The multiconfiguration Dirac-Fock method: principles and recent applications to heavy ions and super-heavy elements

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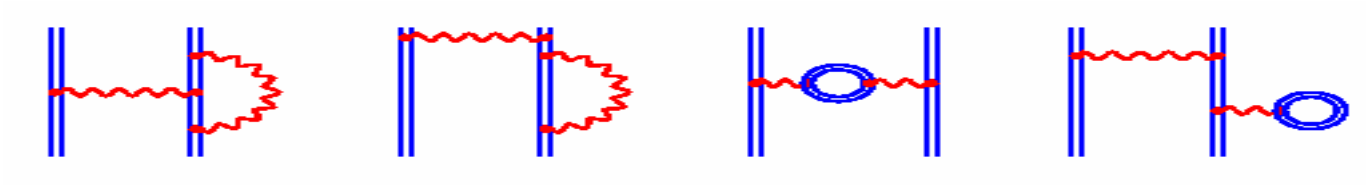
Outline

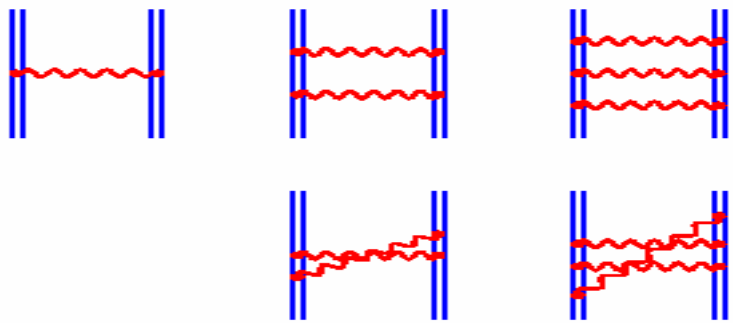
- Introduction
  - The MultiConfiguration Dirac-Fock method
- What are the limits?
  - Why must-we care about the non-relativistic limit?
    - History: fine structure and correlation in small, light atoms
    - Basics of Relativistic Many-Body Perturbation Theory
    - The NR limit beyond the MCDF method
    - Solution
  - Other effects at high-Z
  - Conclusion
- Perspectives:
  - high precision calculations and measurements
  - beyond energy
  - super-heavy elements $Z\alpha \rightarrow 1$ or beyond

Collaborations

- S; Boucard, Université Pierre et Marie Curie
- J.P. Desclaux
- E. Lindroth, Stockholm University
- F. Parente, J.P. Santos, Faculdade de Ciências e Tecnologia Universidade Nova de Lisboa
- J. Marques, M.C. Martins, A.M. Costa, Universidade Nova de Lisboa



“Screening of S.E. and V. P.”



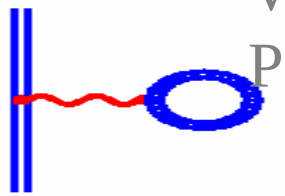
➔RMBPT or MCDF

➔Non Radiative QED (no Hamiltonian or potential form!)

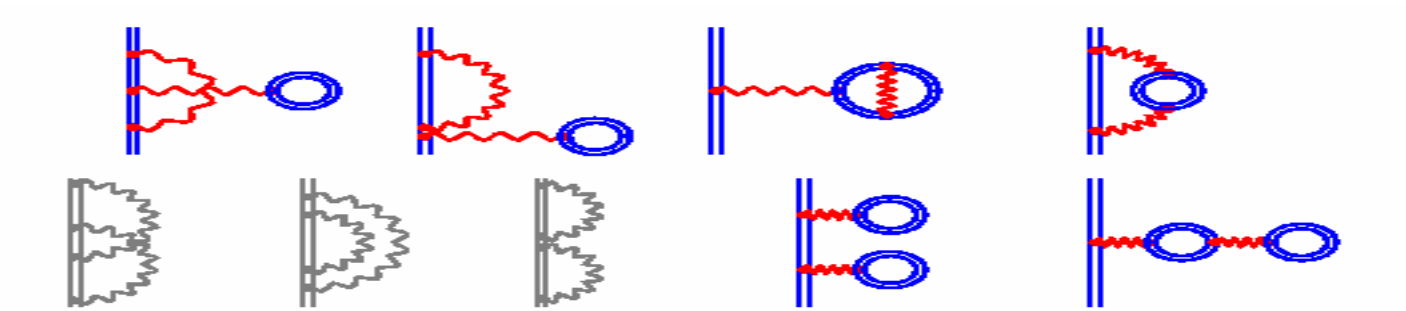
Non Radiative QED (QED correction to correlation and projection operators…)

H-like "One Photon"

Self Energy

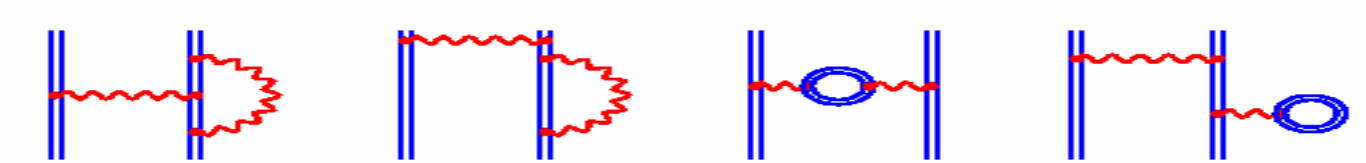


Vacuum Polarization



H-like "Two Photon"

?



"Screening"

Approximately

From QED to practical many-body calculations

- QED at presents cannot be used to get accurate correlation energy in many-body systems (just too hard!)
- One has developed approximation techniques, but their limitations and constraints should not be forgotten!
  - MCDF: all-order variational method (powerful and general, but more difficult to link properly to QED)
  - RMBPT: partly all order, more easily linked to QED but mostly limited to closed-core ± 1 or 2 electrons

Symmetries of spin-orbitals

In relativity and Quantum-electrodynamics, space is invariant by:

- Rotation
- Translation
- Reflection in a mirror
- Time inversion
- Change of inertial frame of reference
- Particle-antiparticle replacement

Symmetries define operators that commute with the Hamiltonian➔they fix degeneracy of the problem

Extra symmetry of the Coulomb problem:

- Non-relativistic symmetry: Lenz vector➔In hydrogen the symmetry group is O(4), energy depend only on the principal quantum number

Symmetries of spin-orbitals: Relativistic vs. non-relativistic

- Non-relativistic
- Rotation:
  - Total orbital angular momentum L (L^2, L_z)
  - Total Spin S
- Parity
- Lenz vector (Coulomb problem):

$$\vec{\ell} = \vec{r} \times \vec{L}$$

- For hydrogen energy is independent of l and s
- For multielectron atoms, energy is specified by L and S, and independent of J

- Relativistic
- Rotation
  - Only total angular momentum J=L+S is preserved
- Parity
- Dirac quantum number κ

$$K = \beta k = \beta(\vec{\sigma} \cdot \vec{L} + 1)$$

- For hydrogen energy does not depends on the sign of κ (parity) p1/2 and s1/2 have the same energy

Symmetries of spin-orbitals: consequences

p orbital: l=1 s=1/2:

- j=1/2, κ=1
- j=3/2, κ =-2

κ =1: p behavior

- κ =-1: s behavior

Configuration like
$2p^5\ {}^2P$ can now be:

- $(2p_{1/2})^2\,(2p_{3/2})^3$ J=3/2
- $(2p_{1/2})\,(2p_{3/2})^4$ J=1/2

$$\phi_{n\kappa}(\vec{x}) = \begin{bmatrix} f_1(x)\chi^{\mu}_{\kappa}(\hat{x}) \\ i f_2(x)\chi^{\mu}_{-\kappa}(\hat{x}) \end{bmatrix}$$

κ =-2: p behavior

- κ =+2: d behavior

The MCDF method (1)

One must solve:

$$\mathcal{H}^{npp}\Psi_{\Pi,J,M}(\ldots,\mathbf{r}_i,\ldots) = E_{\Pi,J,M}\Psi_{\Pi,J,M}(\ldots,\mathbf{r}_i,\ldots),$$

Where (as dictated by Quantum Electrodynamics-QED):

$$\mathcal{H}^{\text{no pair}} = \sum_{i=1}^{N}\mathcal{H}_{\rm D}(r_i) + \sum_{i<j}\mathcal{V}(|\mathbf{r}_i - \mathbf{r}_j|)$$

Not a real Hamiltonian (Relativity!)

$$\mathcal{V}_{ij} = \Lambda_{ij}^{++} V_{ij} \Lambda_{ij}^{++}$$

$$V_{ij} = \frac{1}{r_{ij}} - \frac{\boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_j}{r_{ij}} - \frac{\boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_j}{r_{ij}}[\cos(\omega_{ij}r_{ij}) - 1]$$

$$+(\boldsymbol{\alpha}_i\cdot\boldsymbol{\nabla}_i)(\boldsymbol{\alpha}_j\cdot\boldsymbol{\nabla}_j)\frac{\cos(\omega_{ij}r_{ij}) - 1}{\omega_{ij}^2 r_{ij}},$$

The MCDF method (2)

For that use a variational method, using Slater determinants

superposition of configuration state functions (CSF):

$$|\Psi_{\Pi,J,M}\rangle = \sum_{\nu} c_\nu |\nu \Pi J M\rangle. \qquad (4)$$

$$|\nu \Pi J M\rangle = \sum_i d_i \begin{vmatrix} \Phi_1^i(r_1) & \cdots & \Phi_N^i(r_1) \\ \vdots & \ddots & \vdots \\ \Phi_1^i(r_N) & \cdots & \Phi_N^i(r_N) \end{vmatrix}$$

The CSF are made to be eigenfunctions of parity, total angular momentum (spherical symmetry of the problem) and its projection along an arbitrary axis…

The MCDF method (3)

One gets:

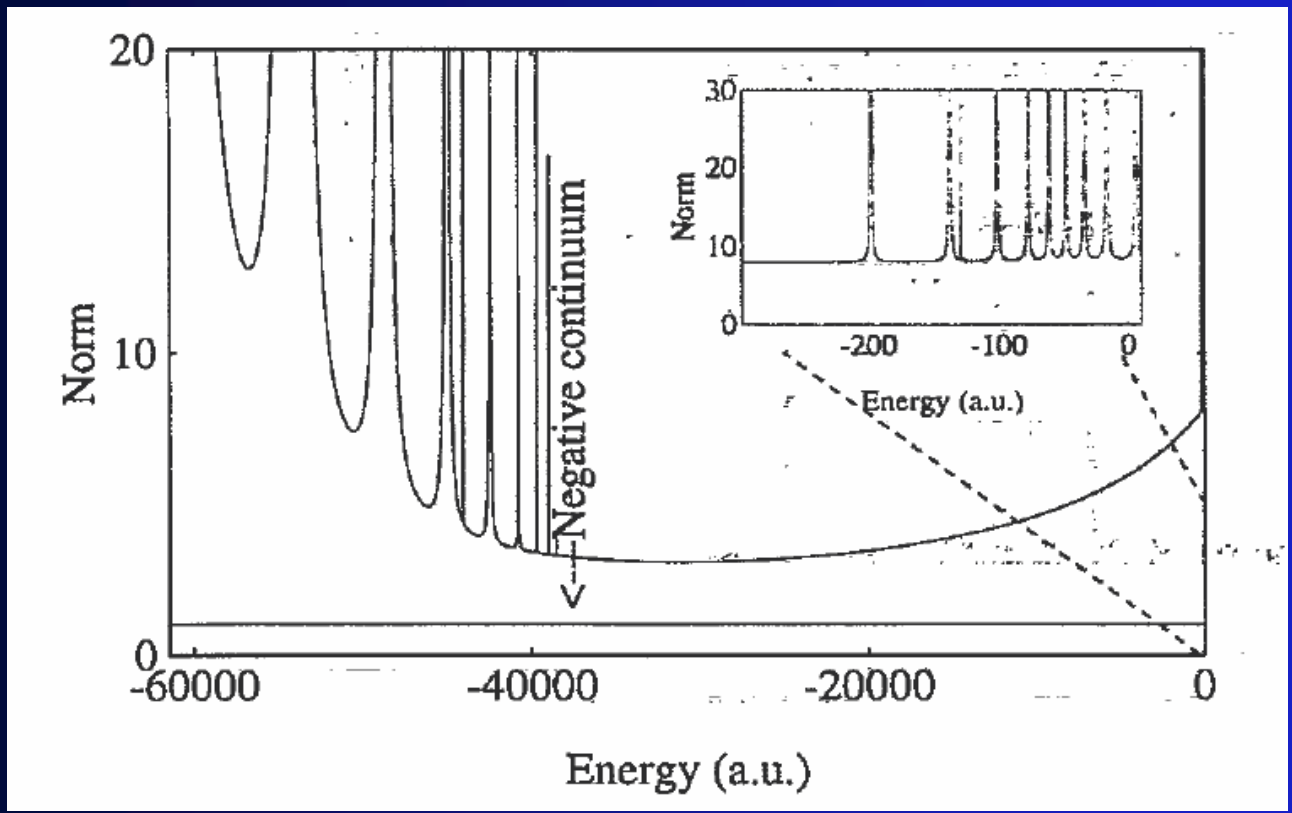
1. a Hamiltonian matrix leading to the c_i mixing coefficients by diagonalization fo given radial wavefunctions (Configuration Interaction method!)
2. Dirac-like, inhomogeneous, integro-differential equations for the radial wavefunctions.
3. Effects can be included to all-orders if presents in both the CI and differential equations

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

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

Projection operators in practice

- What happens if they are not included in the MCDF model?



Indelicato, P., Projection operators in Multiconfiguration Dirac-Fock calculations. Application to the ground state of heliumlike ions., Physical Review A 51: 1132-1145 (1995)

The mdfgme code (P. Indelicato and J.P. Desclaux)

- Can accommodate arbitrary number of open-shells (within your computer memory and disk space)
- Automatic single and double excitation generation, with Brillouin theorem option
- Full JJ➔LSJ recoupling
- Full self- consistent treatment of Breit interaction
- Full self- consistent treatment of Uehling vac.pol.
- First and Second order QED corrections whenever known
- Full projection operator included
- Landé g-j factors, diagonal and non-diagonal hyperfine matrix elements (including Bohr-Weisskopf effect), Shiff moments, pariyt violation, Auger and excitation cross sections, All multipole radiative transition rates, with non-orthogonalinitial and final states
- Available from http://dirac.spectro.jussieu.fr/mcdf

Why must-we care about the non-relativistic limit?

- In 1982 it was found that fluorine-like ions, fine structure ($1s^2\ 2s^2\ 2p^5$ J=1/2-3/2), the disagreement between experiment and relativistic calculation was due to a wrong non-relativistic limit when using a Multi-Configuration Dirac-Fock code
  - Huang, K. N., Y.-K. Kim, K. T. Cheng and J. P. Desclaux, *Correlation and Relativistic Effects in Spin-Orbit Splitting,* Physical Review Letters **48**: 1245-1248 (1982)
- Observation was that when relativistic configurations that have several parents :$1s^2\ 2s^2\ 2p^4\ {}^3P$, ${}^1S$ and ${}^1D$, the $2p_{1/2}$ and $2p_{3/2}$ orbitals do not converge to the non-relativistic 2p: the energy becomes J dependent, which is wrong
- Correlation can lead to the same problem, e.g., boron-like ions: $1s^2\ 2s^2\ 2p + 1s^2\ 2p^3$+…
- The solution proposed was to subtract the faulty non-relativistic limit, a very ad hoc proposal…

Basics of many-body perturbation theory

$$H\Psi = (H_0 + V) \mid \Psi_0 + \rho\rangle = E\Psi = (E_0 + \delta E) \mid \Psi_0 + \rho\rangle$$

H total Hamiltonian, Ψ exact solution, V perturbation
H0 unperturbed Hamiltonian, Ψ_0 set of solutions with E_0
δE energy correction, ρ wave function correction

$$H_0\Psi_0 = E_0\Psi_0$$

$$\delta E = \langle \Psi_0 \mid V \mid \Psi_0 + \rho\rangle$$

We define the model space by Ψ_0 and a wave operator:

$$\Psi = \Omega\Psi_0$$

The projection of the exact solution Ψ onto the model space is represented by P:

$$\Psi_0 = P\Psi$$

$$P = \mid \Psi_0\rangle\langle\Psi_0 \mid$$

Basics of many-body perturbation theory (2)

Using P and Ω we find that the Shrödinger equation is equivalent to the generalized Bloch equation:

$$[\Omega, H_0]\, P = V\Omega P - \Omega P V \Omega P$$

The energy correction is thus given by:

$$H_{eff}\Psi_0 = PH\Omega P\Psi_0 = (E_0 + \delta E)\Psi_0$$

$$H_{eff} - PH_0P = PV\Omega P$$

Ω is found by perturbation expansion replacing $\Omega = 1 + \Omega^{(1)} + \Omega^{(2)} + \ldots$ in the Bloch equation

Basics of many-body perturbation theory (3)

Here we start from a single Slater determinant for Ψ_0:

$$| \alpha \rangle = | \{1s^2 2s^2 2p^5\} \rangle$$

Since V is a two body operator, it can be divided as

$V = V_0 + V_1 + V_2$ V_1 one body potential, V_2 two-body

$$V_1 = \sum_{i,j} \left\{ a_i^\dagger a_j \right\} \left(\langle i \mid -u \mid j \rangle + \sum_a^{core} \langle ia \mid V_{ij} \mid ja \rangle - \langle ai \mid V_{ij} \mid ja \rangle \right)$$

$$V_2 = \frac{1}{2} \sum_{i,j,k,l} \left\{ a_i^\dagger a_j^\dagger a_l a_k \right\} \langle ij \mid V_{ij} \mid kl \rangle$$

u is a one-particle potential included in V_0

If we chose $u=V_{HF}$ then V1=0

Basics of many-body perturbation theory (4)

In this case we have

$$\Omega^1 = \frac{1}{2}\sum_{b,c}^{core}\sum_{r,s}^{exc} \frac{\left\{a_h^\dagger a_s^\dagger a_c a_b\right\}\langle hs \mid V_{ij} \mid bc\rangle}{\varepsilon_b + \varepsilon_c - \varepsilon_h - \varepsilon_s} + \frac{\left\{a_r^\dagger a_s^\dagger a_c a_b\right\}\langle rs \mid V_{ij} \mid bc\rangle}{\varepsilon_b + \varepsilon_c - \varepsilon_r - \varepsilon_s}$$

