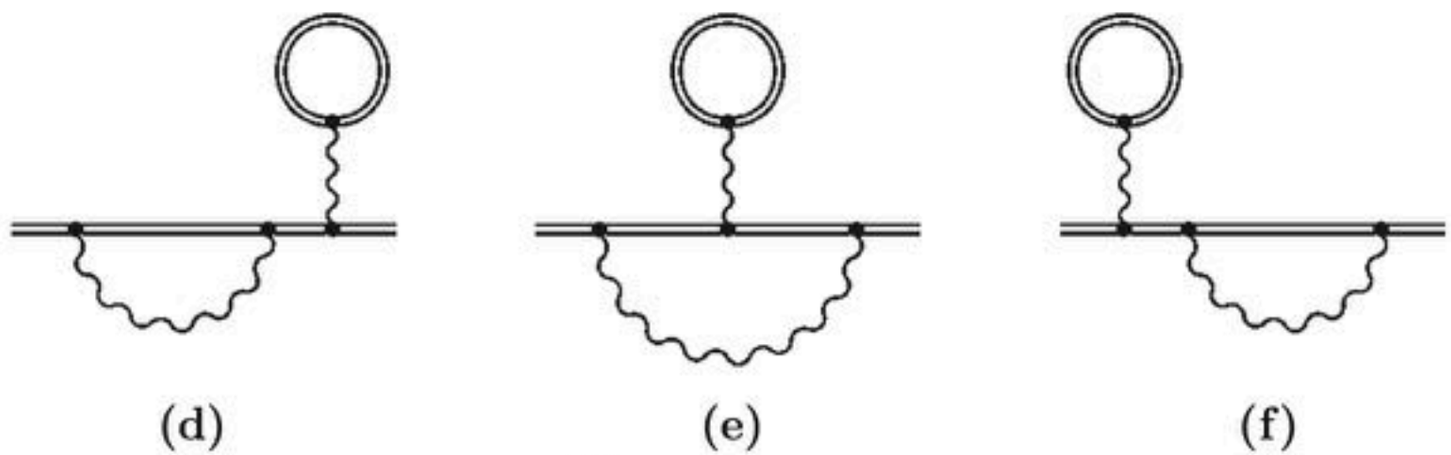
Closed fermion loops 2nd order diagrams

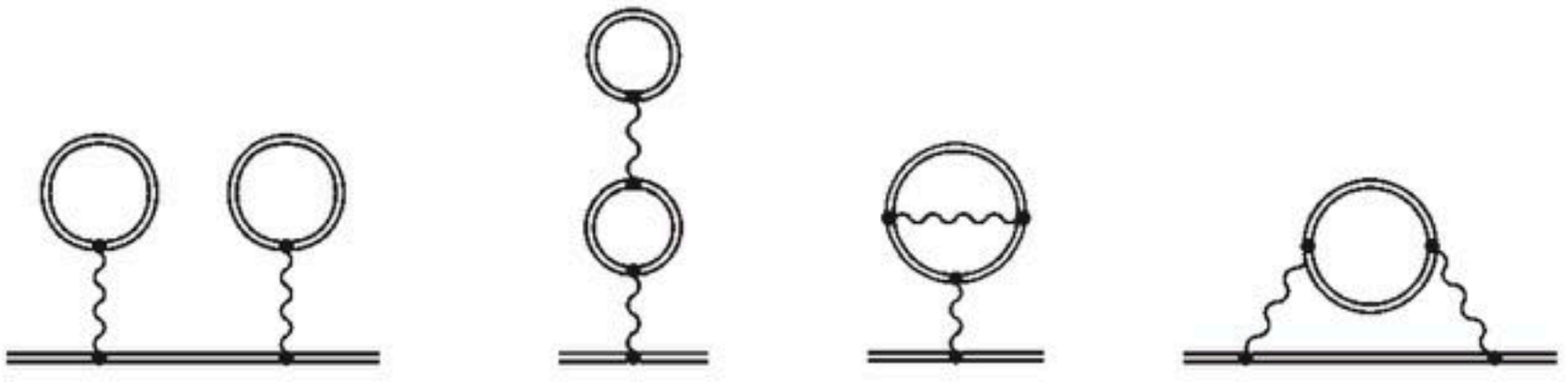
terms of order $(\alpha/\pi)^2$

SE-SE



SE-VP





Uehling in Dirac Eq.

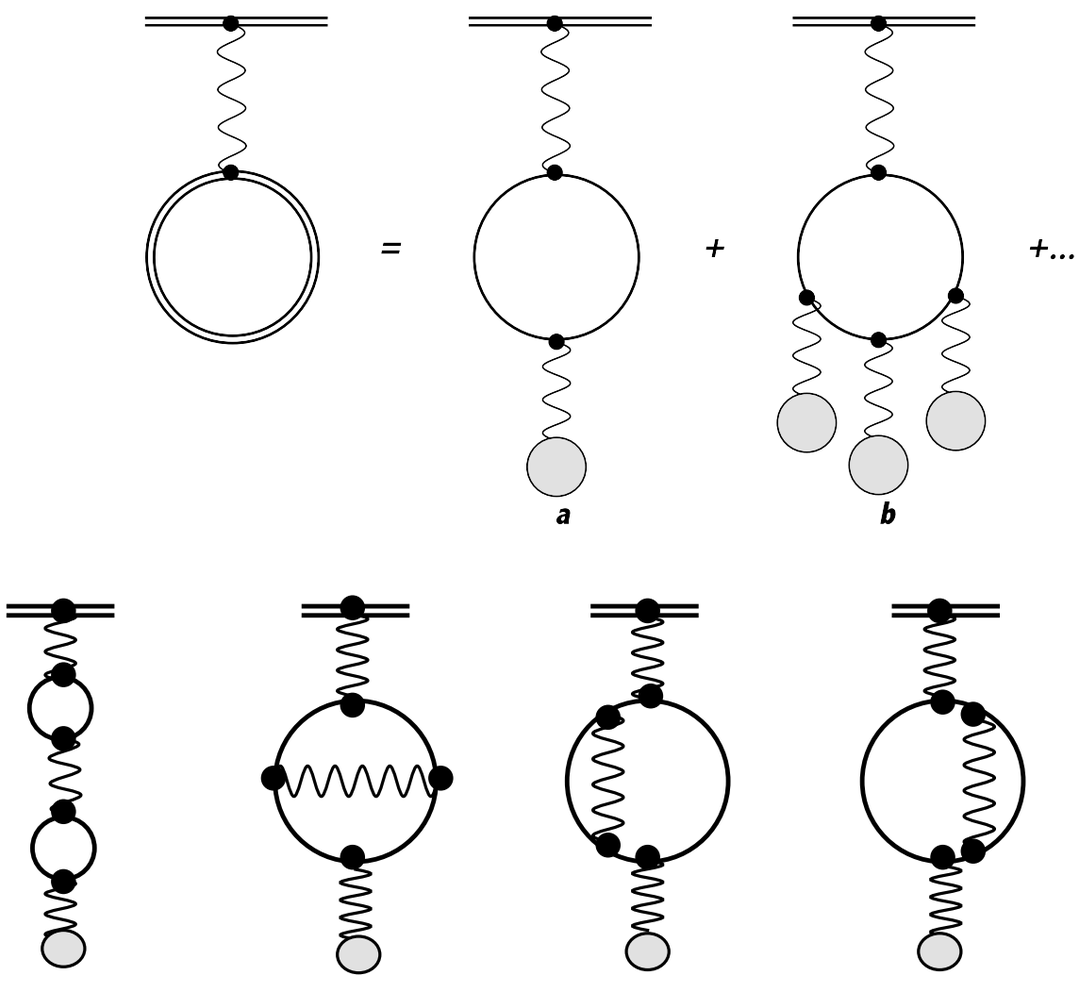
VP-VP

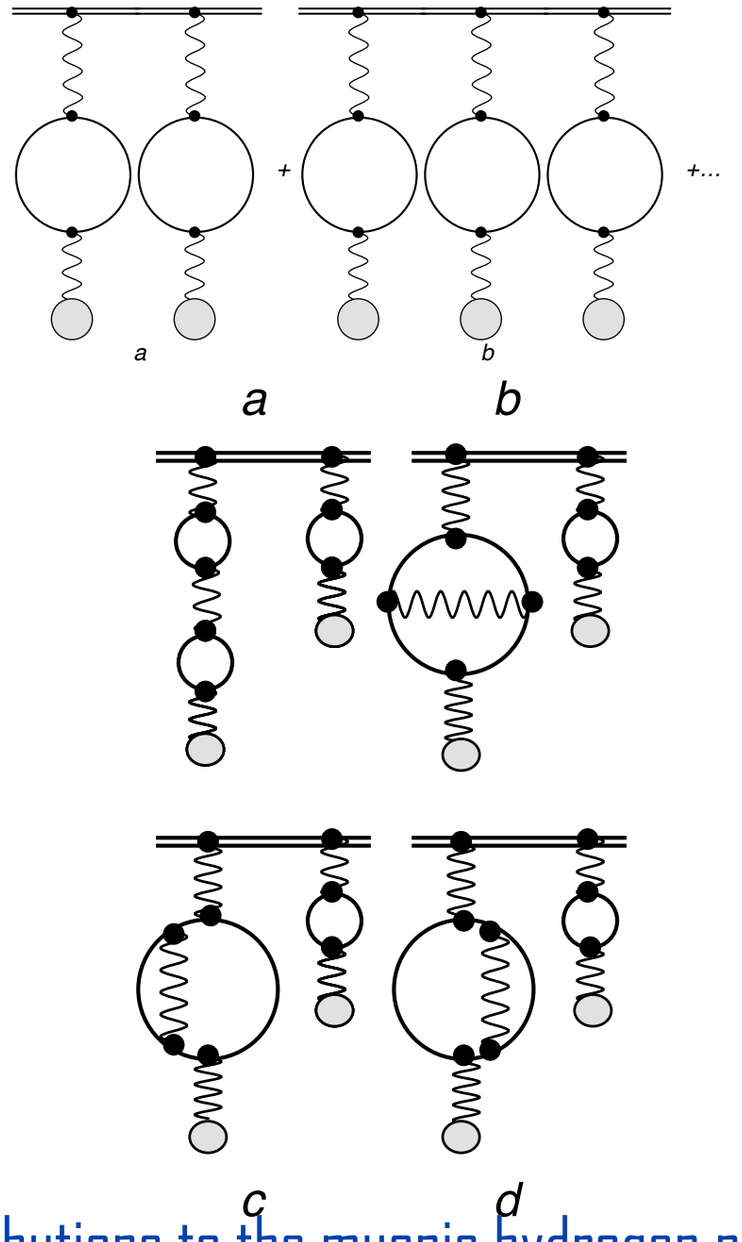
Källén & Sabri potential

S(VP)E

Contributions included to all-order

All-order: the charge distribution is included exactly in the wavefunction and in the operator, when relevant. Higher order Vacuum Polarization contribution included by numerical solution of the Dirac equation



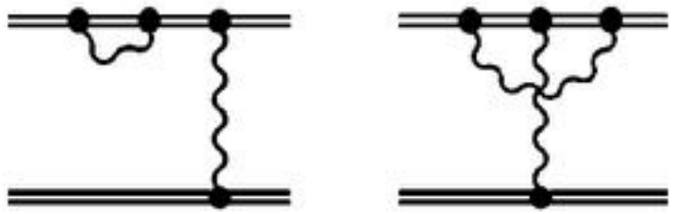


Nonperturbative evaluation of some QED contributions to the muonic hydrogen n=2 Lamb shift and hyperfine structure, P. Indelicato. Phys. Rev. A **87,** 022501 (2013).

Two-electron BSQED corrections

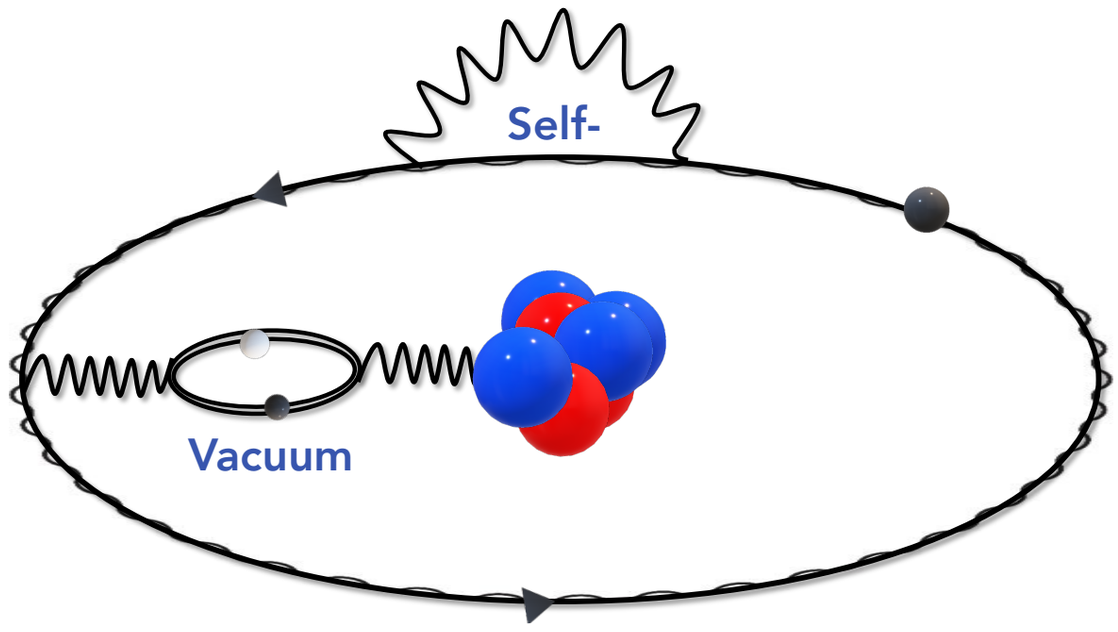
QED, nuclear size corrections…

Self-energy screening



(A) (B)

FIG. 1. Feynman diagrams for radiative corrections to the electron-electron interaction. (A) represents the wave function correction, and (B) is the vertex correction.



Direct QED calculation, e.g.:
Coordinate-space approach to the bound-electron self-energy: Self-Energy screening calculation, P. Indelicato et P.J. Mohr. Phys. Rev. A 63, 052507 (2001).

Approximation: Welton model
MCDF studies of two electron ions II: Radiative corrections and comparison with experiment., P. Indelicato, O. Gorceix et J.P. Desclaux. J. Phys. B 20, 651 (1987).

Self-energy screening

Until recently:

- Welton model $\delta H_{\mathrm{SE}} = \Delta V_n(r)\langle(\delta r)^2\rangle_{\mathrm{vacuum}}$

$$\delta E_{\mathrm{SE}} = \sum \frac{\langle nl|\Delta U_n(r)|nl\rangle_{\mathrm{DF}}}{\langle nl|\Delta U_n(r)|nl\rangle_{\mathrm{Hyd}}} \delta(E_{\mathrm{SE\ Hyd}})_{nl}$$

(P. Indelicato, O. Gorceix, and J. P. Desclaux, J. Phys. B: Atomic 20, 651 (1987).)