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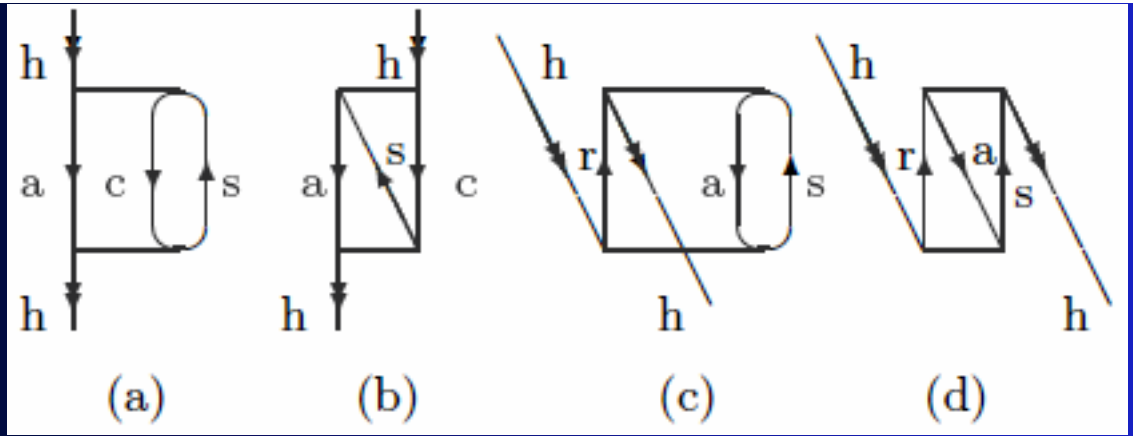
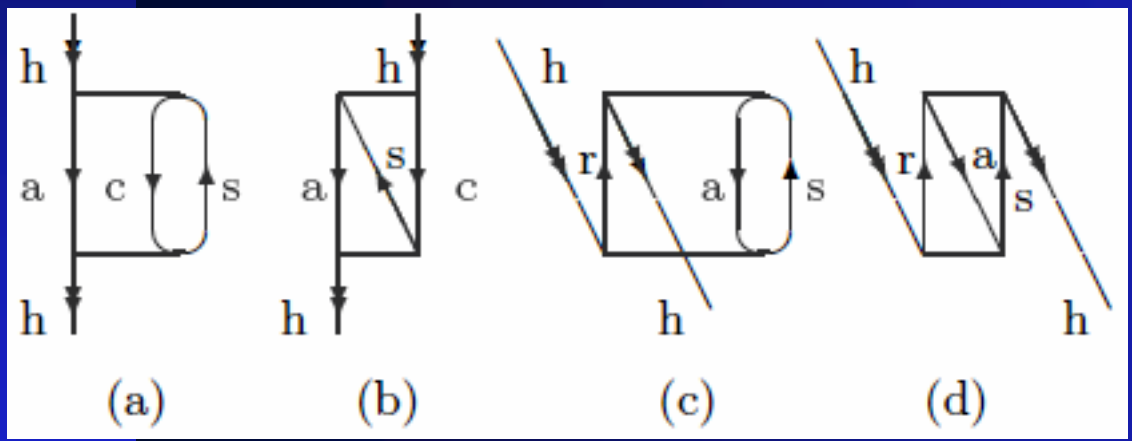


h: hole state (we start from a closed shell, Ne atom with $2p^6$), a, c core electrons, r, s: correlation (unoccupied orbitals)

Can we understand in detail the origin of the problem

- First step: understand if this is a physical problem or a problem specific to the MCDF method
- Many-body perturbation theory can make it easier to understand



Second order energy correction:

•(a) and (b) fluctuation around the reference state (two holes and one excited orbitals)—like vacuum-polarization in QED

•(c) and (d) doubly excitation to two unoccupied orbitals (correlation)

Relaxation in MBPT

- Relaxation (readjustment of the orbitals due to the presence of the hole) is obtained when (single excitation with same κ!)

$$\rho_b^{\text{relax}}(\ell_s = \ell_b, j_s = j_b) = -\sum_s^{\text{exc}} \frac{|\,s\rangle\langle\{hs\}\,|\,V_{12}\,|\,\{hb\}\rangle}{\varepsilon_b - \varepsilon_s},$$

The relaxation energy is $\sum_b^{\text{core}} \langle\{bh\}\,|\,V_{12}\,|\,\{\rho_b^{\text{relax}} h\}\rangle$

We take an example diagram 1a $a = h$ and $\ell_s = \ell_b$

To go from jj to LS coupling one needs to sum over j:

$$|\,\ell m_\ell s m_s\rangle = \sum_{jm_j} |\,(\ell s) j m_j\rangle\langle(\ell s) j m_j\,|\,\ell m_\ell s m_s\rangle$$

Relaxation in MBPT (2)

$$\frac{1}{r_{12}} = \sum_k \frac{r_<^k}{r_>^{k+1}} \mathbf{C}^k(1) \cdot \mathbf{C}^k(2)$$

Non-relativistic

$$\sum_b^{\text{core}} \sum_k 2 \frac{1}{2k+1} \frac{1}{2\ell_h + 1} \langle \ell_h \| \mathbf{C}^k \| \ell_h \rangle^2 \langle \ell_b \| \mathbf{C}^k \| \ell_b \rangle^2$$

Relativistic

$$\sum_b^{\text{core}} \sum_k \frac{1}{2k+1} \frac{1}{2j_h + 1} \langle j_h \| \mathbf{C}^k \| j_h \rangle^2 \langle j_b \| \mathbf{C}^k \| j_b \rangle^2$$

Example: relativistic contribution for k=2

For $p_{1/2}$ =0 but for $p_{3/2} \neq 0$, even when $c \to \infty$

Numerically, RMBPT relaxation with $c \to \infty$ gives a 0.024 eV shift between J=1/2 and J=3/2 in F-like Ar for 2nd order relaxation.

Partial conclusion

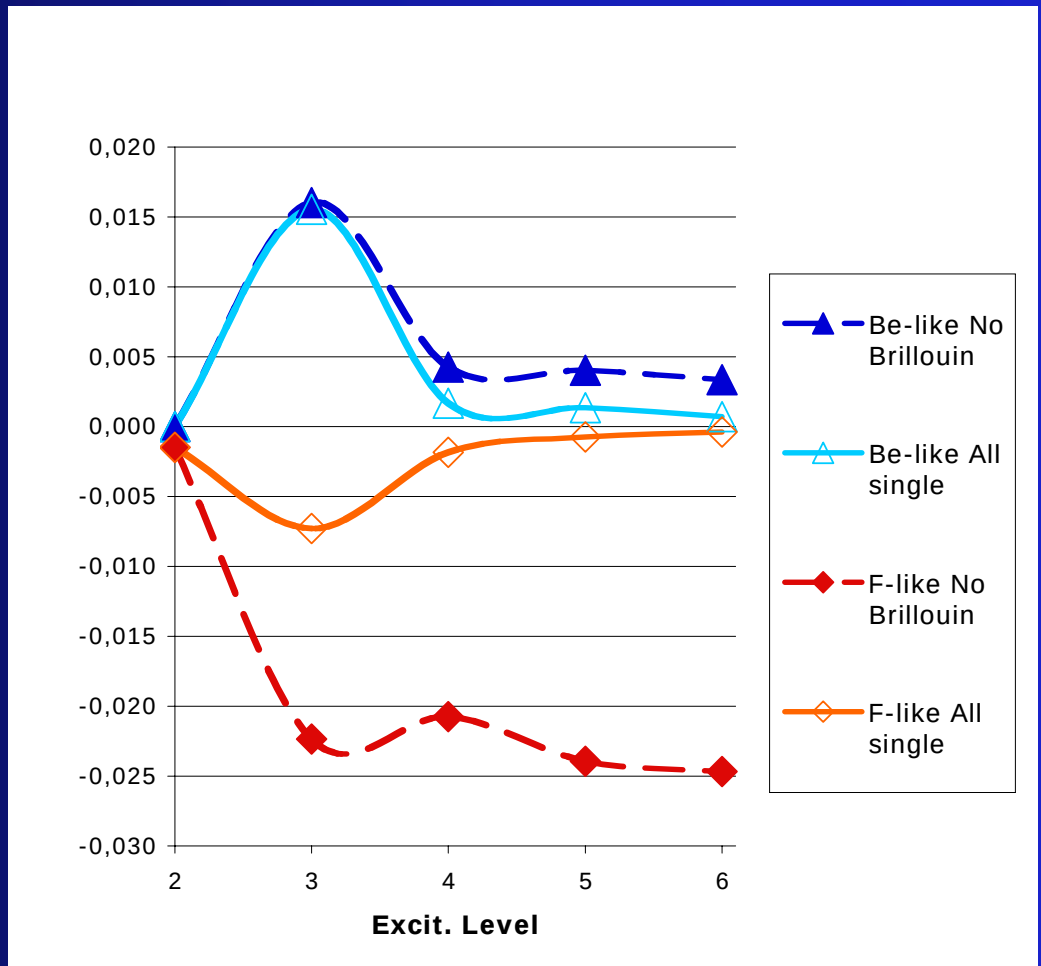
- Relaxation leads to a spurious energy shift
  - RMBPT with high orders: ΔE=-0.050 eV
  - MCDF relaxation Δ E=-0.049 eV
- This N.R. offset is thus consubstantial to relaxation
- It has experimental consequence, even for a Z as large as 18, due to very high-accuracy of experiments

Is there a solution to this problem?

- With RMBPT, the shift is zero if you calculate complete orders
  - Yet people usually use “all-orders” methods to re-sum classes of diagrams
- With MCDF, one could think that including many configurations will solve the problem
  - We showed that one must include single excitations that gives no contributions following the Brillouin theorem in the non-relativistic HF case
  - These are the excitations $n_a\kappa_a \rightarrow n\kappa_a$ (exactly single excitation to be added to RMBPT, that are already present in MCDF and should not contribute to the energy!)

Effect of Brillouin single excitations on the MCDF result (F-like Ar)

- The N.R. offset increases when adding single and double excitations, without the Brillouin ones
- Adding the Brillouin single excitations lead to a zero offset for large configuration spaces



Comparison with experiment

	$2p_{1/2}$	$2p_{3/2}$	Δ
	Contributions		
Ne-like DF orbital energy	426.500 02	424.132 11	2.367 91
Δ DF Breit	−0.226 59	−0.135 76	−0.090 83
Higher order retardation	−0.000 11	0.000 79	−0.000 90
QED correlation	0.013 53	0.007 55	0.005 98
	Contributions specific to RMBPT		
Second order core-core, Coulomb	−4.485 09	−4.425 87	−0.059 21
core-core, Breit	−0.011 87	−0.008 14	−0.003 73
Correlation, Coulomb	2.567 26	2.557 63	0.009 62
Correlation, Breit	0.023 91	0.020 18	0.003 73
Higher order contribution (Coul. + Breit)	0.165 59	0.158 85	0.006 74
Δ DF-Breit orbitals	0.001 98	0.000 43	0.001 56
Total (RMBPT)	424.548 63	422.307 77	2.240 86
Experiment			2.240 10
	Contributions specific to MCDF (N.R. offset subtracted)		
Relaxation (Coulomb)	−3.108 00	−3.059 31	−0.048 69
Relaxation (Breit)	−0.004 06	−0.003 14	−0.000 92
Correlation (Coul. → $5g$)	1.424 66	1.396 04	0.028 62
Correlation (Breit → $5g$)	−0.013 59	0.007 41	−0.021 00
Total (MCDF)	424.585 85	422.345 69	2.240 16
Experiment			2.240 10

Indelicato, P., E. Lindroth and J. P. Desclaux, *Nonrelativistic limit of Dirac-Fock codes: The role of Brillouin configurations,* Phys. Rev. Lett. **94**: 013002 (2005)

Conclusion

The NR problem affects also the ground state energy

Configuration	No Brillouin	All single	Difference
corr. → $3d$	−5.1792	−5.1989	−0.0196
corr. → $4f$	−7.7349	−7.7603	−0.0255
corr. → $5g$	−8.6551	−8.6871	−0.0320

- The N.R. offset is due to relaxation and goes away when doing a complete calculation
- In the MCDF case, the offset is going to zero if a large enough configuration space is used, but only if all single configurations are included
- In practice, excluding Brillouin single excitations and then subtracting the N.R. offset leads to the same value for **transition energy**, with better numerical convergence
- Failing to account for the N.R. offset leads to poor results, even at a moderately large Z
- Similar problems can happen in RMBPT calculations if subclasses of important effects are singled out and are treated to higher order

Does that happens to other quantities than energy?