- Model potential: calculate the self-energy in a non-coulomb, screened potential

Self-energy screening: new method

A model operator has been defined:

This operator can be easily incorporated in any calculations employing the Dirac-Coulomb-Breit Hamiltonian.

$$h^{\mathrm{SE}} = V_{\mathrm{loc}}^{\mathrm{SE}} + \sum_{i,k=1}^{n} |\phi_i\rangle B_{ik} \langle\phi_k| \,,$$

The model operator reproduces very precisely exact evaluation of the Self-energy values for one-electron ions

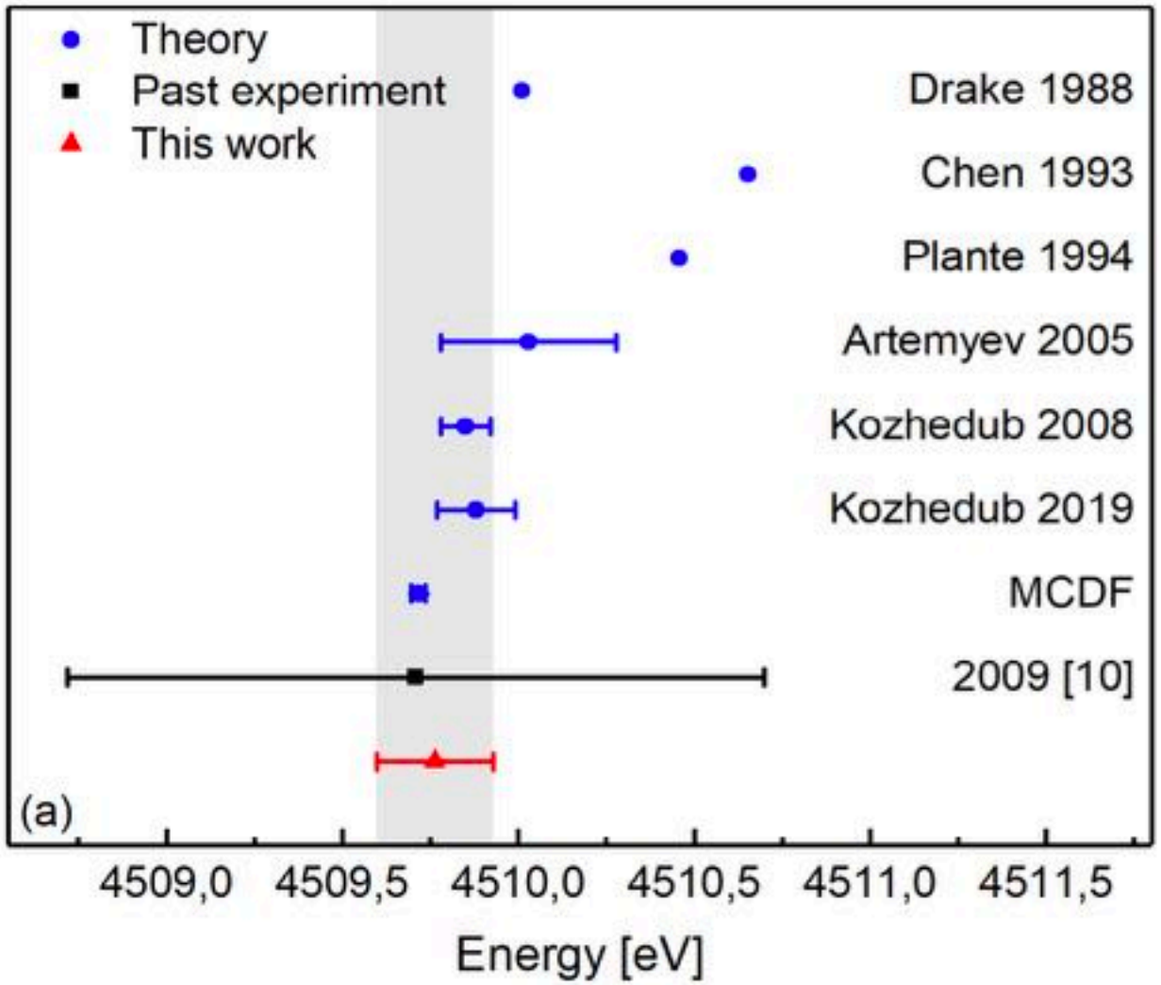
Now implemented since the 2016 version of the MCDFGME code (Indelicato and Desclaux)

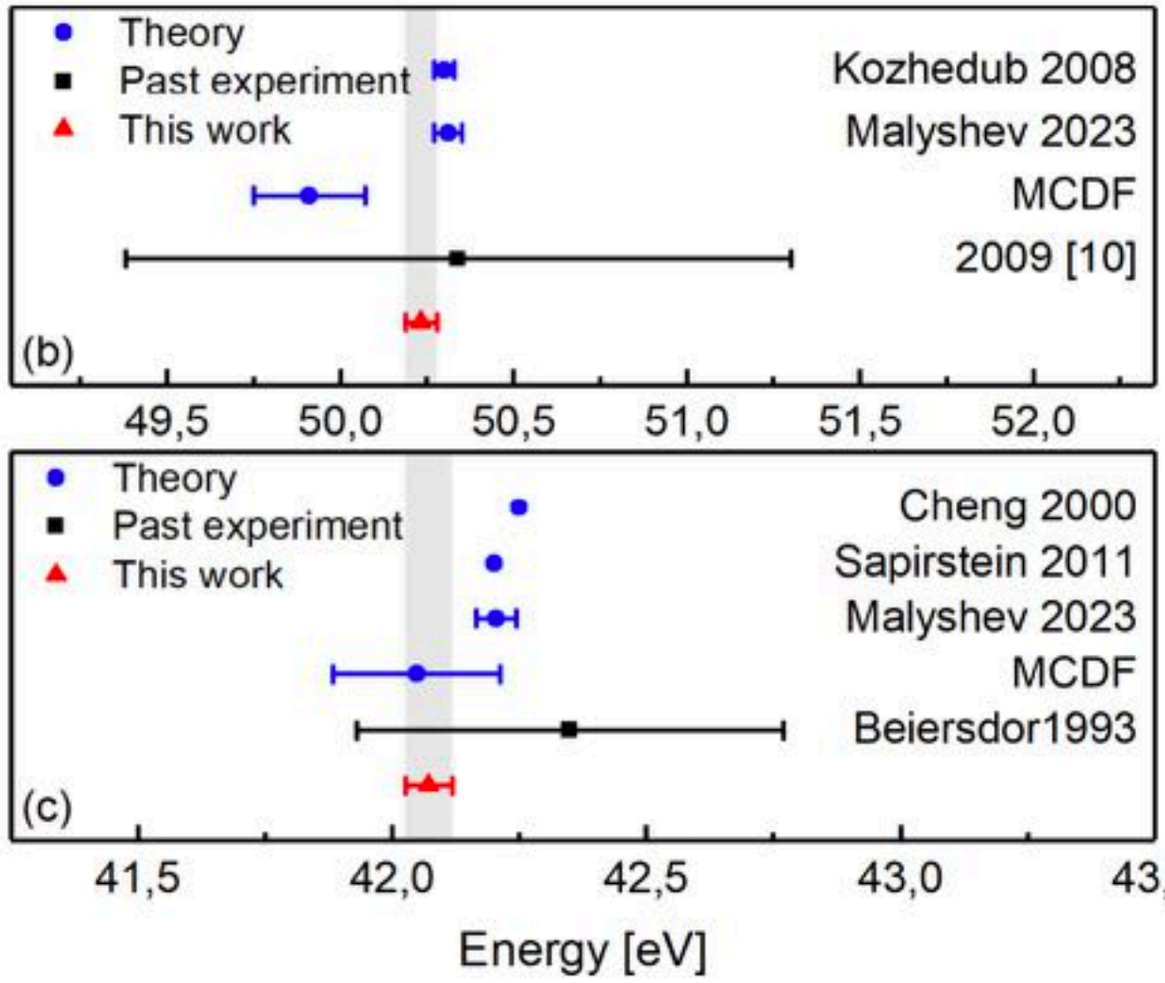
Shabaev, V. M., I. I. Tupitsyn and V. A. Yerokhin (2013),Physical Review A88(1): 012513.

High-precision measurements Δn=0 few-electrons U ions

Crystal spectroscopy at ESR

Highly-charged U ions

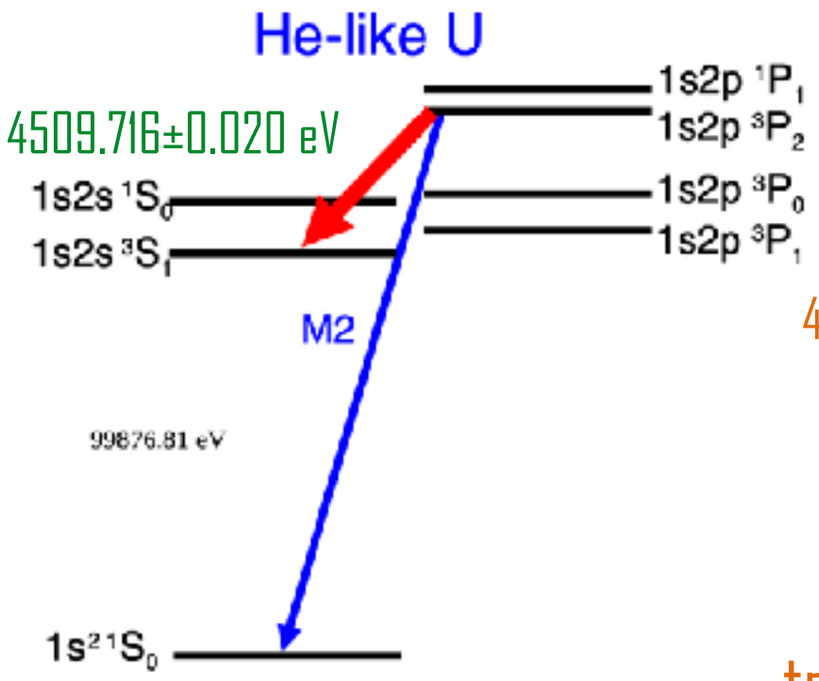




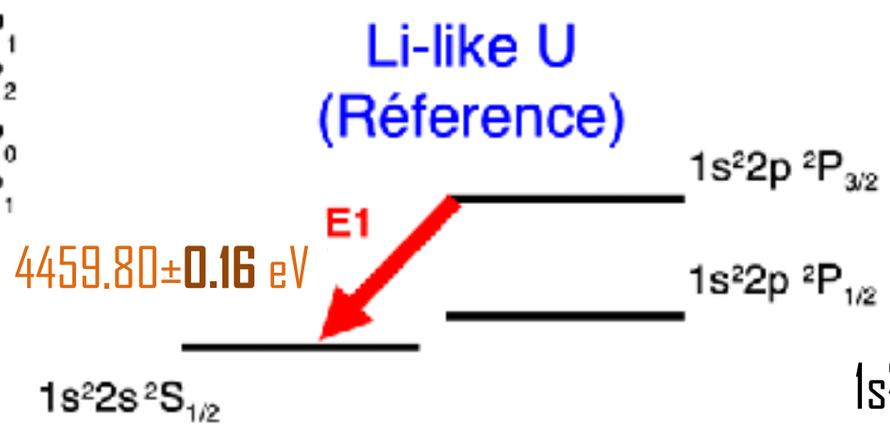
R. Loetzsch, H.F. Beyer, L. Duval, U. Spillmann, D. Banas, P. Dergham, F.M. Kröger, J. Glorius, R.E. Grisenti, M. Guerra, A. Gumberidze, R. Heß, P.-M. Hillenbrand, P. Indelicato, P. Jagodzinskil, E. Lamour, B. Lorentz, S. Litvinov, Yu.A. Litvinov, J. Machado, N. Paul, G.G.Paulus1,6, N.Petridis, J.P.Santos, M.Scheidel, I. Uschmann, G. Weber, Th. Stöhlker, M. Trassinelli, accepted to Nature (2024)

Spectroscopy of Intrashell He-like U transition

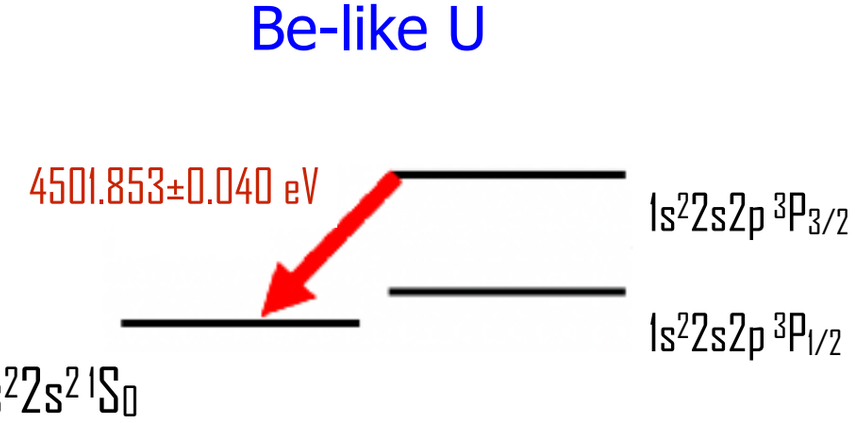
Comparing two states of charges allows to bypass the nuclear uncertainties



accuracy reached for
correlation orbitals up to 7i
1s 2s $^3S_1$: **39** configurations,
7.6k Coulomb integrals
26k Breit Integrals

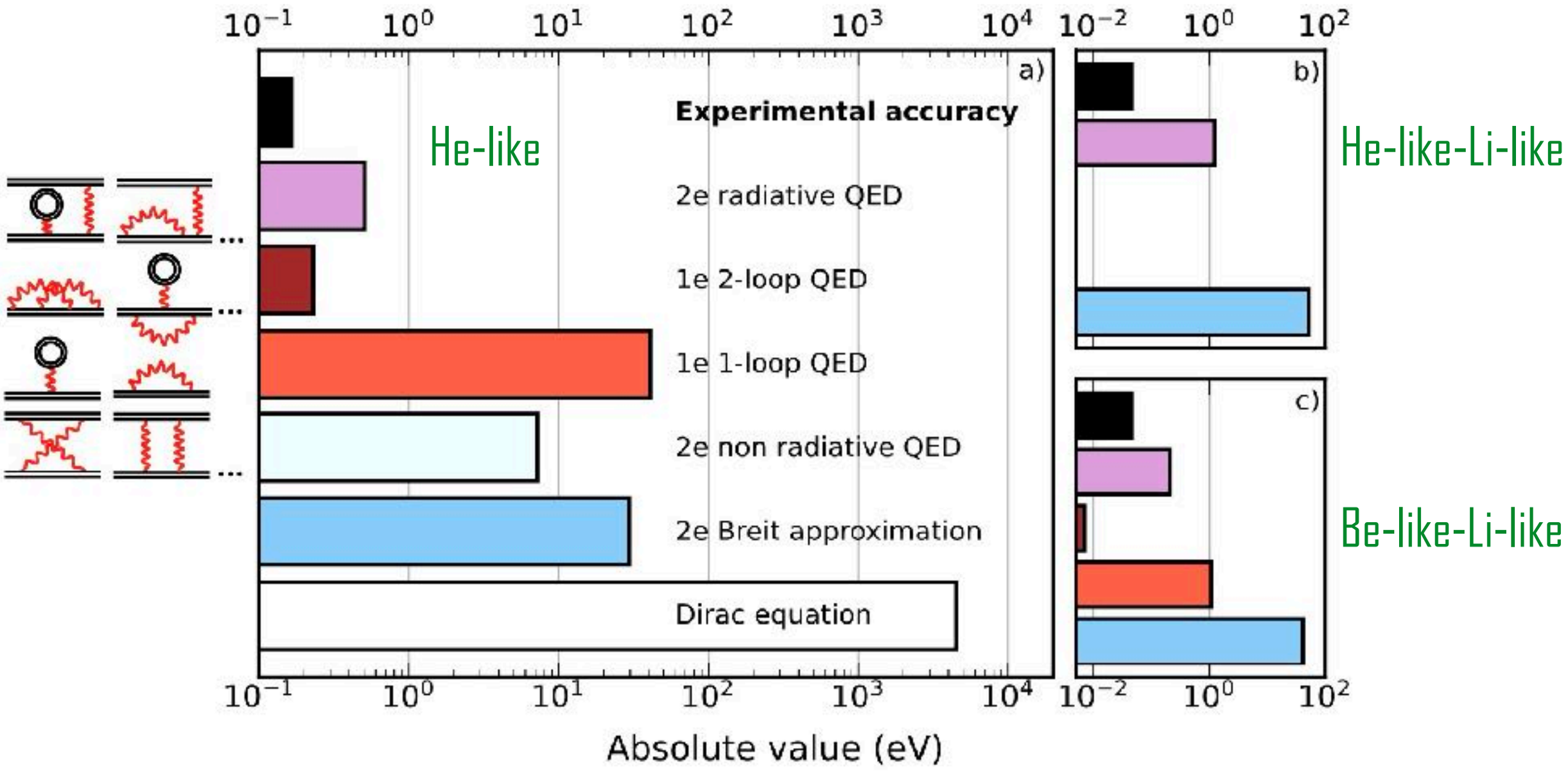


triples to 8k
accuracy reached for
correlation orbitals up to 8k
$1s^2$ 2s $^2S_{1/2}$: **21.7k** config.,
102M Coulomb integrals
too many Breit Integrals



<u>triples only to 4f</u>
accuracy reached for
correlation orbitals up to 7i
$1s^2$ 2s2p $^1P_1$: **9.1k** configurations,
17.4M Coulomb integrals
3.6M many Breit Integrals

Contributions

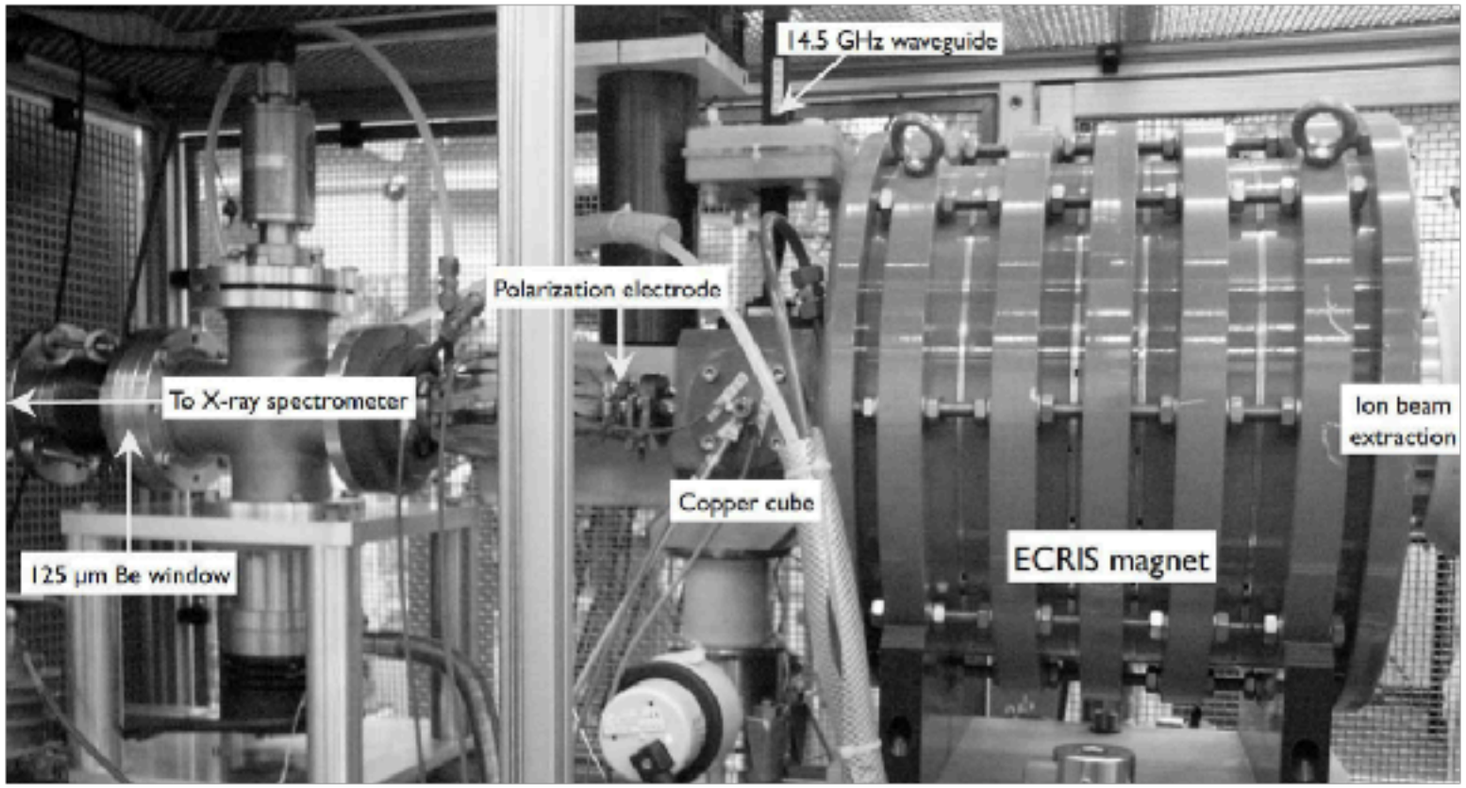


Medium-Z few-electron ions

Reference-free measurements in 2-5 ions

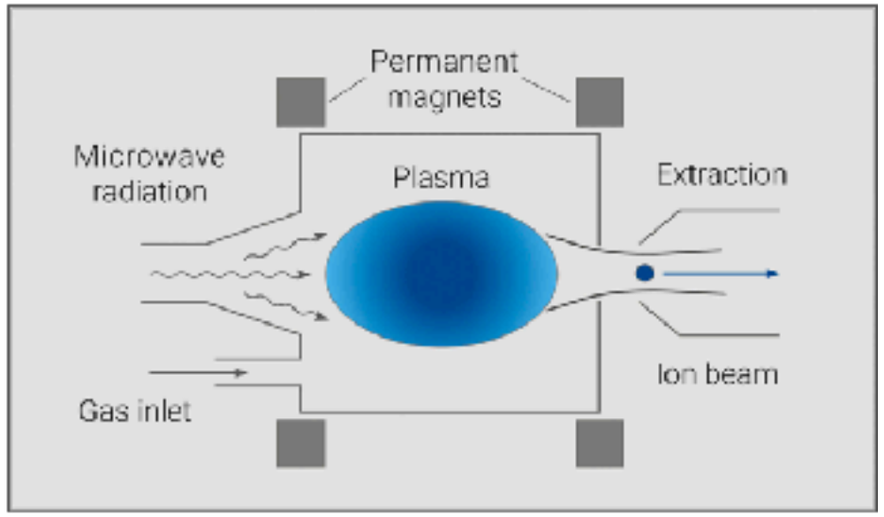
comparison with theory and astrophysics benchmarks

The Source "SIMPA" for highly-charged ion production



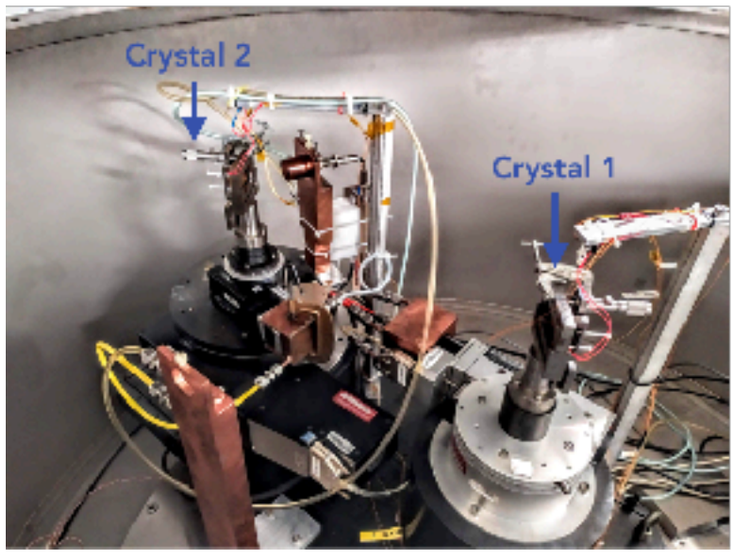
Microwaves : 14.5 GHz

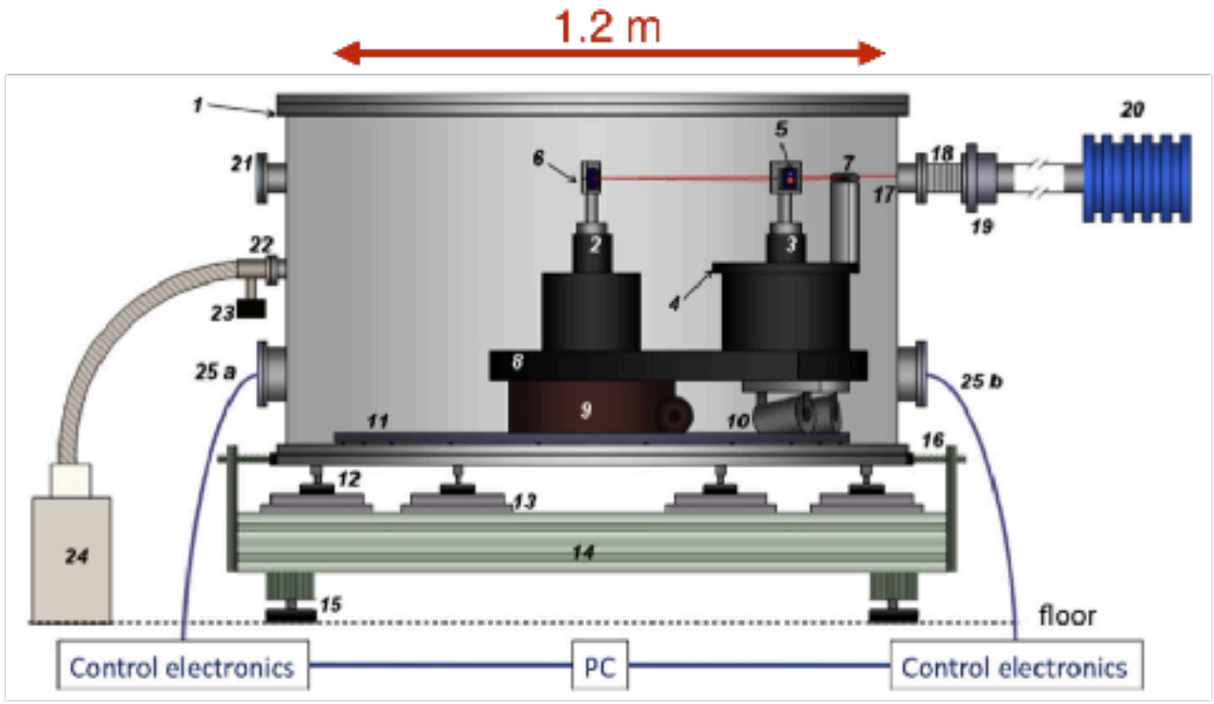
Extraction voltage: 0 V to 25 kV



- Direct connection to plasma, 50µm thick Be window
- In the plasma the ions are trapped in the space charge of the electrons (~10^{11} e^-/cm^3), ~ few eV trapping depth
- Intense source, provides access to forbidden transitions, narrow linewidths

The Paris Double Crystal Spectrometer

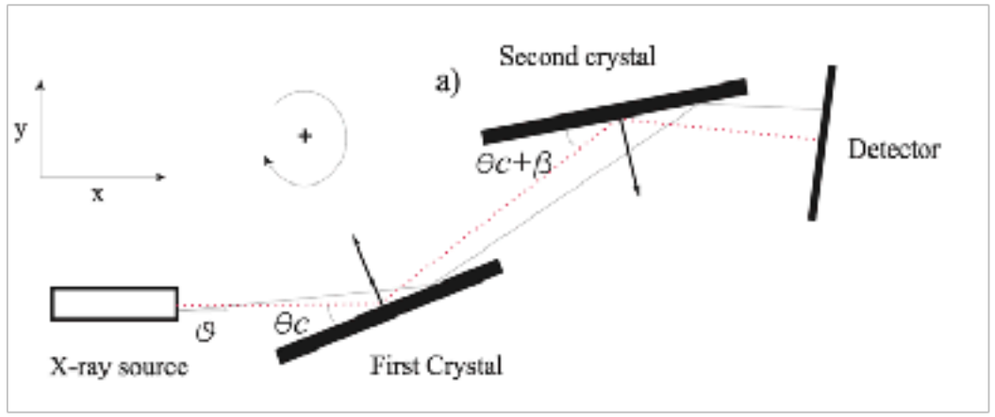


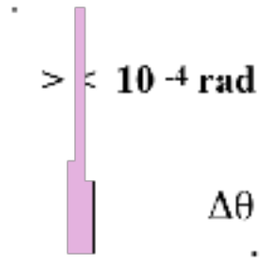


- Si_{111} crystals from NIST, lattice spacing (d) known to 10^{-8}
- Angular encoder for second axis: Heidenhain RON 905 with AWE 1024 interpolator →0.2" of arc angular accuracy
- Detector : LAAPD (large area avalanche photodiode) cooled at -10°C

The Paris Double Crystal Spectrometer

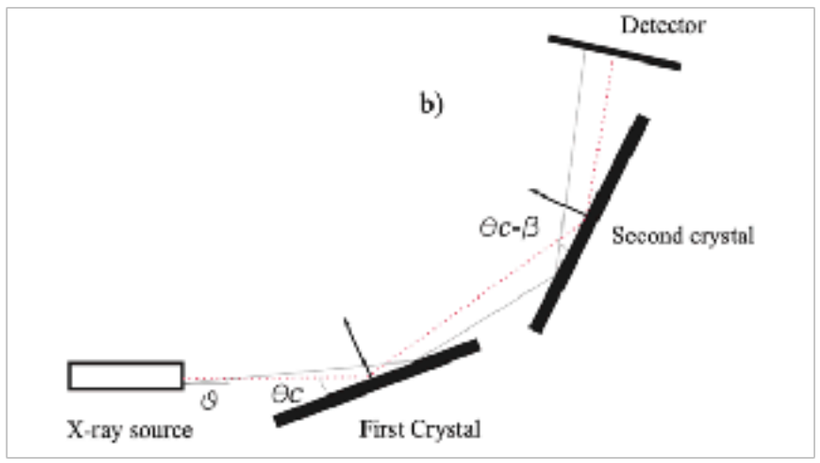
Parallel
Energy
Non-dispersive

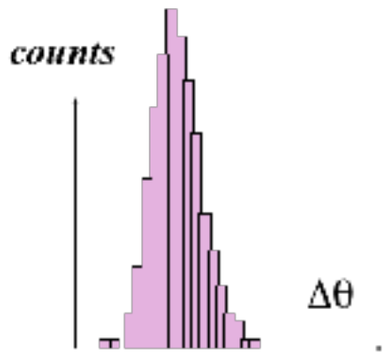




width :
DCS response function

Antiparallel
Energy Dispersive

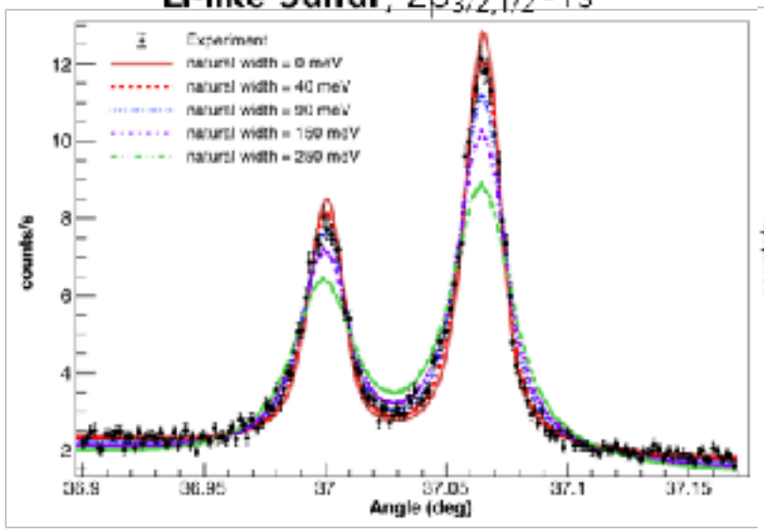




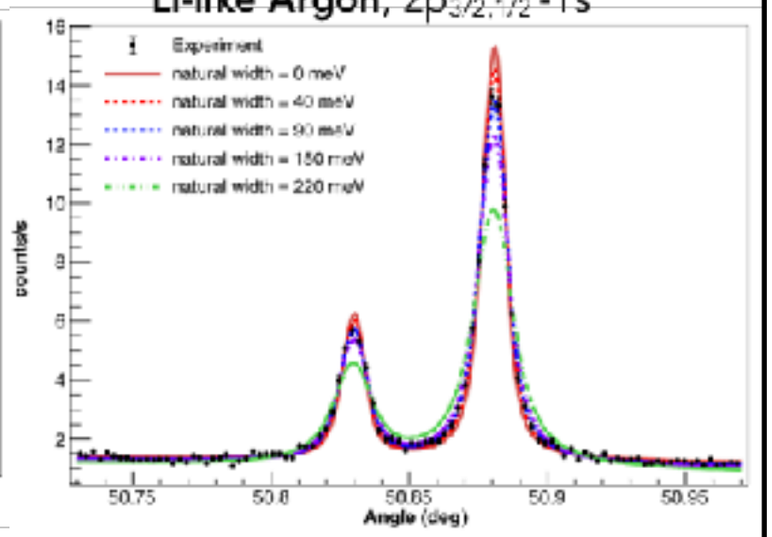
width :
intrinsic line width
Doppler broadening
DCS response function

DCS Recent Results

Li-like Sulfur, $2p_{3/2,1/2}$ -1s



Li-like Argon, $2p_{3/2,1/2}$ -1s

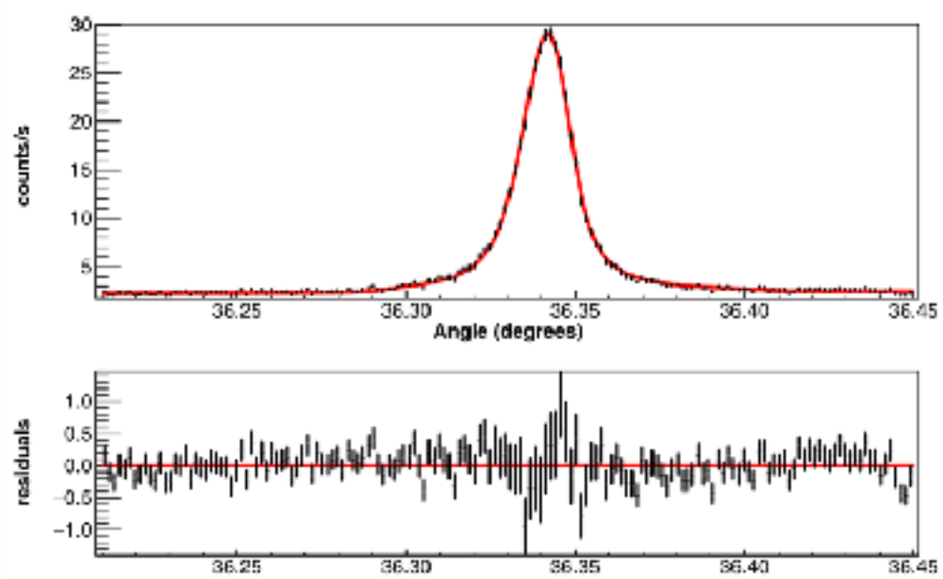


Highest precision, reference-free measurements in core-excited Li-like ions

Sulfur peak ratio : 0.46 [theory], 0.627(22) [exp]
Argon peak ratio : 0.44 [theory], 0.397(14) [exp]
Cannot be explained by known contaminant lines

J. Machado, G. Bian, N. Paul, et al,
PRA 101, 062505 (2020)

He-like Sulfur



First ppm measurements of the relativistic magnetic dipole transition in He-like S