- Example:
  - Forbidden spin-flip transition probability $1s^2 2s2p\ ^3P_1$ ➔ $1s^2 2s^2\ ^1S_0$ in Be-like ions (intercombination line)
- To get high-accuracy thee are two ways:
  - one does optimize separately initial and final wave functions with a moderately large basis set
  - one use the same (huge) basis set for both states
- Does one recover the non-relativistic limit (0) in an MCDF calculation?

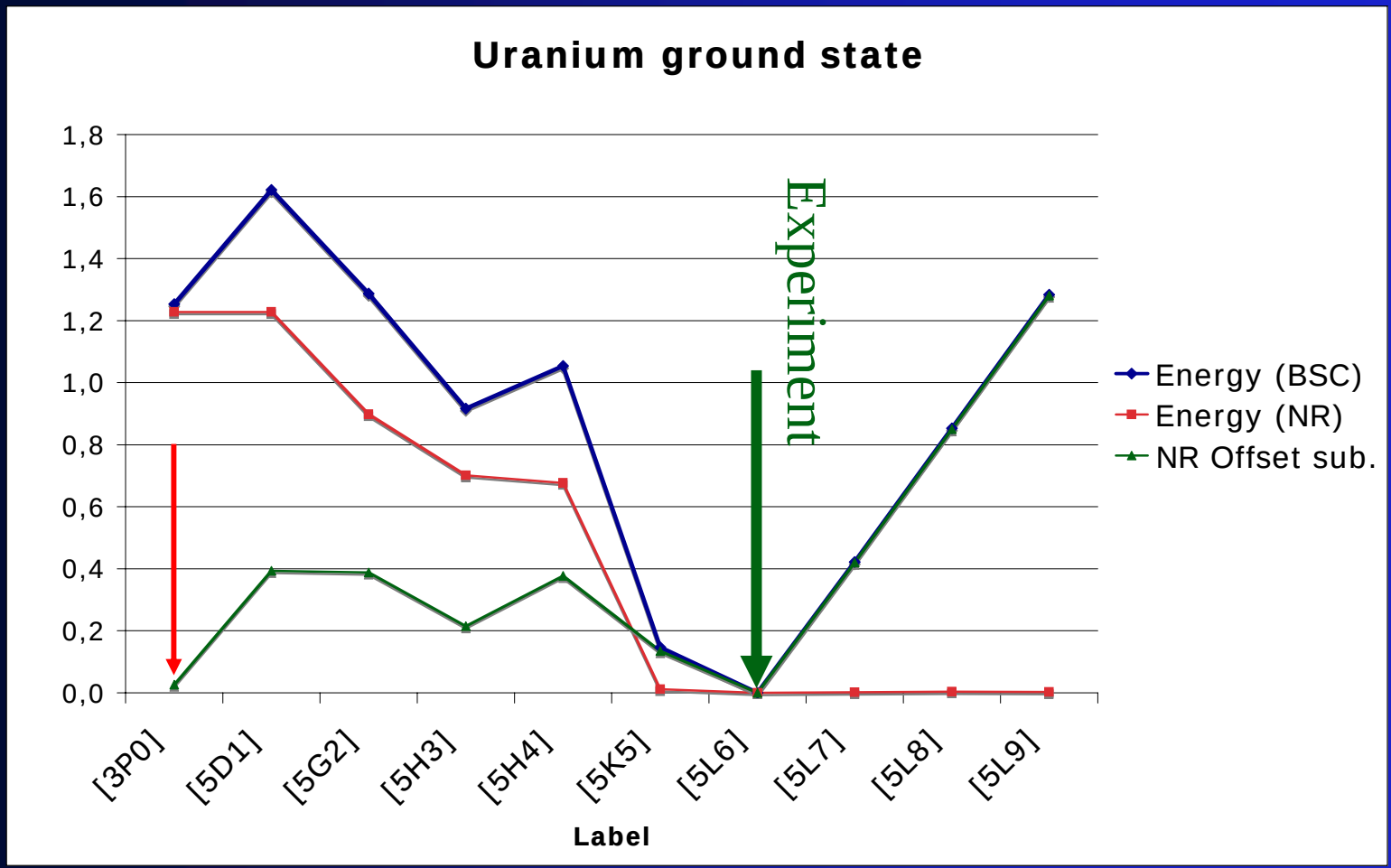
Does that happens to other quantities than energy (2) ?

Source	$A_{ki}(B^{+})$	$A_{ki}(C^{2+})$
Weiss, large scale MCHF [8]		106.7
Froese Fischer and Gaigalas, large scale MCHF [9]	10.27±0.20	103.0±0.4
Present work, MCDF		
Orthogonal orbitals, without the Breit interaction		
$2s2p+2p3d$ without the NR offset subtracted	341.3	301.7
with the NR offset subtracted	11.43	113.2
Orthogonal orbitals, with the Breit interaction		
$2s2p+2p3d$ without the NR offset subtracted	317.2	248.2
with the NR offset subtracted	7.38	81.4
Nonorthogonal orbitals		
$2s2p+2p'3d$ without the Breit interaction	11.46	113.7
with the Breit interaction	7.37	81.8
$n\leqslant 4$ + Breit + core excited configurations	9.01	94.4
$n\leqslant 5$ + Breit + core excited configurations	9.13	100.1
Jönsson and Froese Fischer, relativistic, $n\leqslant 8$ [10]		102.9±1.5
Doerfert *et al.*, experiment [11]		102.9±0.14

Kim, Y. K., F. Parente, J. Marques, P. Indelicato and J. P. Desclaux, Failure of multiconfiguration Dirac-Fock wave function in the nonrelativistic limit, Physical Review A 58: R1885-R1888 (1998)

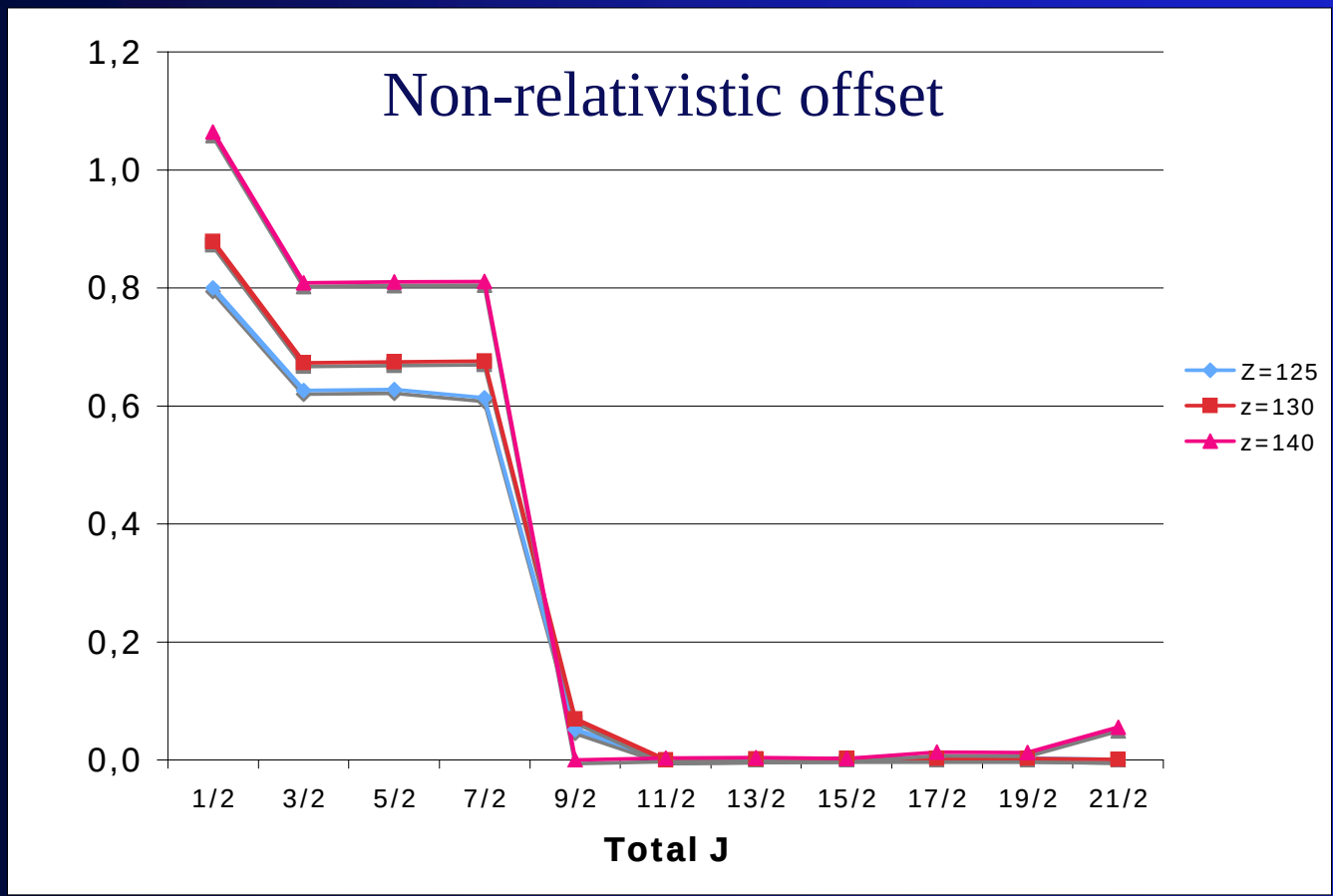
Is this problem surviving at high-Z? Uranium (know ground state)