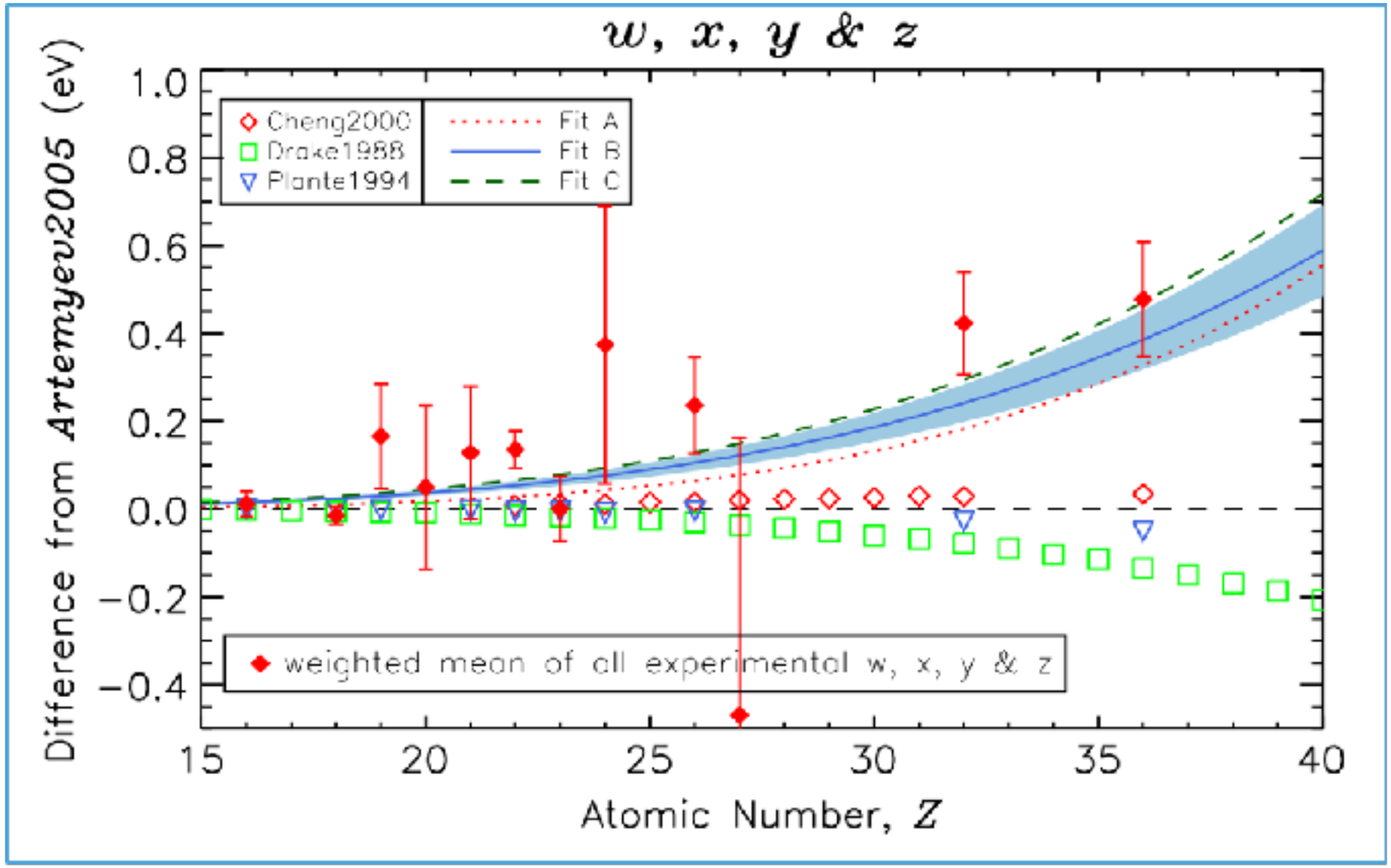
Test of 2e QED effects, sensitive to crystal form factors

J. Machado, N. Paul, et al,
PRA 107, 032821 (2023)

Comparison theory-experiment for He-like ions

$n=2 \rightarrow n=1$

Z^4 dependence claimed for fit B

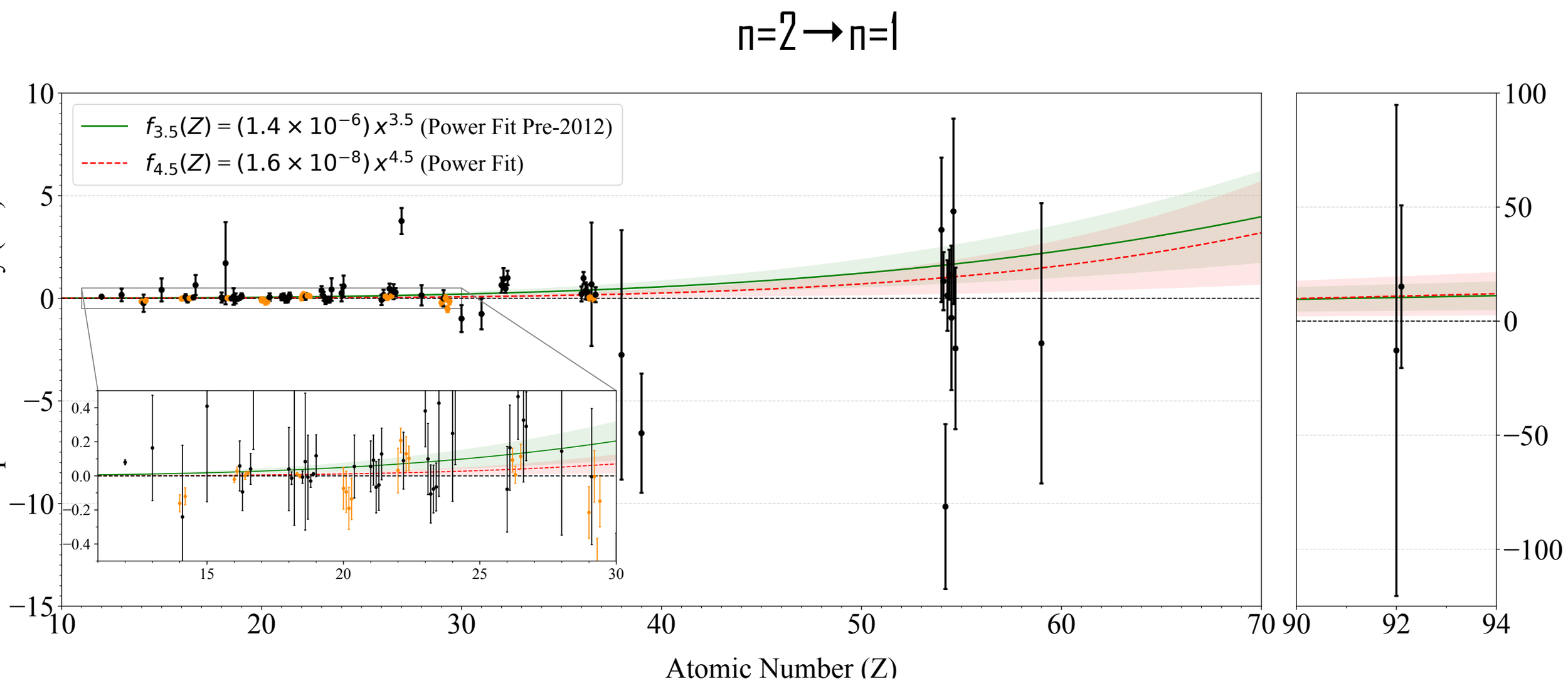


deviation at
Z=92 ~16.8 eV

C T Chantler et al. 2014 New J. Phys. 16 123037

C T Chantler et al. 2014 New J. Phys. 16 123037

Comparison theory-experiment for He-like ions



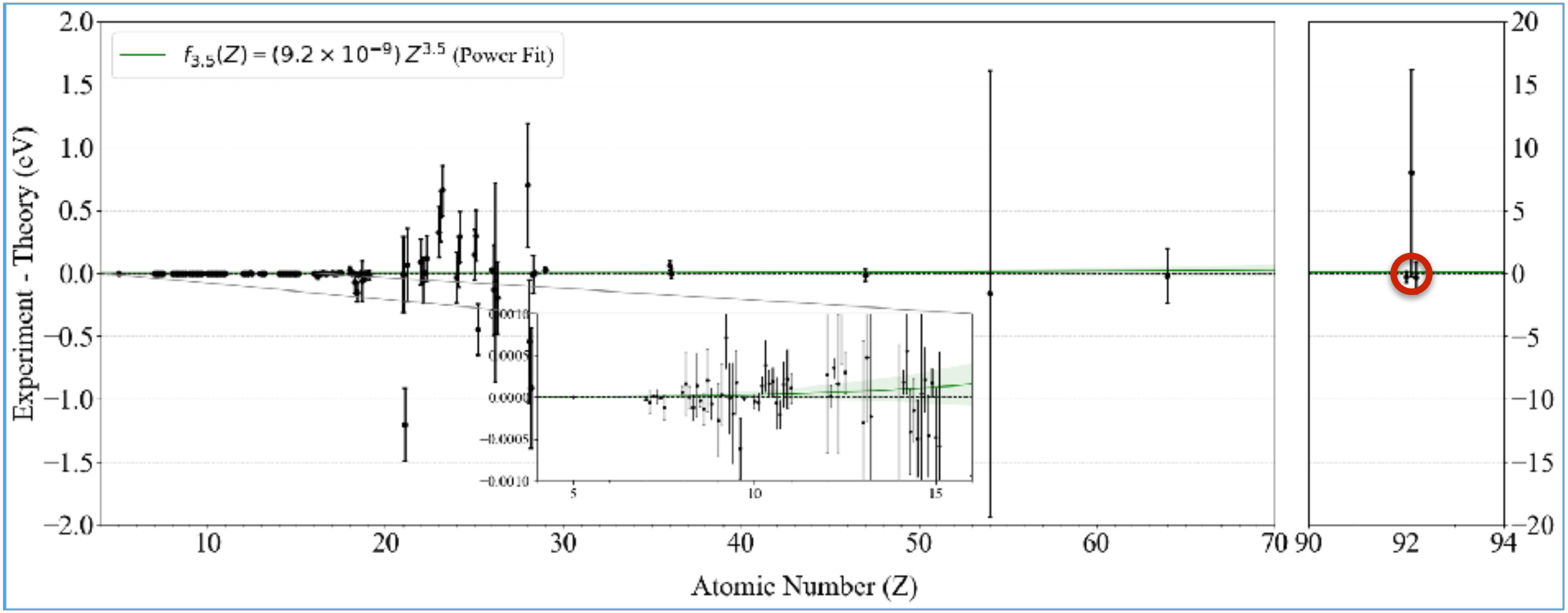
with new measurements (LKB DCS, MPIK Heidelberg, Livermore) reduced deviation

next improvement: He-like U improved (analysis in progress)

C. Godinho, J. Machado, N. Paul, M Guerra, P. Indelicato and M. Trassinelli (2023, unpublished)

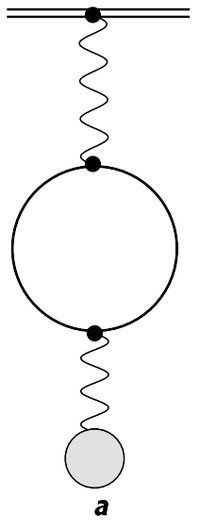
Comparison theory-experiment for He-like ions

$\Delta n=0$



weak constraint on 5th force

particle of charge: ϵq_e and mass μ

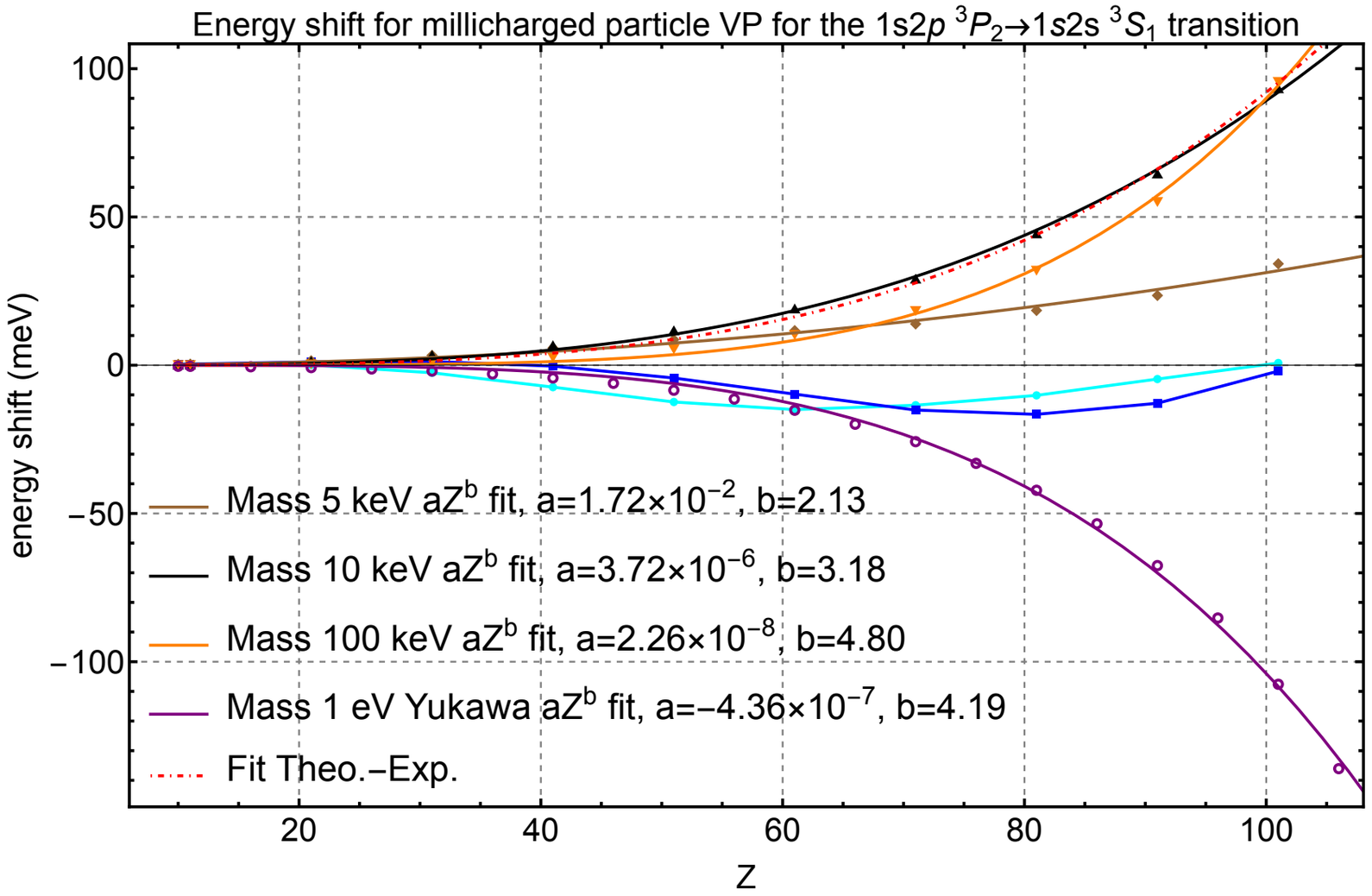


Uehling approximation

creation of a virtual pair m_{μ^+} m_{μ^-}

Comparison theory-experiment for He-like ions

Δn=0 constraints on dark matter interactions



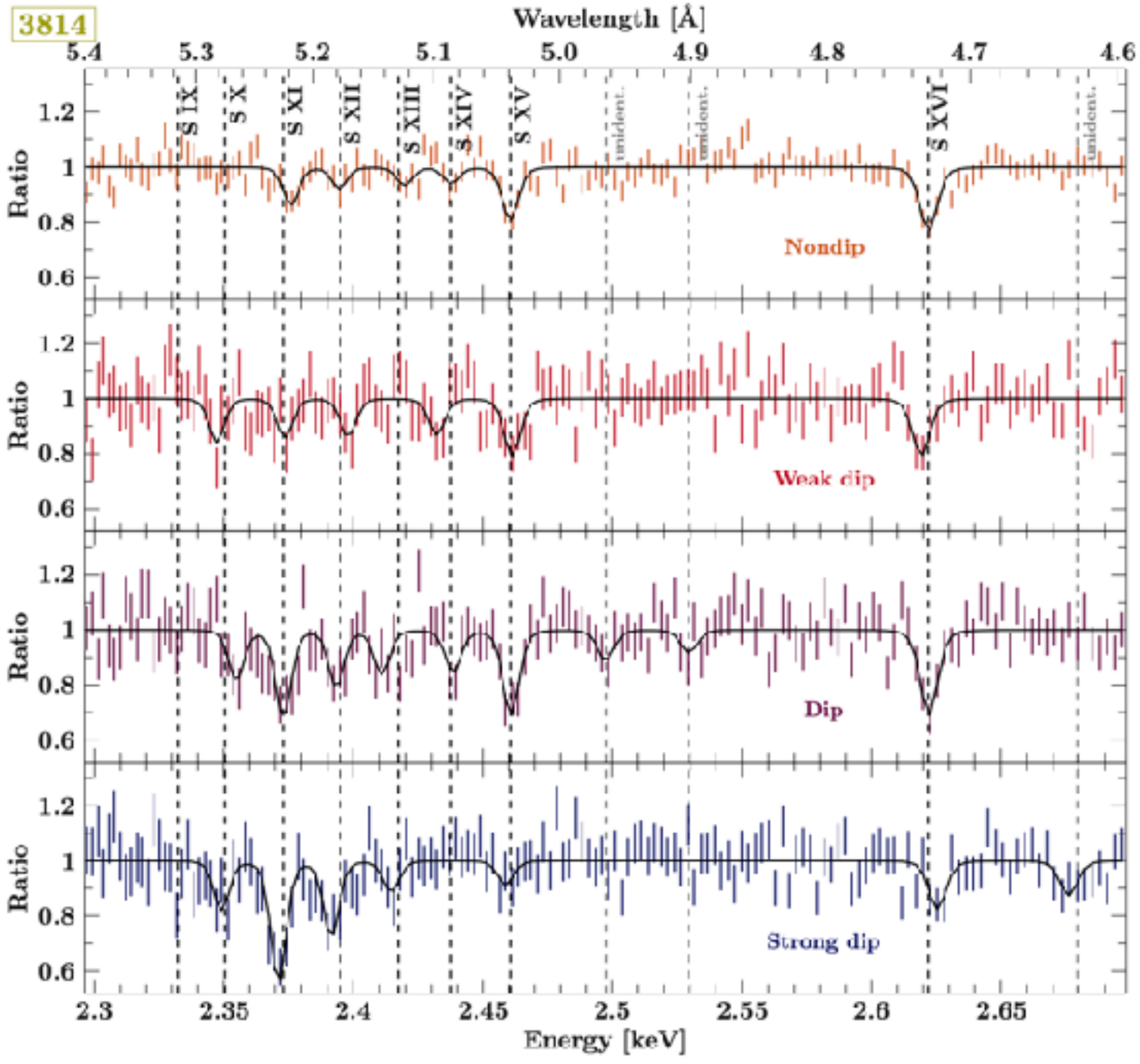
- milliCharged Particle mass 1 keV, q=$10^{-3}q_e$
- milliCharged Particle mass 2 keV, q=$10^{-3}q_e$
- milliCharged Particle mass 5 keV, q=$10^{-3}q_e$
- milliCharged Particle mass 10 keV, q=$10^{-3}q_e$
- milliCharged Particle mass 100 keV, q=$10^{-3}q_e$
- Yukawa boson mass 1 eV, $q_Y q_e$=0.2