Example Uranium 92 electrons, ground state, [Rn] $5f^3\ 6d\ 7s^2\ ^5L_6$

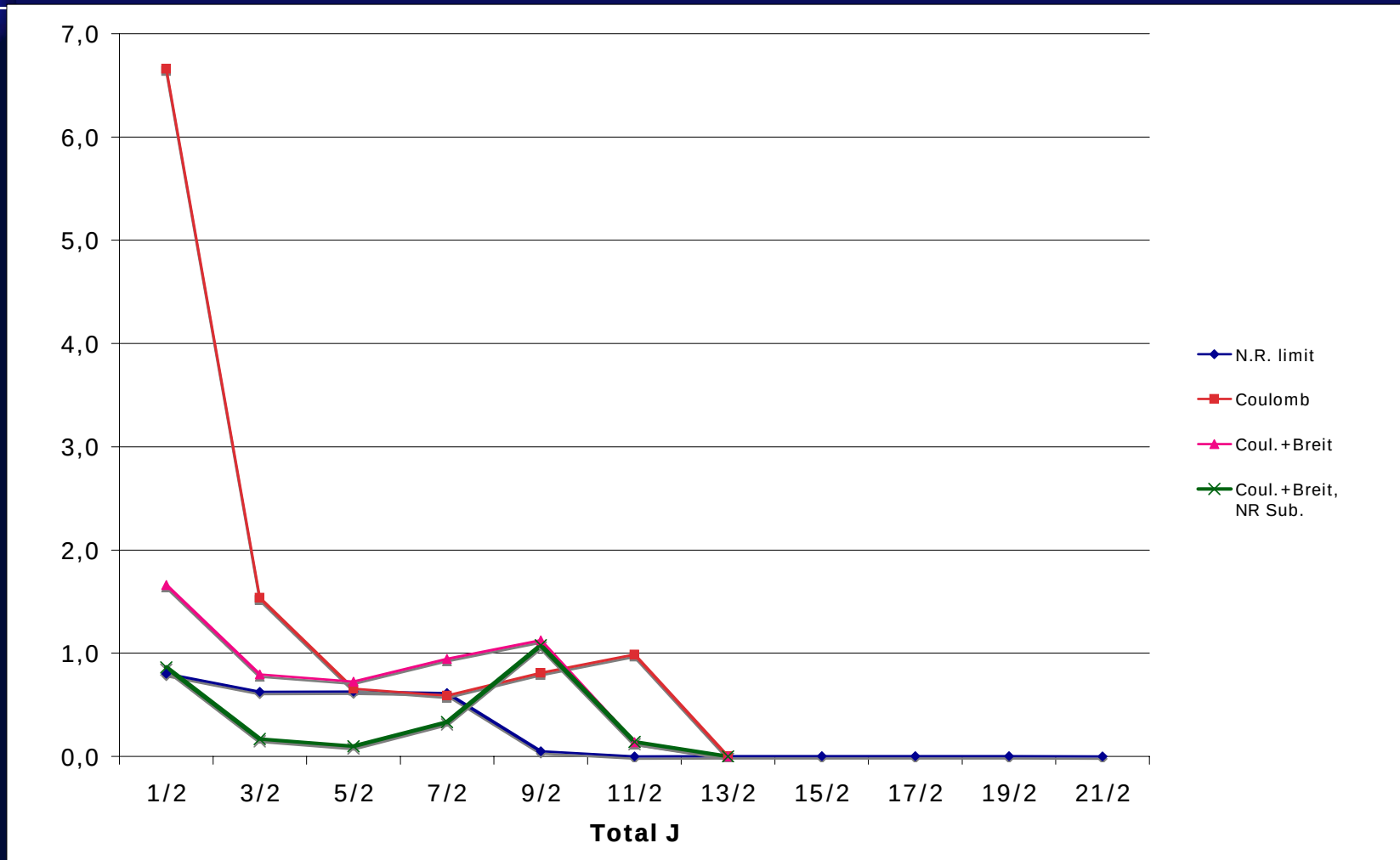


Is this problem surviving at high-Z? Element 125 isoelectronic sequence

Example Atom with 125 electrons, ground state, first with a 5g orbital: [Rn] $5f^{14}\ 6d^{10}\ 7s^2\ 7p^6\ 8s^2\ 6f^3\ 5g\ 8p$

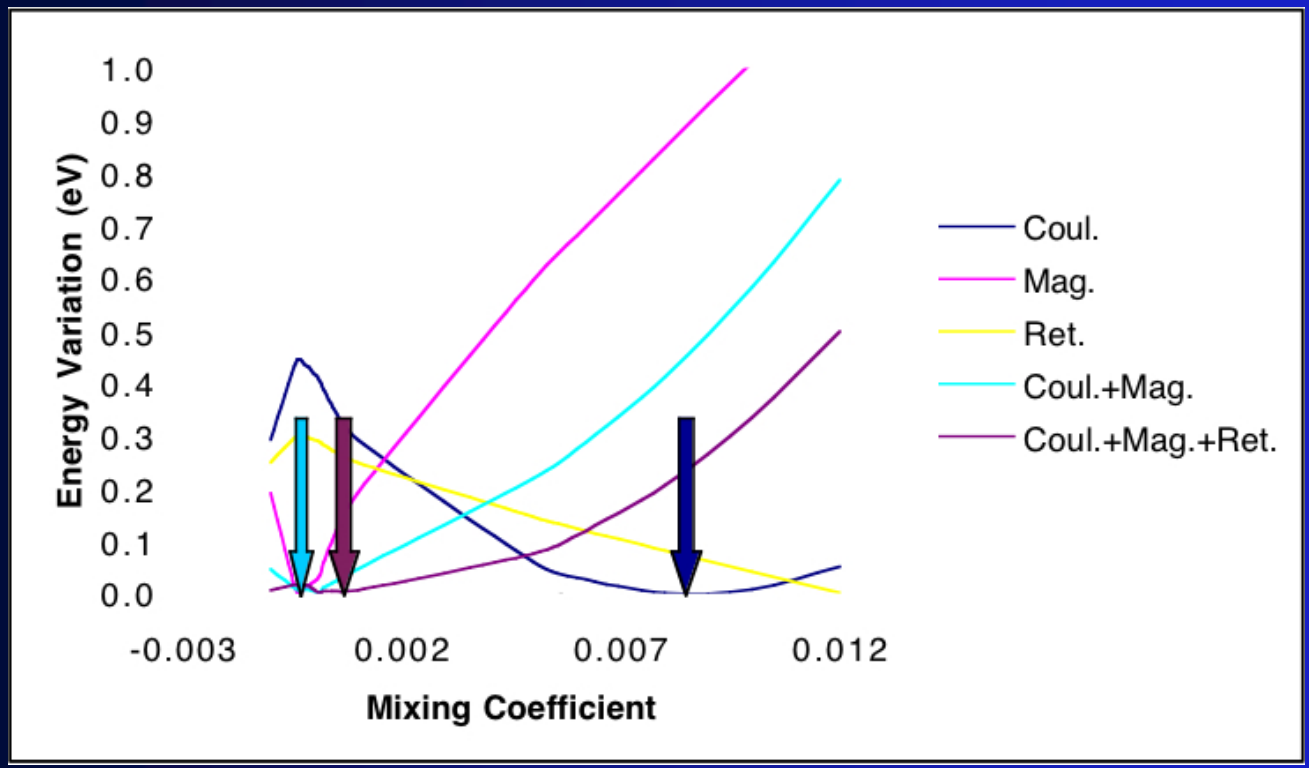


Variation of the binding energy with total angular momentum (Z=125)



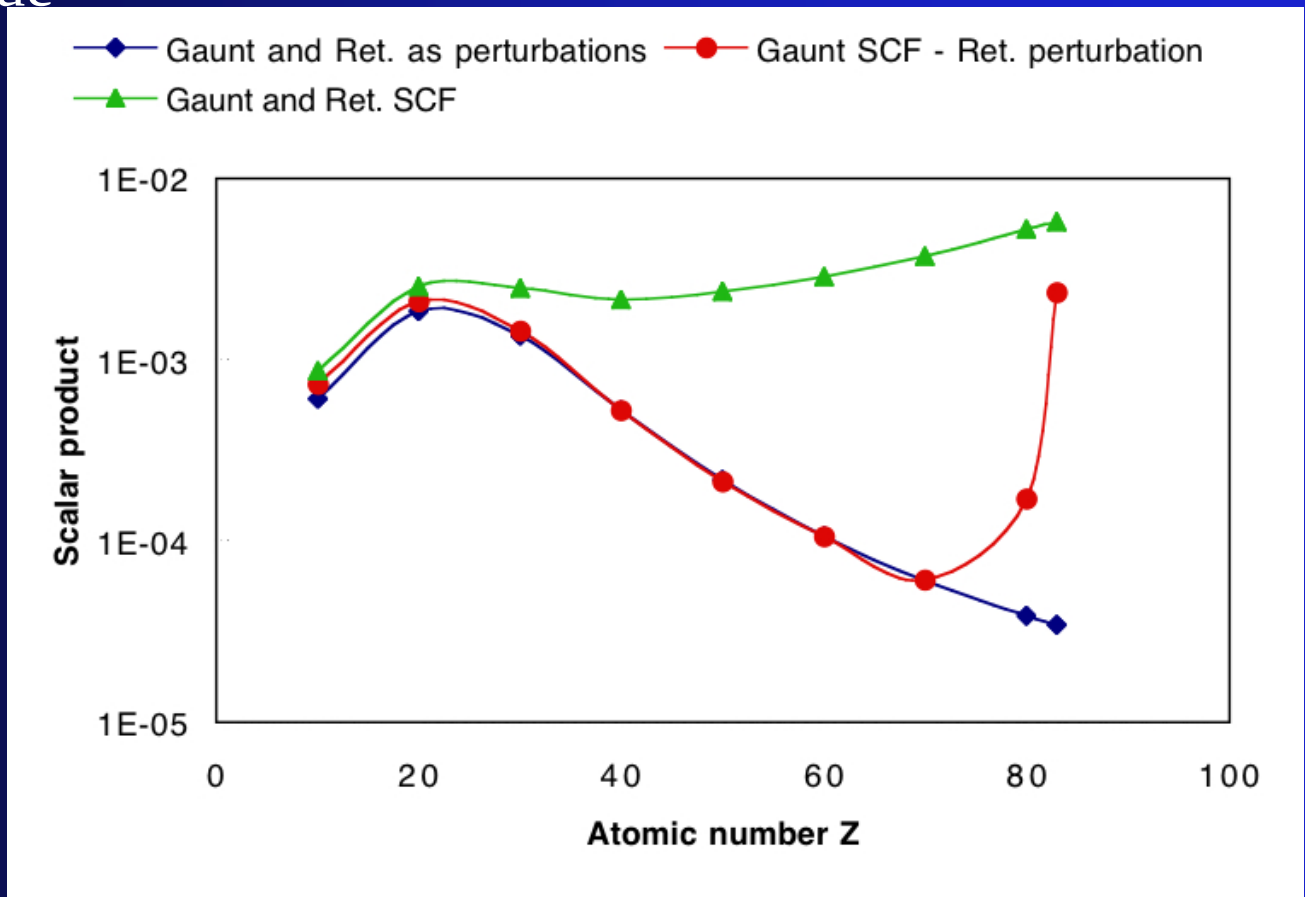
Other unsolved problems
(1) No minimum for the 1s 2p J=1

- Very simple case: $c_1|1s\ 2p_{1/2}>+c_2|1s\ 2p_{3/2}>$with the full relativistic electron-electron interaction, there is no energy minimum at high-Z!

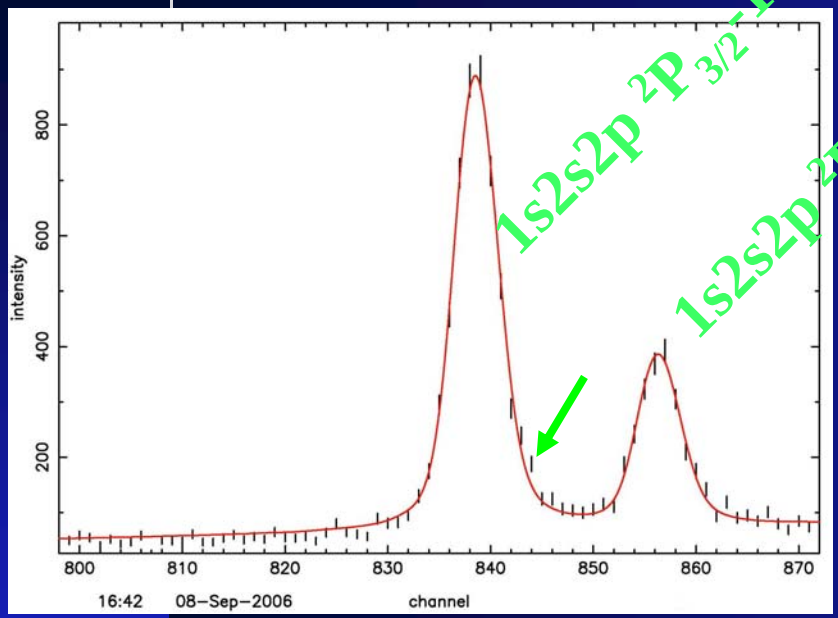


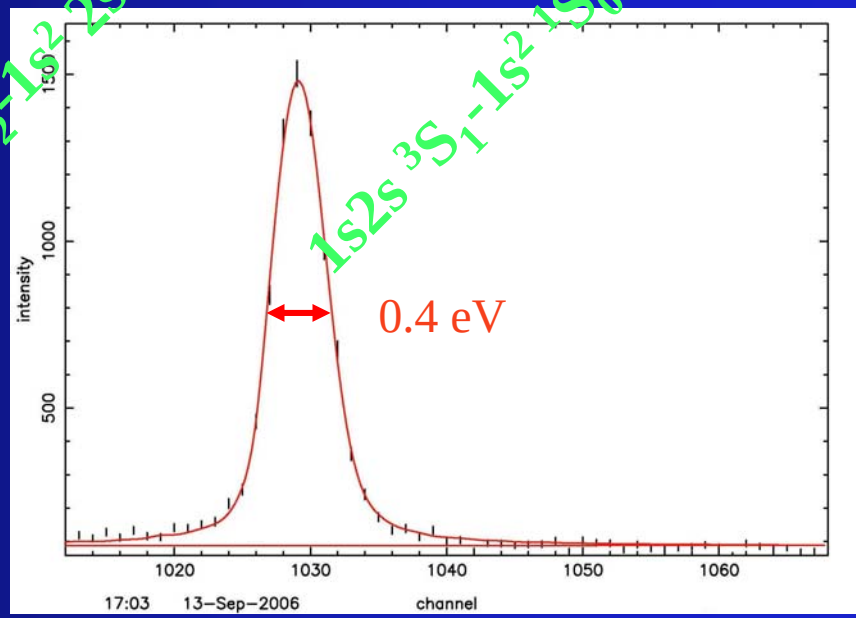
Other unsolved problems
(2) No orthogonality between 1s 2p J=1

- Very simple case $c_1|1s\ 2p_{1/2}J=1\rangle+c_2|1s\ 2p_{3/2}J=1\rangle$ one obtains the "$^3P_1$" as the lower energy eigenvalue and "$^1P_1$" as the higher energy eigenvalue



High precision studies of medium-Z highly charged ions





Li-like Ar

Natural width:

$^2P_{3/2}$-Radiative 66 meV Auger: 6 meV

$^2P_{1/2}$-Radiative 57 meV Auger: 65 meV

We use the M1 He-like line as a reference

He-like Ar

Natural width 3 neV

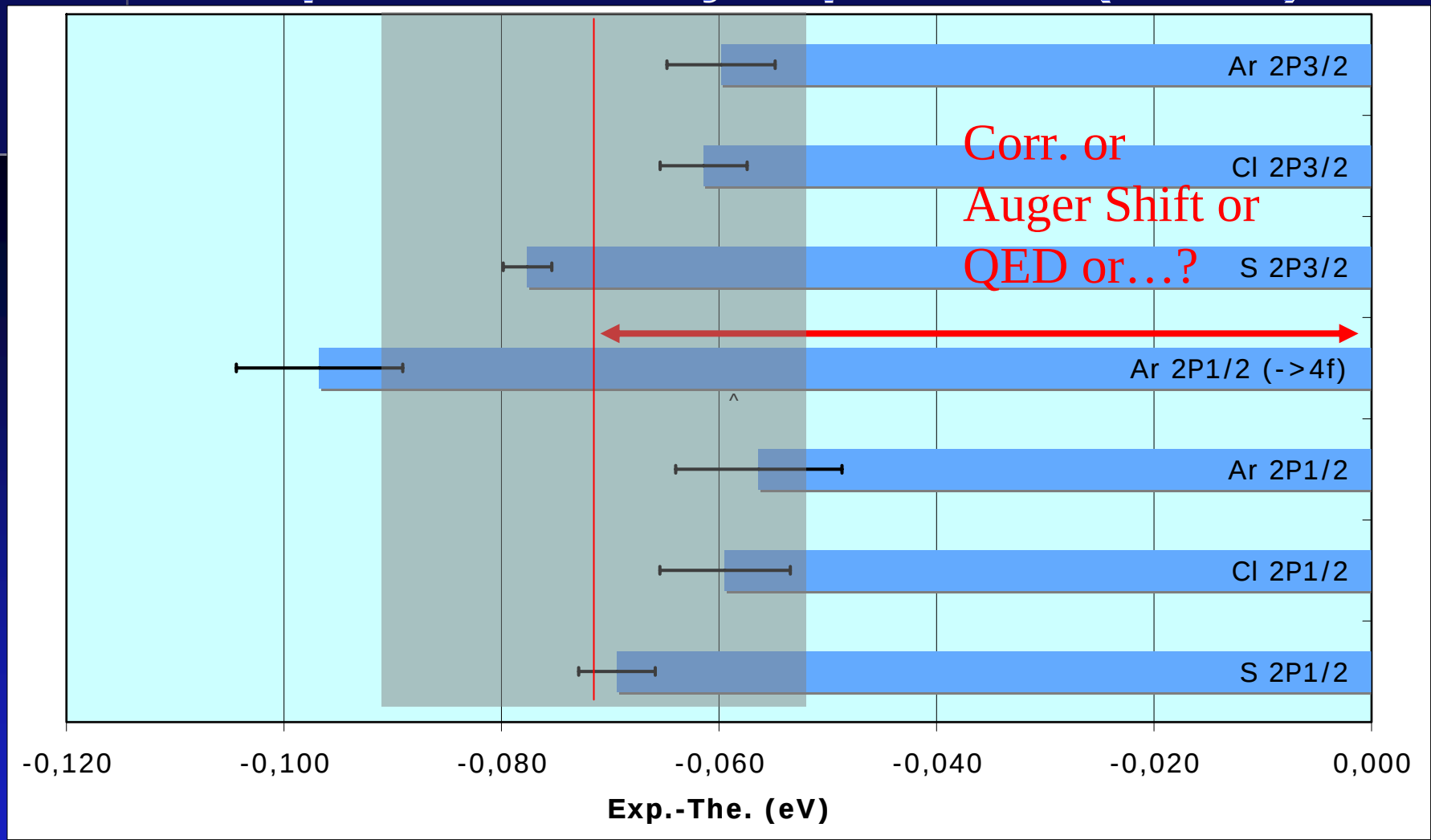
Doppler width 40meV

What do we learn from doubly-excited states

Contribution	$1s\,2s\,2p\ {}^2P_{1/2}$	$1s^2\,2s\ {}^2S_{1/2}$	transition
Coulomb	-6353,455	-9468,188	3114,734
Magnetic	0,180	2,203	-2,023
Retardation	0,048	-0,022	0,069
Higher order ret.	0,001	0,000	0,001
Coul. + Breit Corr.	-0,632	-1,453	0,822 (41)
S.E.	1,380	2,597	-1,218
S.E. Screening	-0,038	-0,123	0,085
V11	-0,094	-0,173	0,079
V13	0,000	0,001	0,000
2nd order QED	-0,001	-0,002	0,001
Recoil	0,000	0,000	0,000
Total	-6352,610	-9465,160	3112,550
Experiment			3112,453
Obs.-Calc.			-0,097 (8)(41)
S.E. Screen (I&M)	-0,03127	-0,153	0,122
Total	-6352,60349	-9465,19077	3112,587
Obs.-Calc.			-0,134 (8)(41)