Few-electron ions for astrophysics

Laboratory astrophysics

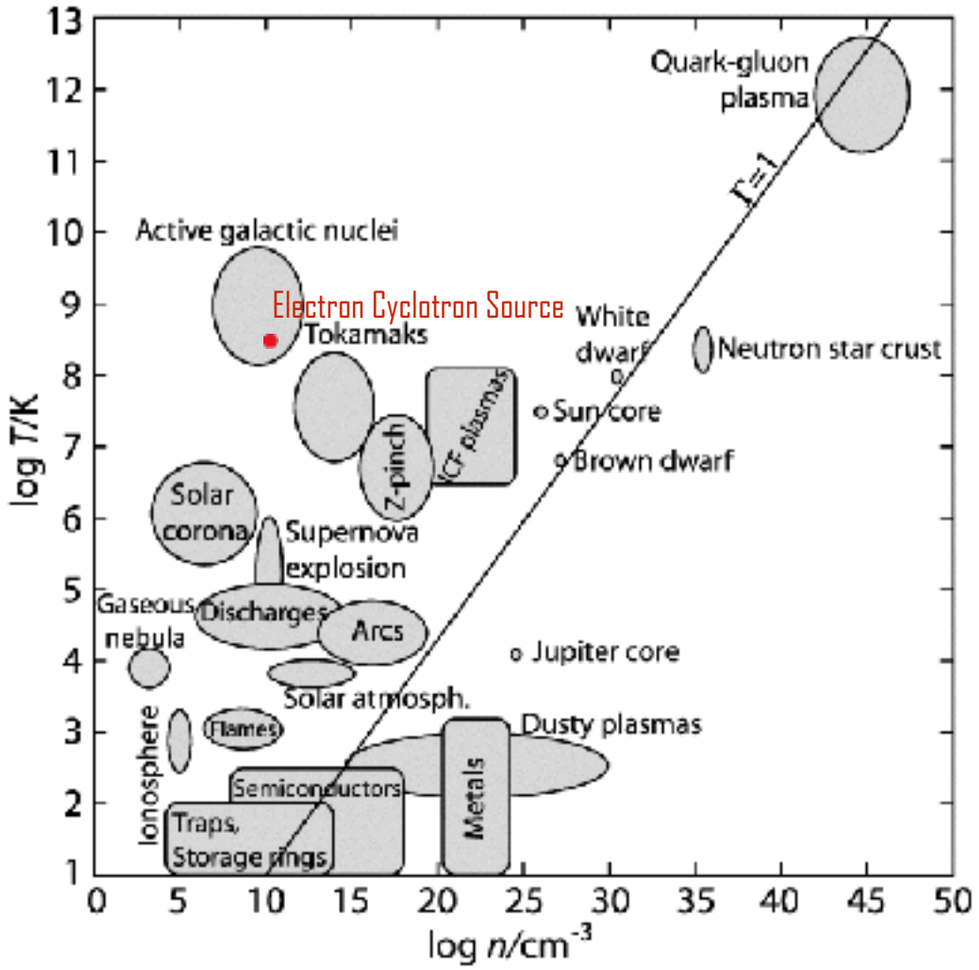
Sulfur in astrophysics

- Absorption or emission of sulfur
- black hole binary Cyg X-1/ HDE 226868
- Bumps or holes are signatures from inhomogeneities in temperature and densities in the stellar wind powered by the accretion



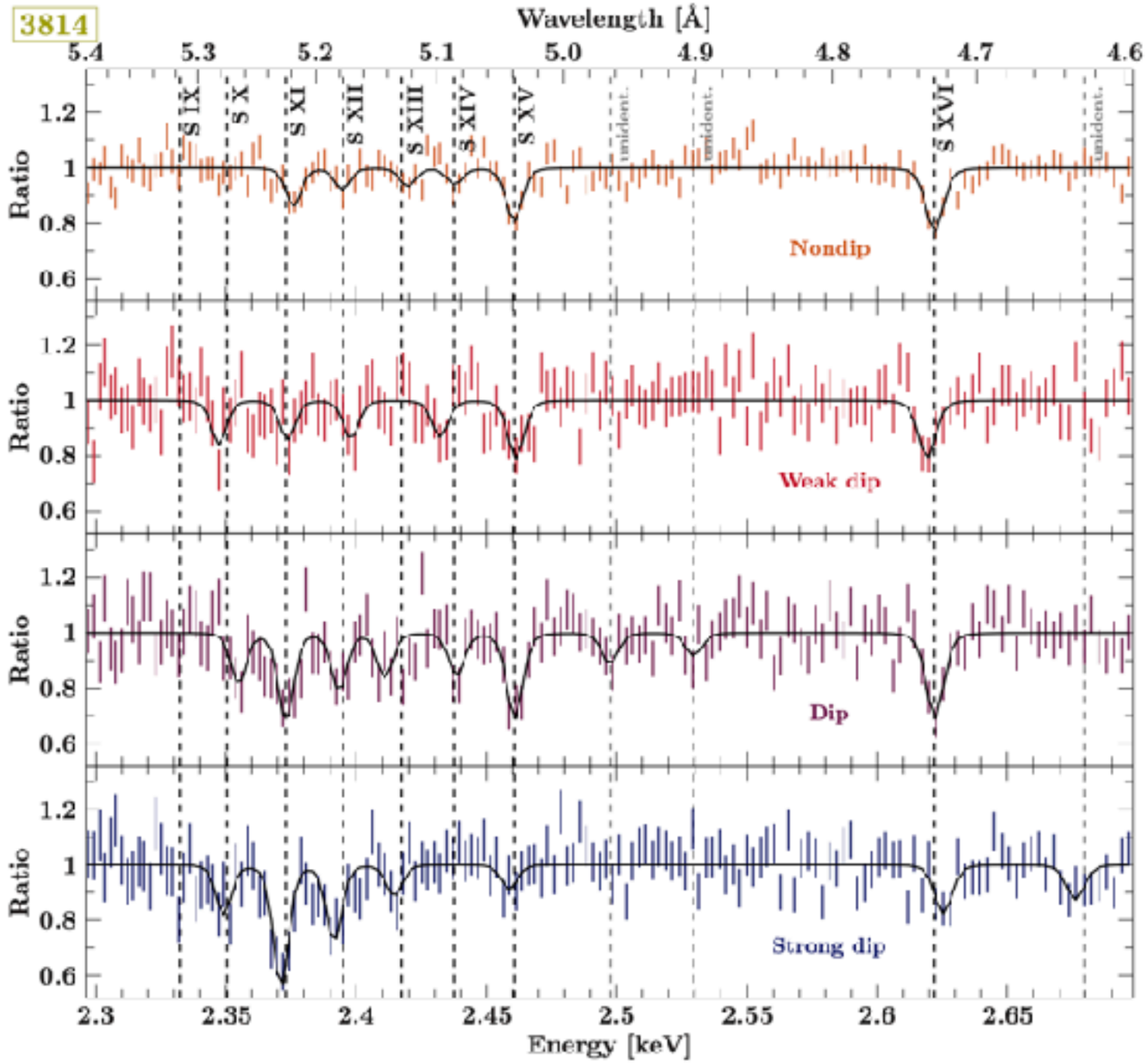
M. Hirsch, N. Hell, V. Grinberg et al, A&A 626, A64 (2019)

Sources of Highly Charged Ions



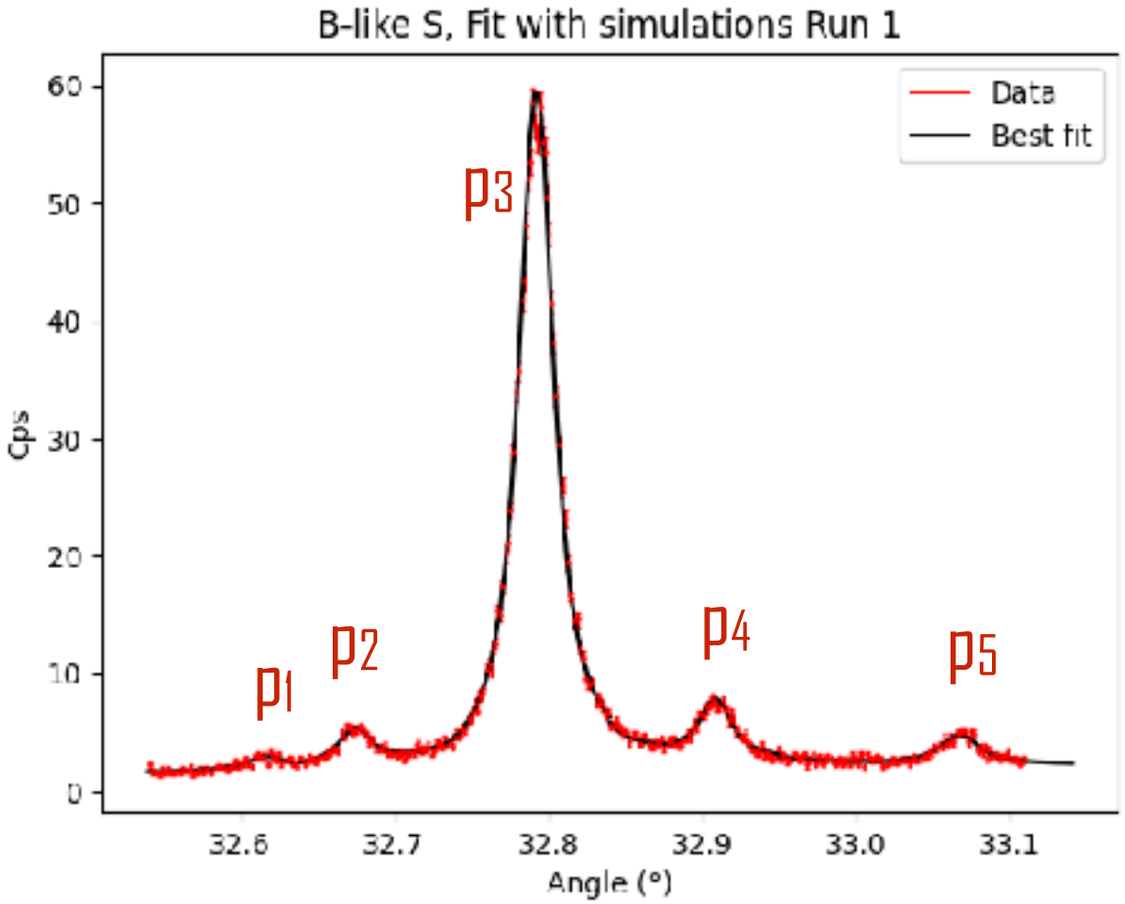
Temperature and electron densities of different plasmas

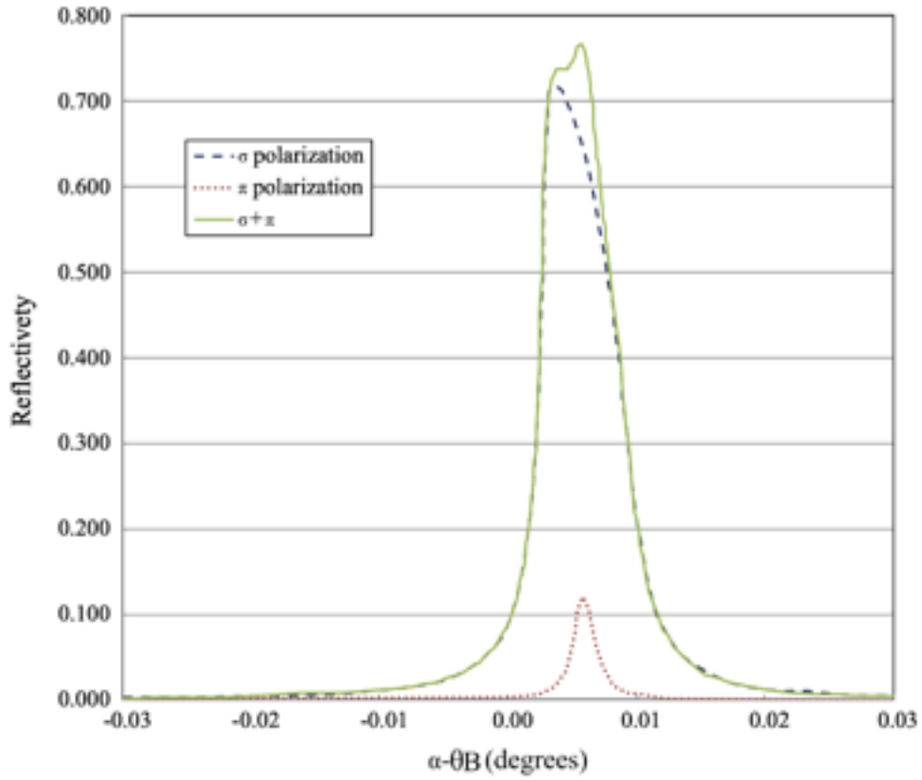
Donkó, Hartmann and Kalman. (2007). Strongly Coupled Plasma Liquids.