S.E. screening is not under control at the needed accuracy
Correlation must be improved
Auger shift completely unknown

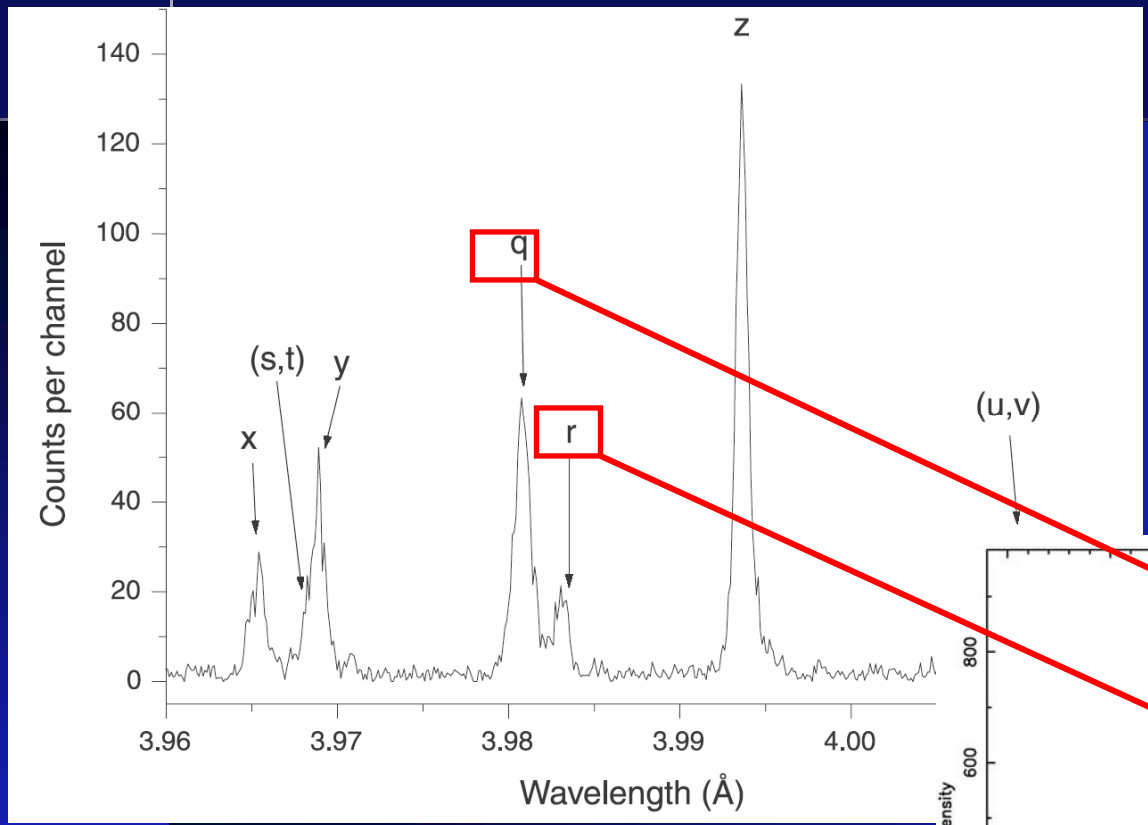
Comparison Theory-experiment (Li-like)

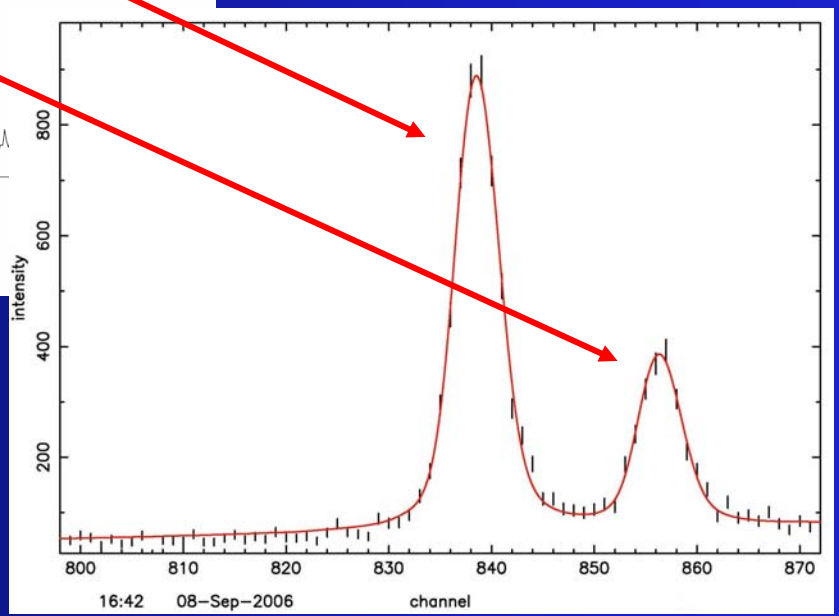


Experiment: statistical err. only

Theory correlation within (n=1 to n=2) active state except Ar $^2P_{1/2}$ (4f) (n=1 to n=4)

EBIT measurements





M. R. Tarbutt, R. Barnsley, N. J. Peacock, et al., J. Phys. B: At. Mol. Opt. Phys. 34, 3979 (2001).

Selectivity vs. intensity

Indelicato et al. NIM in press (2006)

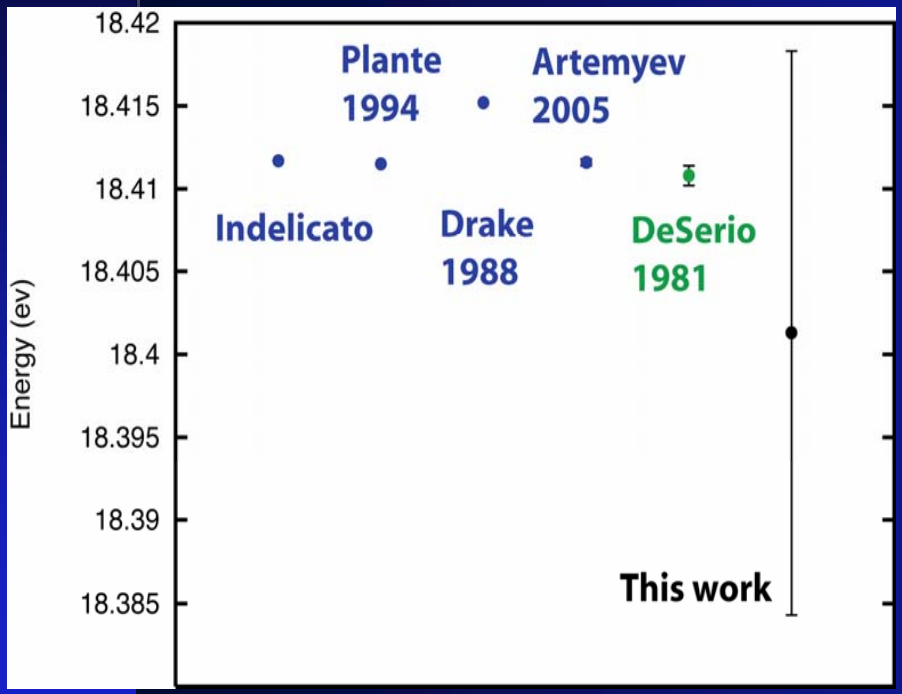
Comparison between EBIT, ECRIS and MCDF

	Tarbutt et (EBIT 200		ECRIT (2006)		MCDF Diff.	
$1s2s2p\ ^3P_{3/2} -> 1s2\ ^2S_{1/2}$	3114,130	0,078	3114,117	0,023	3114,19	0,07
$1s2s2p\ ^3P_{1/2} -> 1s2\ ^2S_{1/2}$	3112,405	0,078	3112,440	0,023	3112,51	0,06
$1s2s2p\ ^4P_{(1/2-3/2)} -> 1s2s\ ^2S_{1/2}$	3091,780,15		3091,810,01			
$1s\ 2s2p\ ^1P_1 - 1s2s\ ^1S_0$					3091,95	0,14
$1s2s2p\ ^4P_{3/2} -> 1s2s\ ^2S_{1/2}$			3087,20		3087,07	0,12

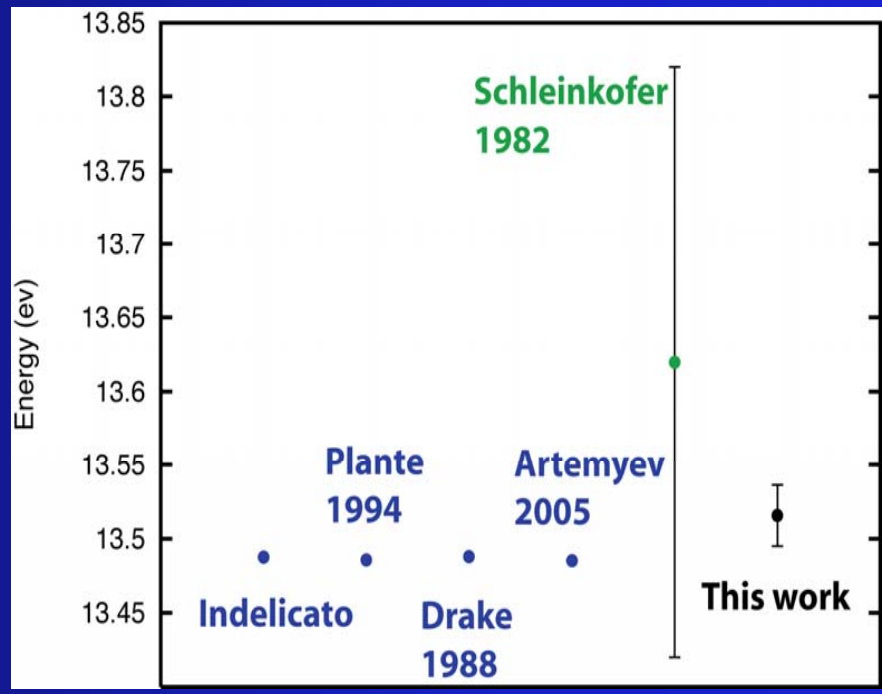
Preliminary Results for He-like Sulphur

Comparison against theory and previous experiments

1s2p $^3P_2$- 1s2s $^3S_1$ transition (preliminary)