M. Hirsch, N. Hell, V. Grinberg et al, A&A 626, A64 (2019)

B-like S



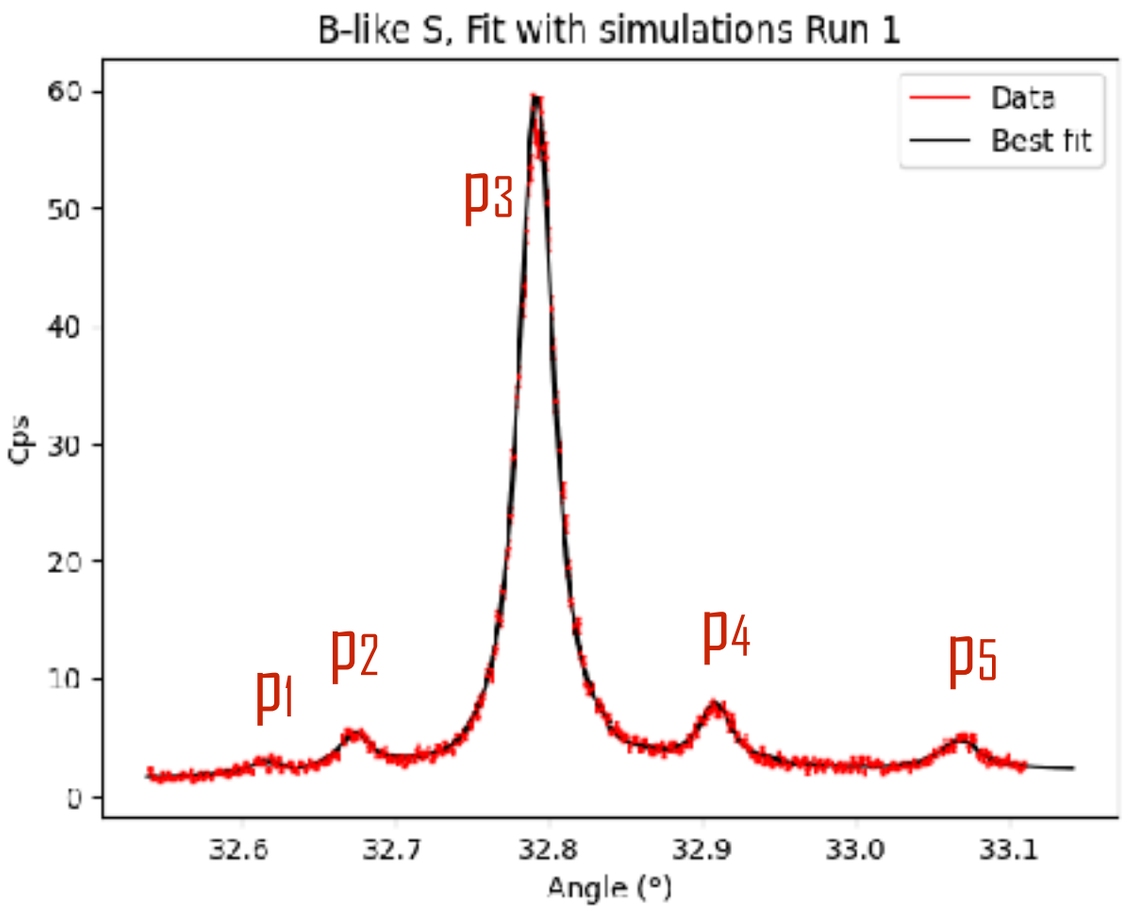


Bayesian evidence suggests only a single peak for the large one

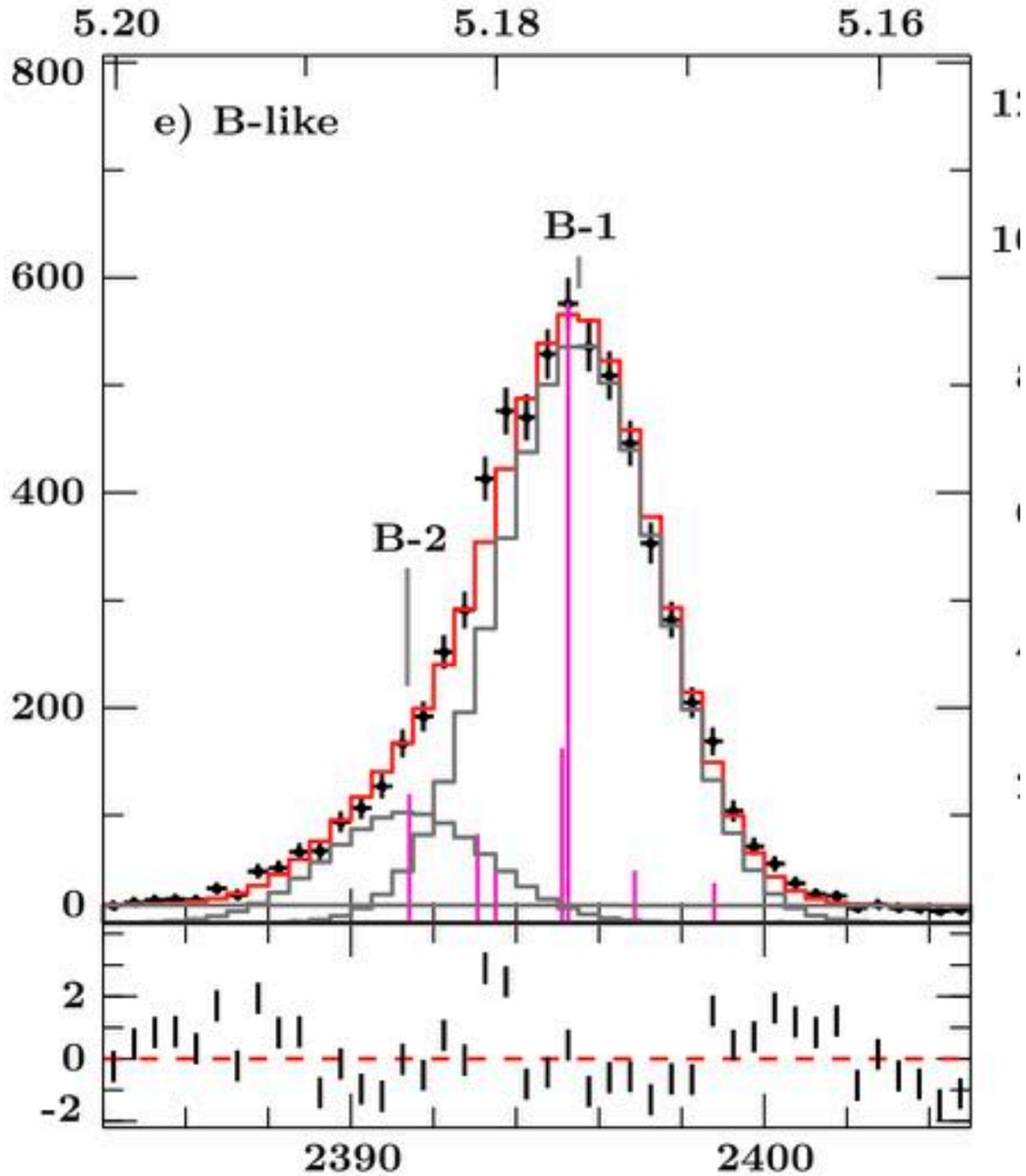
Bayesian analysis to determine the number of components in each peak.

Louis Duval, Jorge Machado, Martino Trassinelli, Nancy Paul, Paul Indelicato

B-like S



2392.9 eV 2395.5 eV 2399.4 eV



LABORATORY MEASUREMENTS OF THE K-SHELL TRANSITION ENERGIES IN L-SHELL IONS OF SI AND S, N. Hell, G.V. Brown, J. Wilms et al. The Astrophysical Journal 830, 26 (2016). using NASA/GSFC Calorimeter ~4.5 eV resolution

B-like S

Table run per run:

peak	energy (eV)	width (meV)
p1	2392.979(11)	456(35)
p2	2393.778(4)	156(46)
p3	2395.462(5)	182(8)
p4	2397.128(4)	153(25)
p5	2399.405(9)	136(17)

each spectrum analyzed independently
weighted averaging

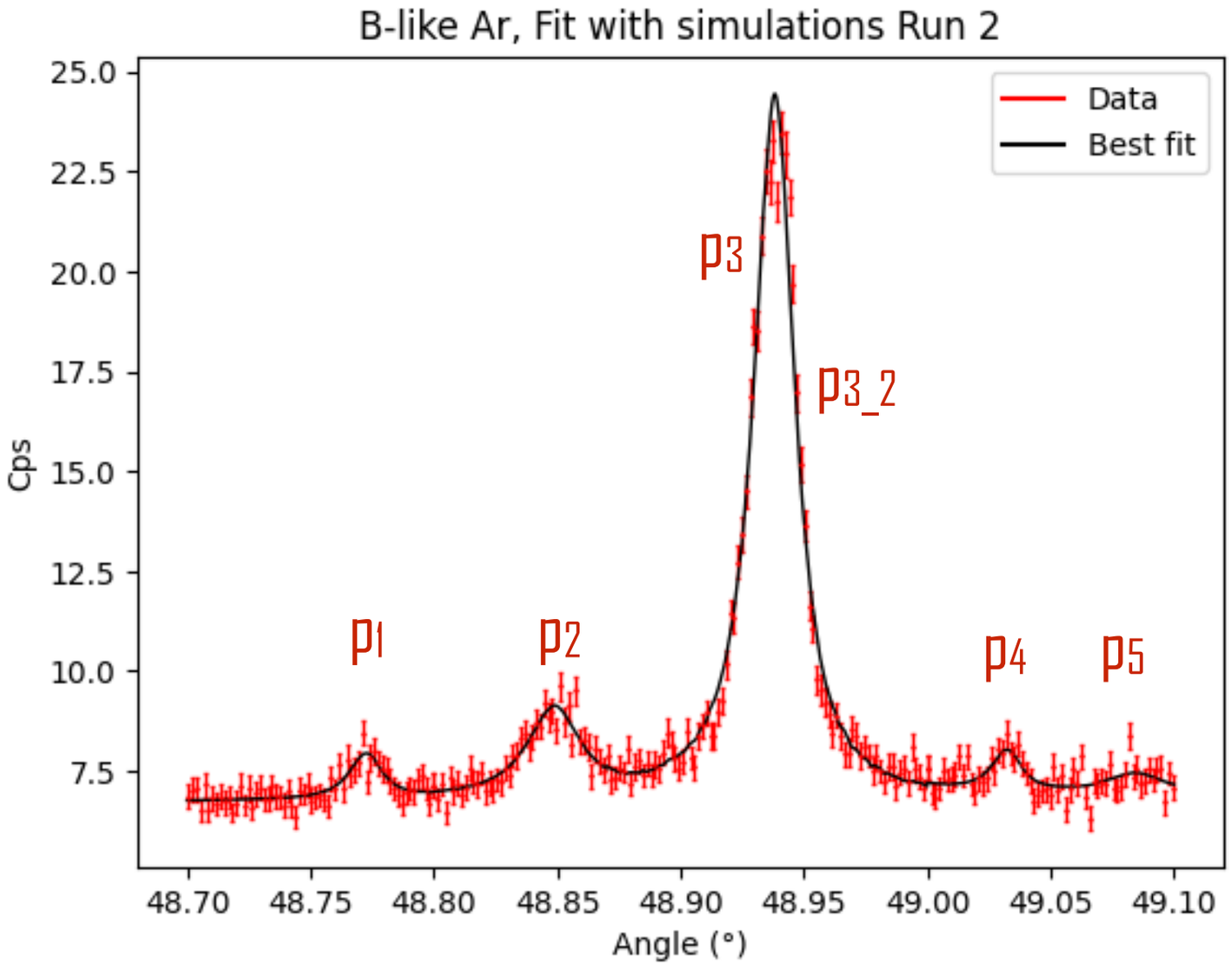
Table with sets:

peak	energy (eV)	width (meV)
p1	2392.940(11)	256(35)
p2	2393.778(4)	154(30)
p3	2395.462(5)	192(3)
p4	2397.126(4)	140(17)
p5	2399.405(7)	208(28)

all spectra fitted together

Louis Duval, Jorge Machado, Martino Trassinelli, Nancy Paul, Paul Indelicato

B-like Ar



Bayesian evidence suggests two lines for the large peak

	peak	energy	sd_energy	amp	sd_amp	gamma	sd_gamma
0	p1	3059.495258	0.052857	0.027862	0.031746	0.104780	0.000005
1	p2	3062.055544	0.025286	0.119467	0.123285	0.351441	0.000008
2	p3	3064.730654	0.010460	0.352798	0.259878	0.241471	0.000002
3	p3_2	3064.999118	0.015824	0.093331	0.224209	0.156352	0.000002
4	p4	3067.783640	0.282822	0.030394	0.117646	0.208913	0.000052
5	p5	3069.349237	0.093624	0.110213	0.146690	0.571780	0.000048

Theory becomes very challenging!

- Example: $1s\ 2s^2\ 2p^2\ {}^2P_{1/2}$
  - 40 000 configurations with single, double and triples excitations up to n=5
  - 141 Million Coulomb Integrals
  - obliged to neglect non-diagonal Breit integrals
  - new 2TB machine to test larger cases
- Convergence:
  - In many cases convergence is hard or impossible up to now up to even n=4, because of the presence of up to 4 simultaneous holes
  - even worse for $1s\ 2s\ 2p^3$ level
- Line identification
  - p5 peak for S not identified yet
  - Ar seems OK within the calculation accuracy

Understanding the plasma and cascade processes

- Role of excitation process in the ECRIS plasma?
  - ions are normally in their ground state
  - B-like level $1s\ 2s^2\ 2p^2$ hole created by 1s ionization of C-like ions
  - what about $1s\ 2s\ 2p^3$? ionization and excitation? Ionization+Auger from N-like?

Exemple X-IFU simulations

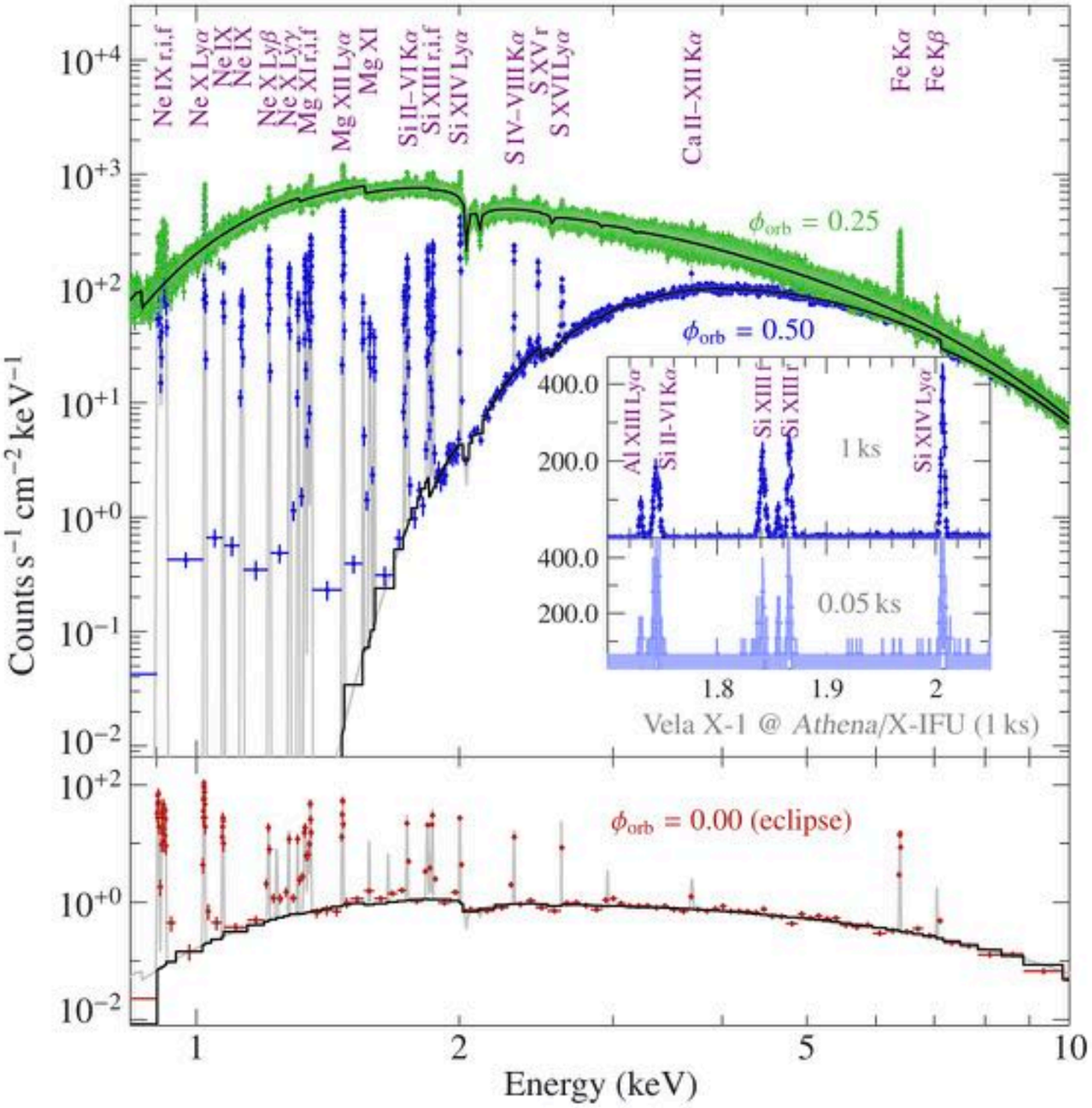


FIGURE 1 Simulations of 1-ks observation with Athena X-IFU of the HMXB Vela X-1 at three orbital phases. The inset compares the Si region of the spectra for 1-ks and 50-s exposures

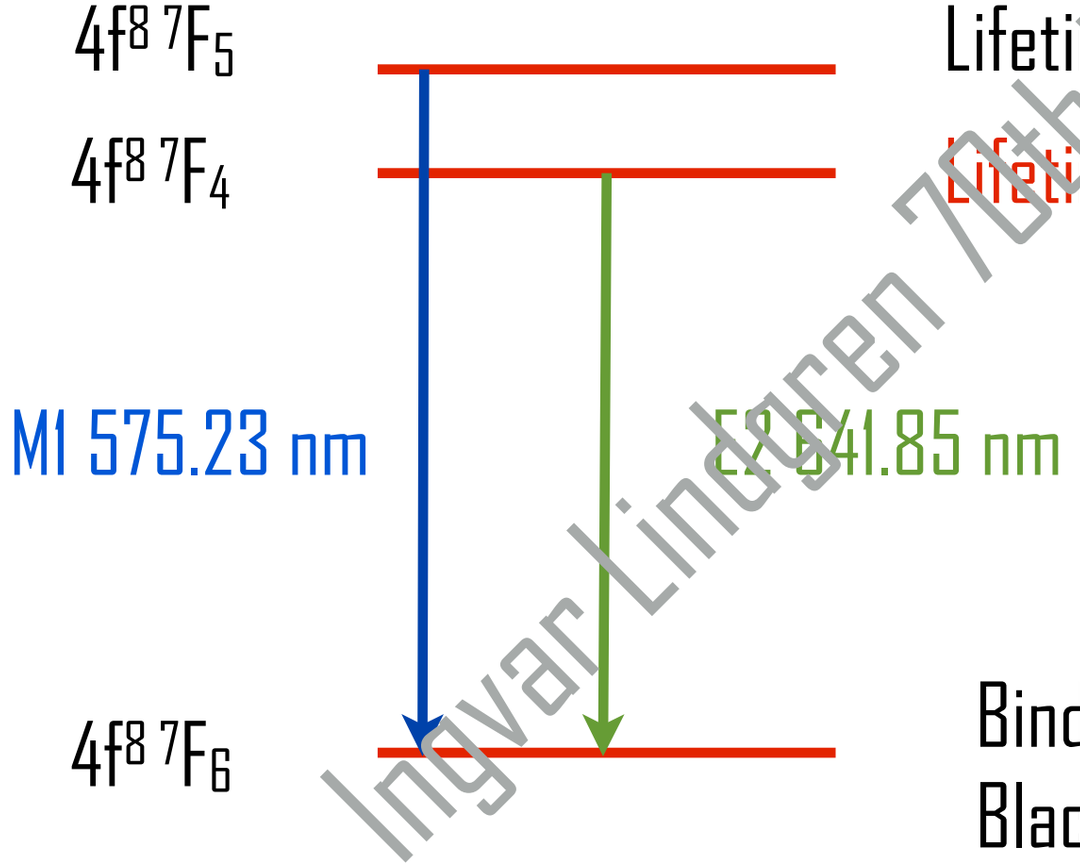
Highly charged ions in a new era of high resolution X-ray astrophysics, N. Hell, P. Beiersdorfer, G.V. Brown et al. X-Ray Spectrometry 49, 218-233 (2020).

Evaluation of long-lived metastable states

Future high-precision atomic clocks?

Example of HCI transition (non HFS)

- Look for reverse level ordering
  - ★Ground configuration of Sm-like ions (62 electrons)
  - ★$_{202}Hg^{18+}$, m/q: 11.2, close to Be^{+} (9)
  - ★Relativity changes the ground state: $4f^8\ ^7F_6$



Binding energy of 4f: 602 eV
Blackbody radiation at 300K: $2.6x10^{-2}$ eV

Other ideas, and uncertainties

Looking at ground state level crossing like 4d-5s ($Z=39, Y^{2+}$), 4f-5s (Nd^{13+})...

J.C. Berengut, V.A. Dzuba, V.V. Flambaum et A. Ong. Phys. Rev. A **86** (2012), p. 022517: "Highly charged ions with E1, M1, and E2 transitions within laser range"

TABLE XI. Scaling dependences for HCIs for various sources of systematic shifts in optical clocks.

Second-order Stark shift	$\sim 1/Z_a^4$
Blackbody shift	$\sim 1/Z_a^4$
Second-order Zeeman shift	suppressed[a]
Electric quadrupole shift	$\sim 1/Z_a^2$
Fine structure	$\sim Z^2 Z_a^3/(Z_{\rm ion}+1)$
Hyperfine A coefficient	$\sim Z Z_a^3/(Z_{\rm ion}+1)$

[a]The Zeeman shift is sensitive to the specific fine and hyperfine structure of the transition, but may be suppressed in HCIs due to a larger energy denominator.

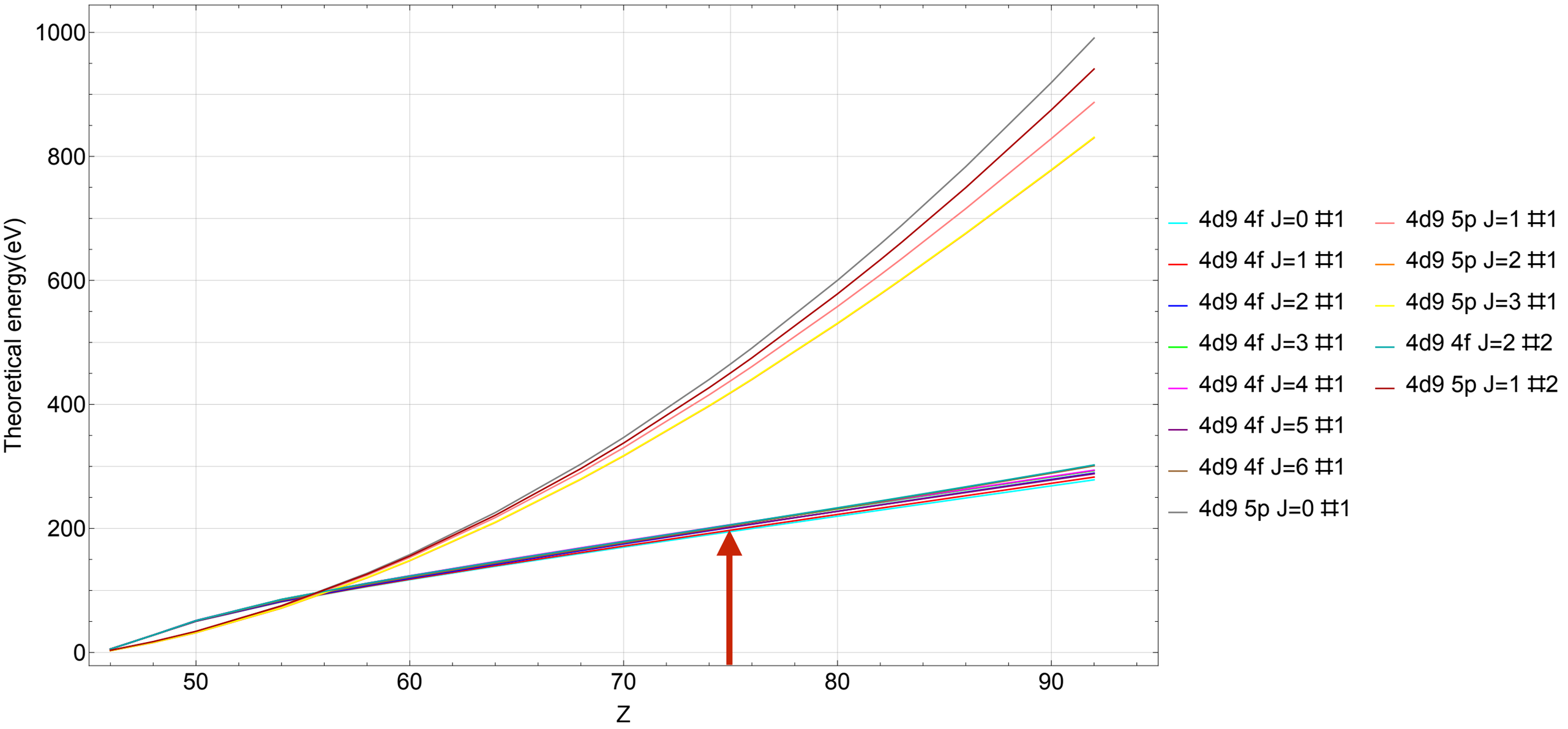
Pd-like ^{187}Re

- Measurement of the total mass to 1 eV accuracy performed for ^{187}Re (Z=75, Pd-like) and ^{187}Os (Z=76, Ag-like) performed with PENTATRAP at the MPIK in Heidelberg (for neutrino mass measurement)
- Pd and Pd-like ions have a closed shell ground state $4d^{10}\ {}^1S_0$
- During the $^{187}Re^{29+}$ measurement, it appeared that around 50% of the time the trapped ion had a different mass
- It soon appeared it was not an experimental problem of some sort
- The measurement time in the PENTATRAP is a couple of hours
- Three methods where independently used to look for possible cases of (very long-lived) metastable states without knowing the value of this mass difference

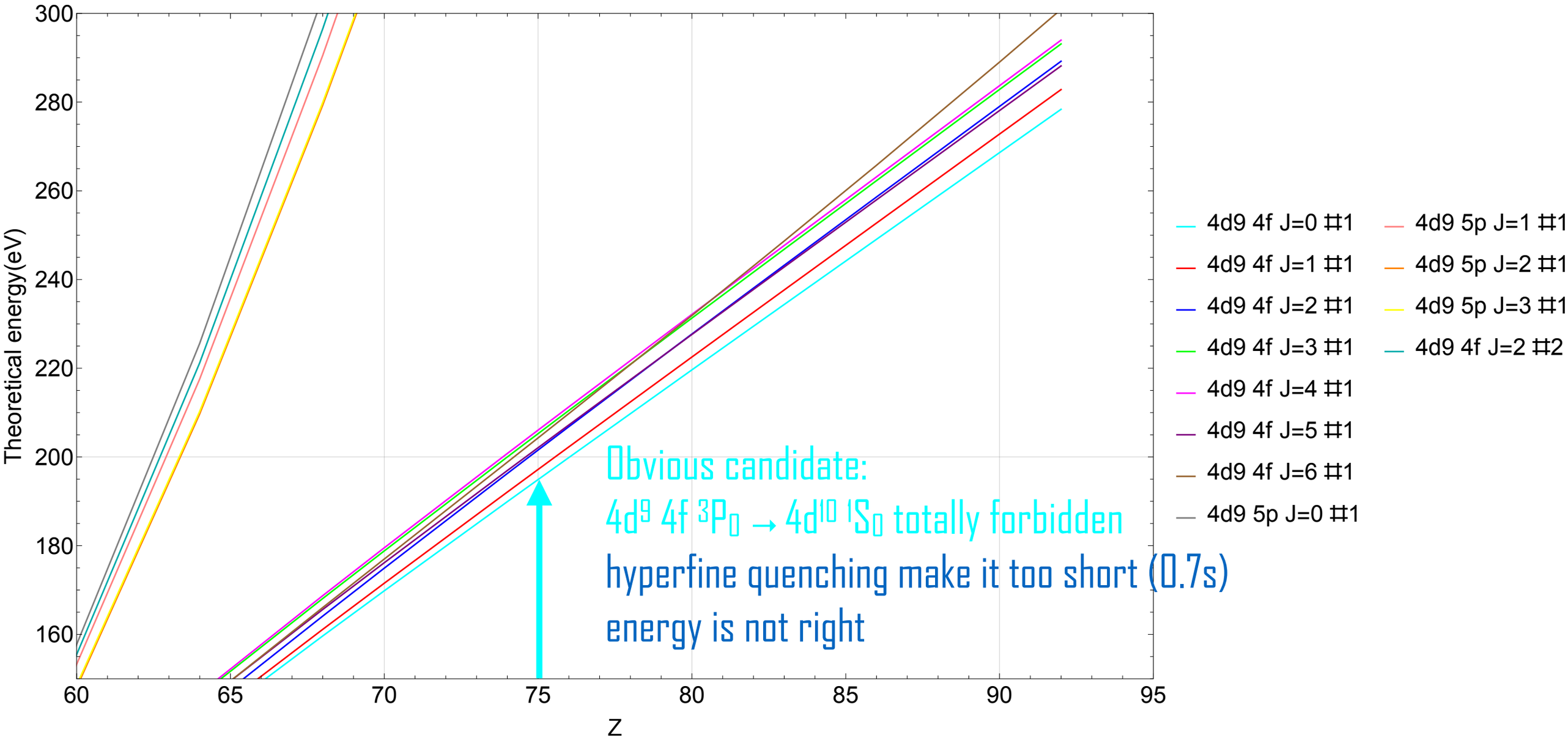
Detection of metastable electronic states by Penning trap mass spectrometry, R.X. Schüssler, H. Bekker, M. Braß et al. Nature 581, 42-46 (2020).

Pd-like ^{187}Re

lower level energies, relative to the $4d^{10}\ {}^1S_0$ ground state

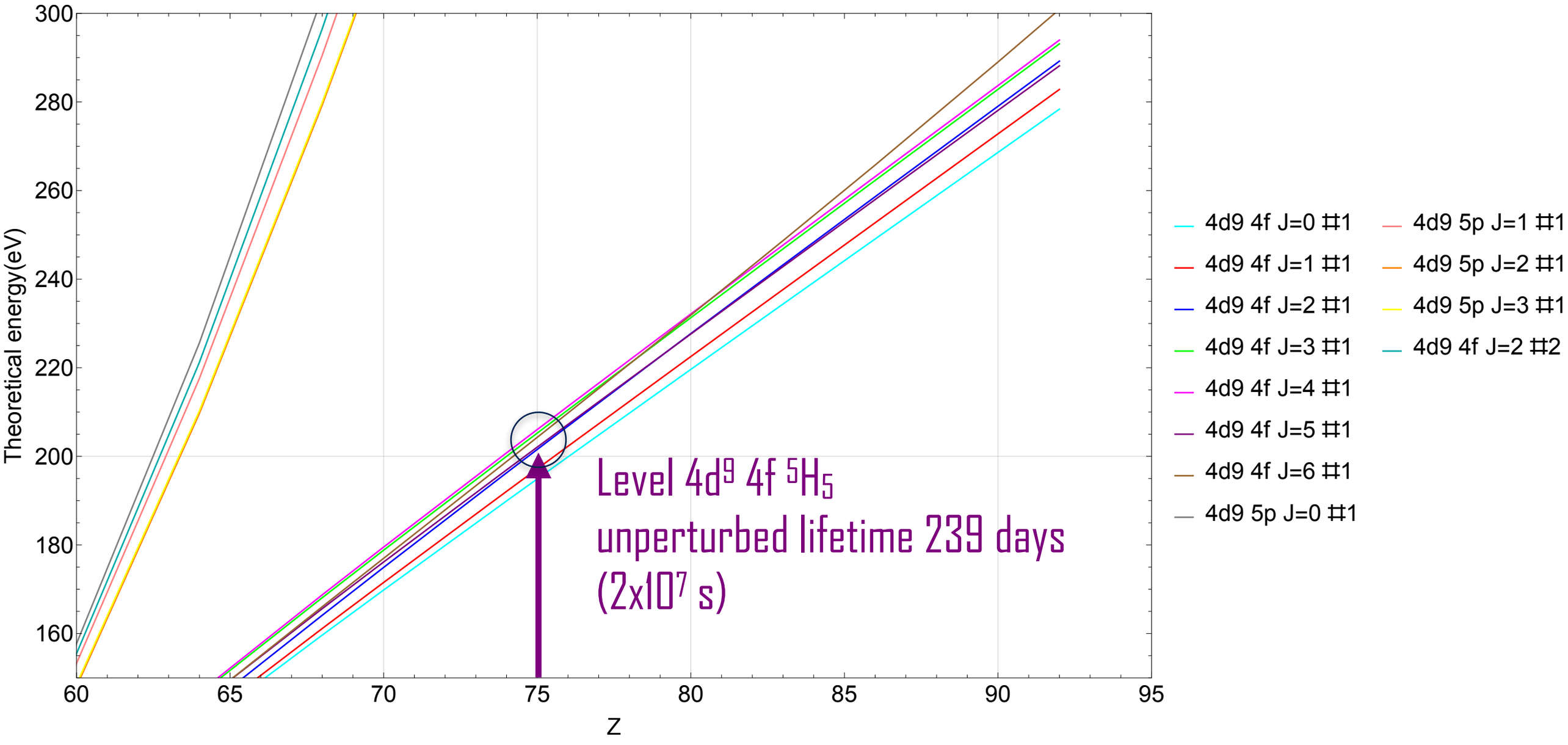


Pd-like ^{187}Re



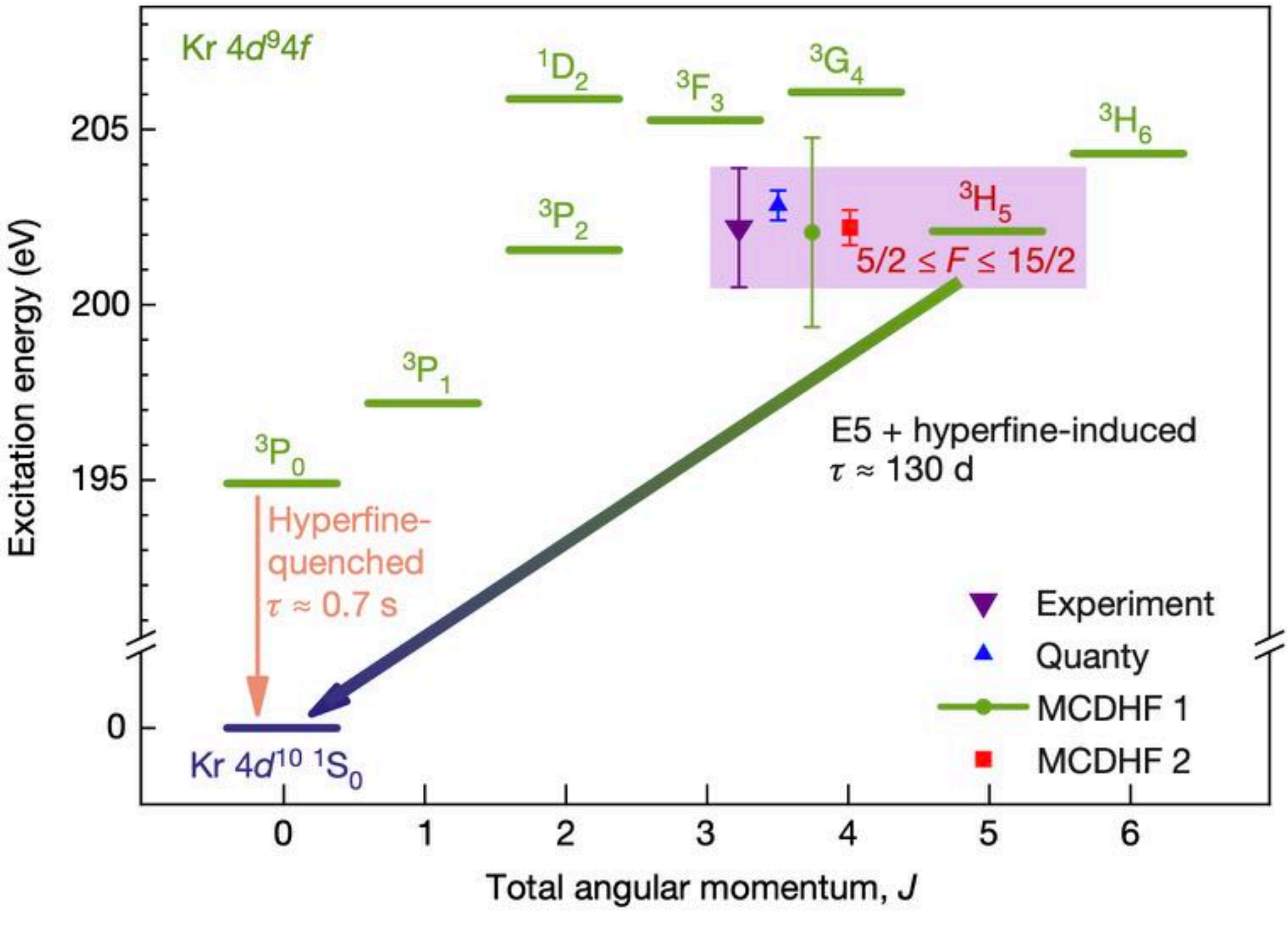
Pd-like ^{187}Re

Pd and Pd-like ions have a closed shell ground state $4d^{10}\ {}^1S_0$



Pd-like ^{187}Re

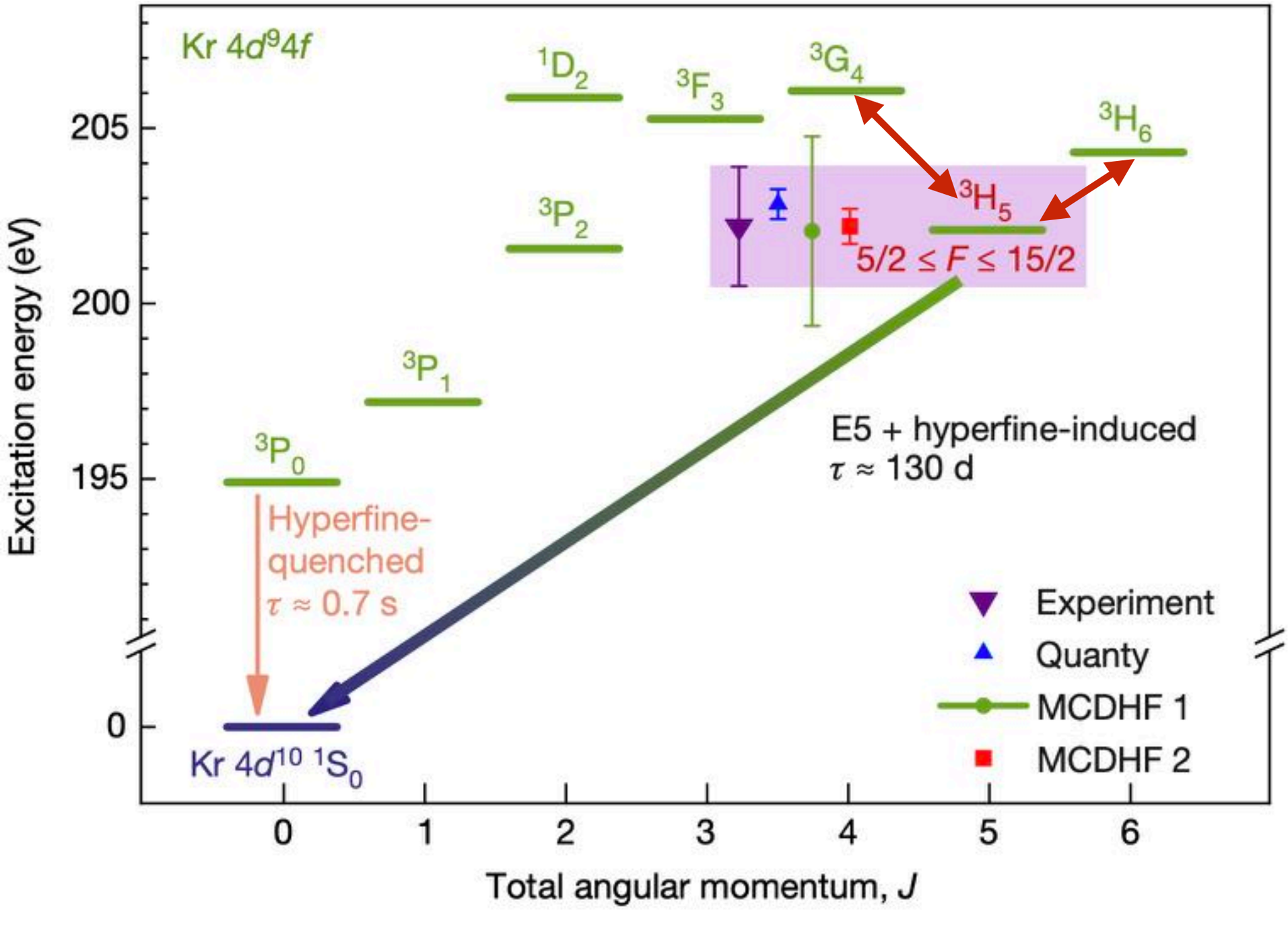
$4d^9\,4f\,{}^3H_5$ unperturbed lifetime 239 days



Pd-like ^{187}Re

$4d^9\,4f\,{}^3H_5$

^{187}Re has a nuclear spin: I=5/2 and a nuclear Q-pole moment

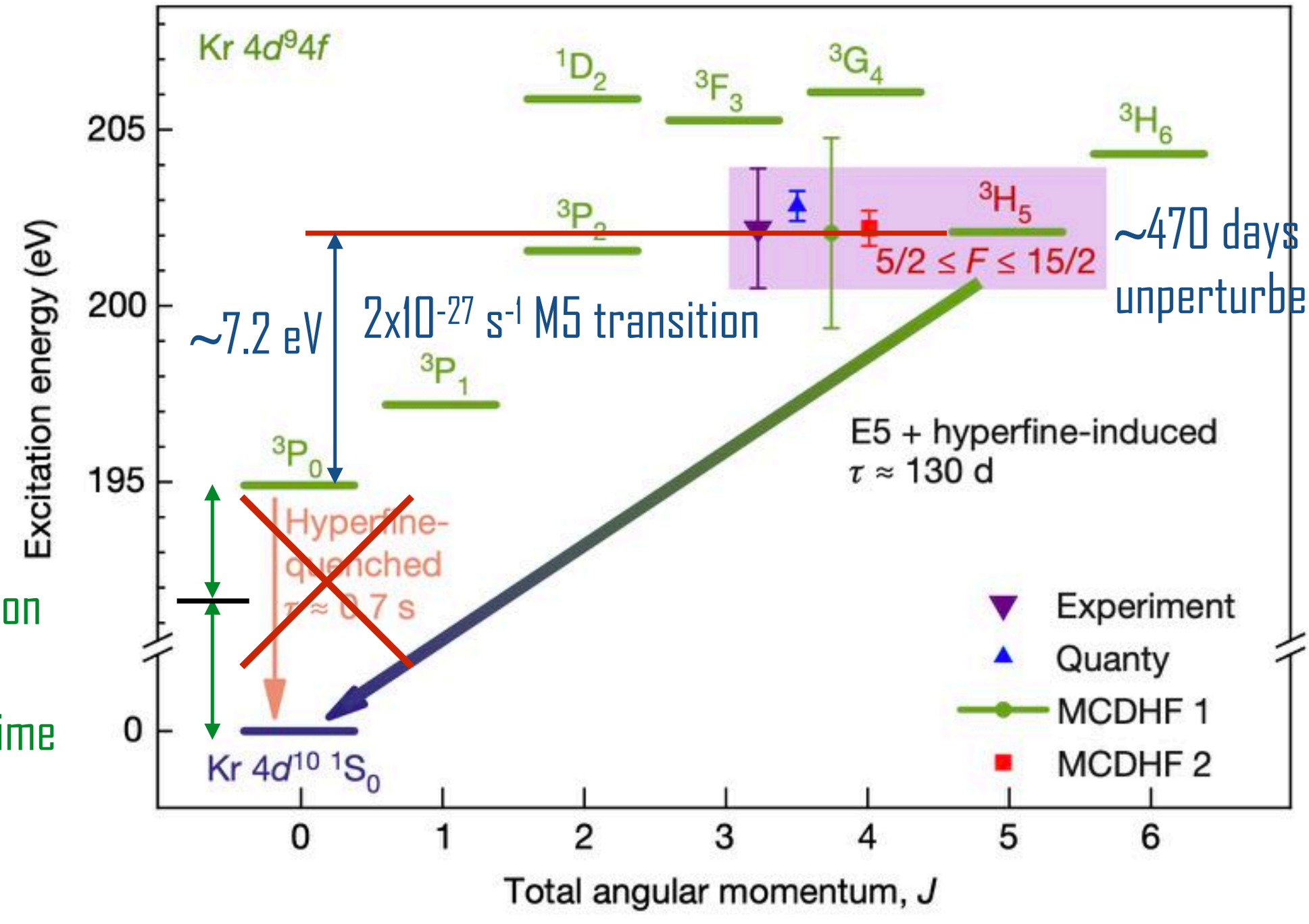


going for Pd-like ^{190}Os?

$4d^9\,4f\,{}^3H_5$

^{190}Os (Z=76) has a nuclear spin I=0 so no hyperfine quenching

^{187}Os: 1.6% abundance, ^{188}Os: 16.1 % abundance, ^{190}Os: 24.6% abundance



two-photon decay ~∞ lifetime

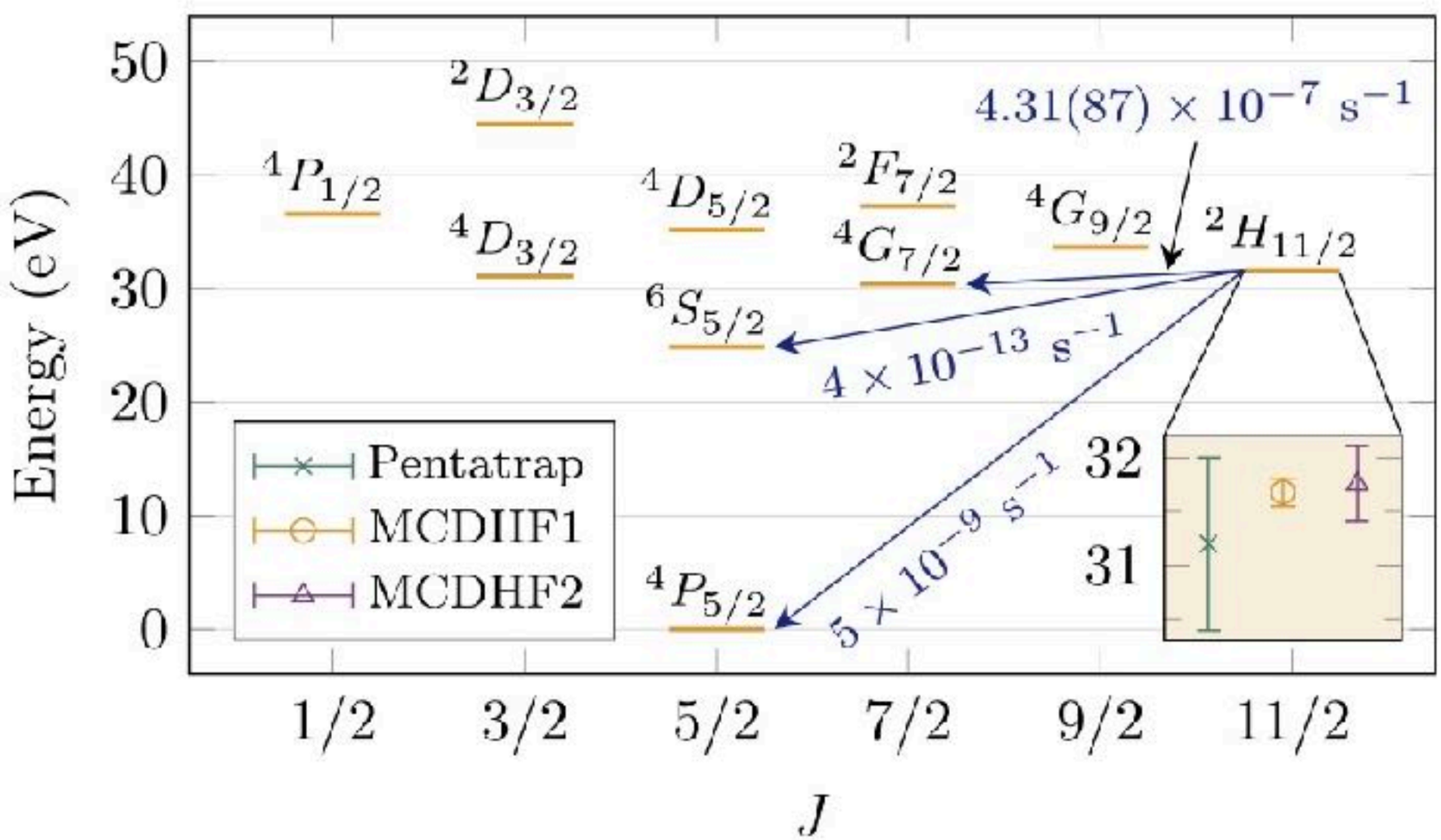
Final result for ^{187}Re and ^{187}Os

- Three different calculations have been performed to check the convergence
  - GRASP 2018* (Zoltan Harman):
    - Layer by layer optimisation
    - excitation of the n=4 orbitals up to 9h
    - **ΔE= 202.2(5) eV**
  - MCDFGME 2020 (PI)
    - smaller set
    - Fully relaxed orbitals
    - Self-consistent magnetic and retardation interaction
    - higher-order QED
    - **ΔE=202.1(27) eV**
  - QUANTY** (M. Haverkort)
    - multi-Slater-determinant states constructed from relativistic Kohn-Sham single-electron orbitals
    - local spin density functional
    - **ΔE=202.41 eV to 203.26 eV**

MCDF issues for $^{187}Re^{29+}$

- $^{187}Re^{29+}$: Pd-like (Z=75, 46 electrons) $[Kr]4d^{10}$ J=0
- total correlation energy double excitations:
  - from 1s to 4f: 472 configurations
  - from 1s to 5g: 4 892 configurations
  - from 1s to 6h: 17 654 configuration. Why not?
    - cannot index all retardation coefficients > 2^{31}-1=2x10^9 integrals =56 Gb memory, integer overflow
    - going to 64 bit (1.7 10^7 TB!) integers will lead to huge computer time for the large cases and require huge RAM to be efficient
    - cannot hold all the coefficients in memory⇒ calculation duration problem…
- limit to excitations from 4s, meaning one assumes inner core orbitals below 4s are weakly affected by the outer shells

Nb-like lead


Energy (eV)
50
40
30
20
10
0
$^2D_{3/2}$
$^4P_{1/2}$
$^4D_{3/2}$
$^4D_{5/2}$
$^2F_{7/2}$
$^4G_{7/2}$
$^4G_{9/2}$
$^2H_{11/2}$
$^6S_{5/2}$
$^4P_{5/2}$
$4.31(87) \times 10^{-7}$ s^{-1}
4×10^{-13} s^{-1}
5×10^{-9} s^{-1}
Pentatrap
MCDHF1
MCDHF2
32
31
1/2
3/2
5/2
7/2
9/2
11/2
J

Conclusions

- Experimental progress and astrophysical needs require improved accuracy for transition energies, lifetime, Auger rates…
- Current methods reach their limit pretty fast due to physics (large number of configuration and interaction integrals), methods and computer limitations (RAM, speed…)
- High-accuracy measurements on highly charged ions with more than 3 electrons, leads to the need of accurate theoretical calculations for complicated systems
  - complex outer-shell structure
  - many holes
- Other challenges:
  - laser spectroscopy, in particular of super-heavy elements ($Z \geq 103$)
  - use of long lived-metastable states for Atomic clock insensitive to black body radiation and with high quality factors
  - improve transition energy calculations to manipulate the clock HCI (shelving…)

Perspectives

- Precision x-ray measurements and predictions needed for astrophysics applications, in particular with the new satellites with micro-calorimeters
  - XRISM launched in September
  - New China x-ray satellite (2030)
  - ATHENA with XIFU (>2030)
- Improvement of the Paris DCS for faster setup and change of energy (done)
- MIVOC method for generating metallic ions of astrophysical interest in the SIMPA ion source
- Code developments
  - full parallelisation (complicated gestion of RAM exchange between processors)
  - self-energy screening self-consistent
  - use AI for initial condition (machine learning?) and convergence (neural networks?)
  - global convergence methods like “nested sampling”

Thank you for your attention