1s2p $^1P_1$- 1s2p $^3P_1$ transition
This work: 13.483(16) eV

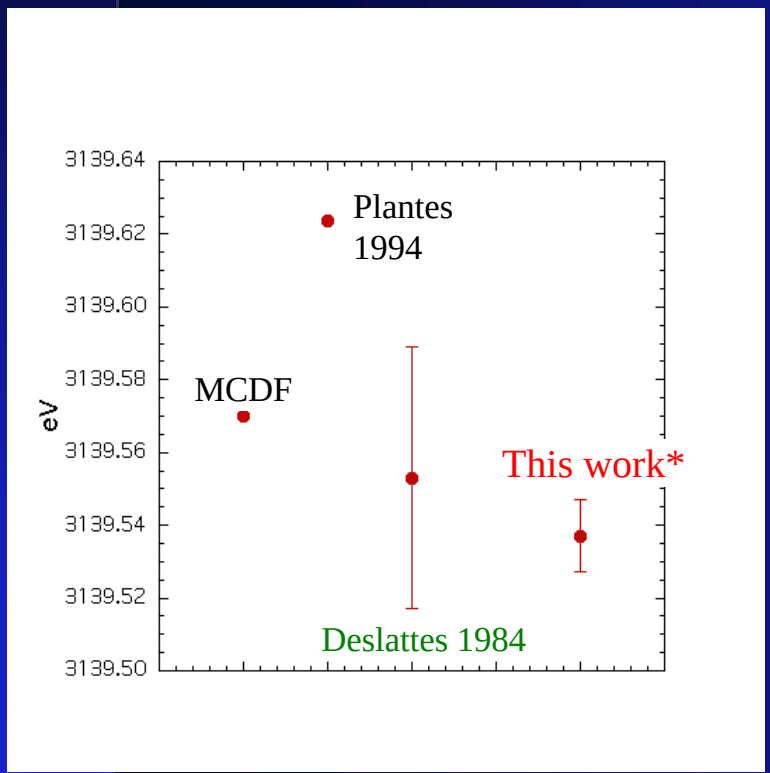


*using the MCDF theoretical value for the M1

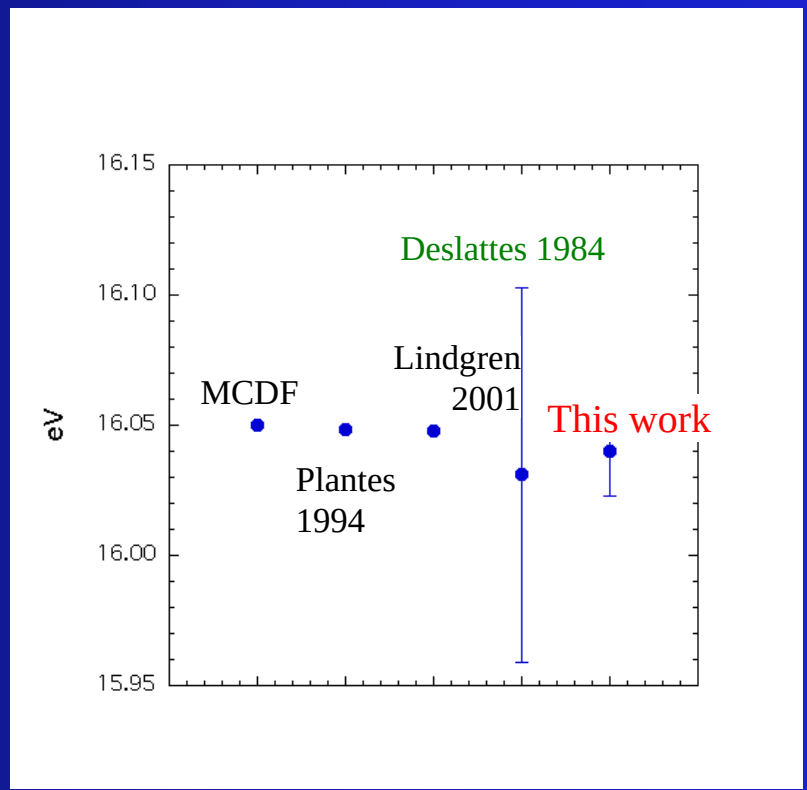
Preliminary results for He-like Ar

Comparison against theory and previous experiments

1s2p $^1P_1$- 1s^2 $^1S_0$ transition
This work: 3139.536(10) eV



1s2p $^1P_1$- 1s2p $^3P_1$ transition
This work: 16.040(17) eV



*using the MCDF theoretical value for the M1

High-field effects in Be-like ions (1)

Be-like ions are a good test case:

- Strong intrashell correlation
- Fast calculation

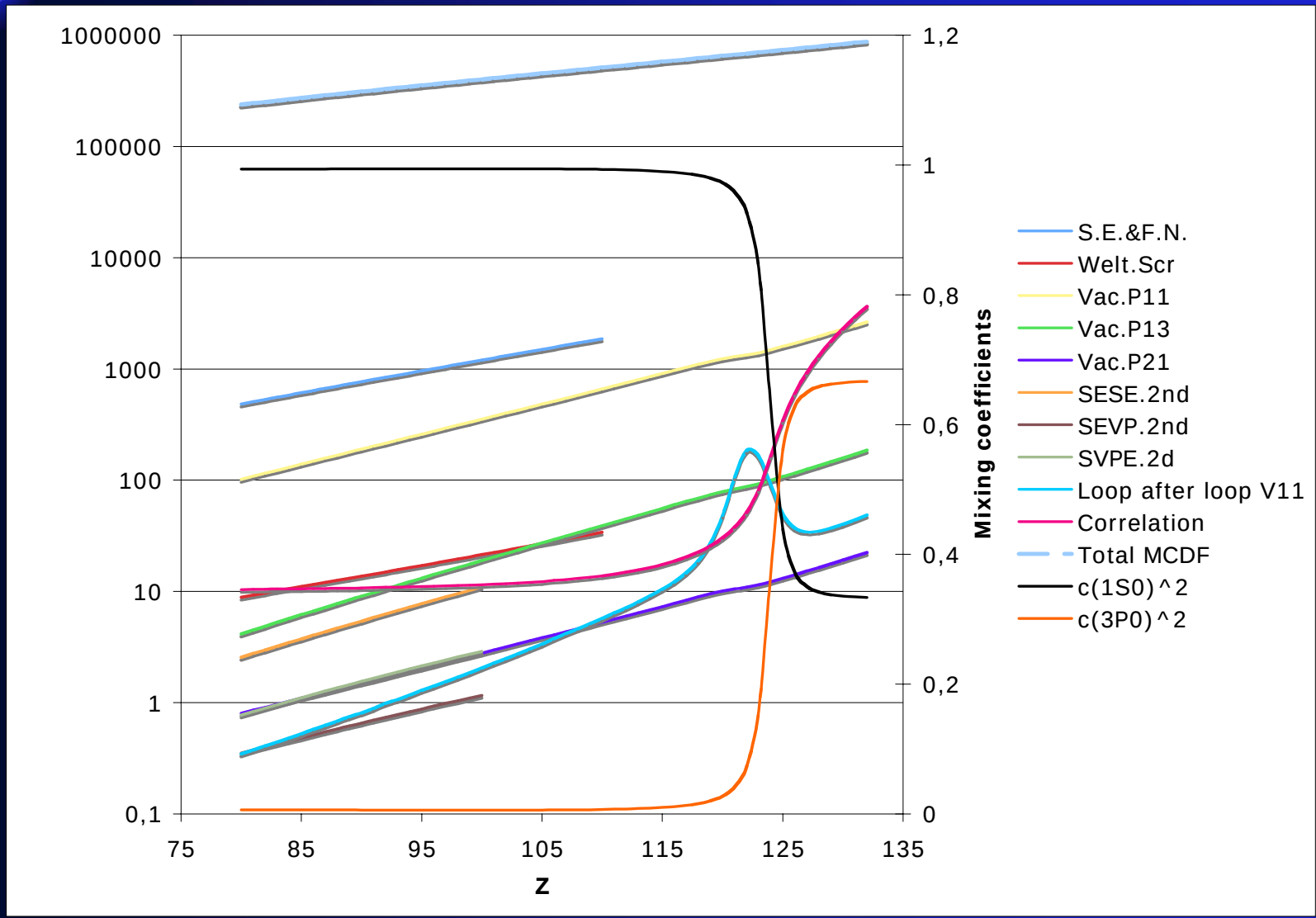
$|\mathrm{Be}\ {}^1S_0\rangle = c_1|\ {}^1S_0\rangle + c_2|\ {}^3P_0\#1\rangle + c_3|\ {}^3P_0\#2\rangle$ (LSJ)

$|\mathrm{Be}\ J=0\rangle = d_1|1s^2 2s^2\ J=0\rangle + d_2|1s^2 2p_{1/2}{}^2\ J=0\rangle + d_3|1s^2 2p_{3/2}{}^2\ J=0\rangle$ (JJ)

Test bench for all-order Breit, non-perturbative vacuum polarization

Can we observe new qualitative effects for SHE?

Be-like ions (2)



Be-like ions (3)

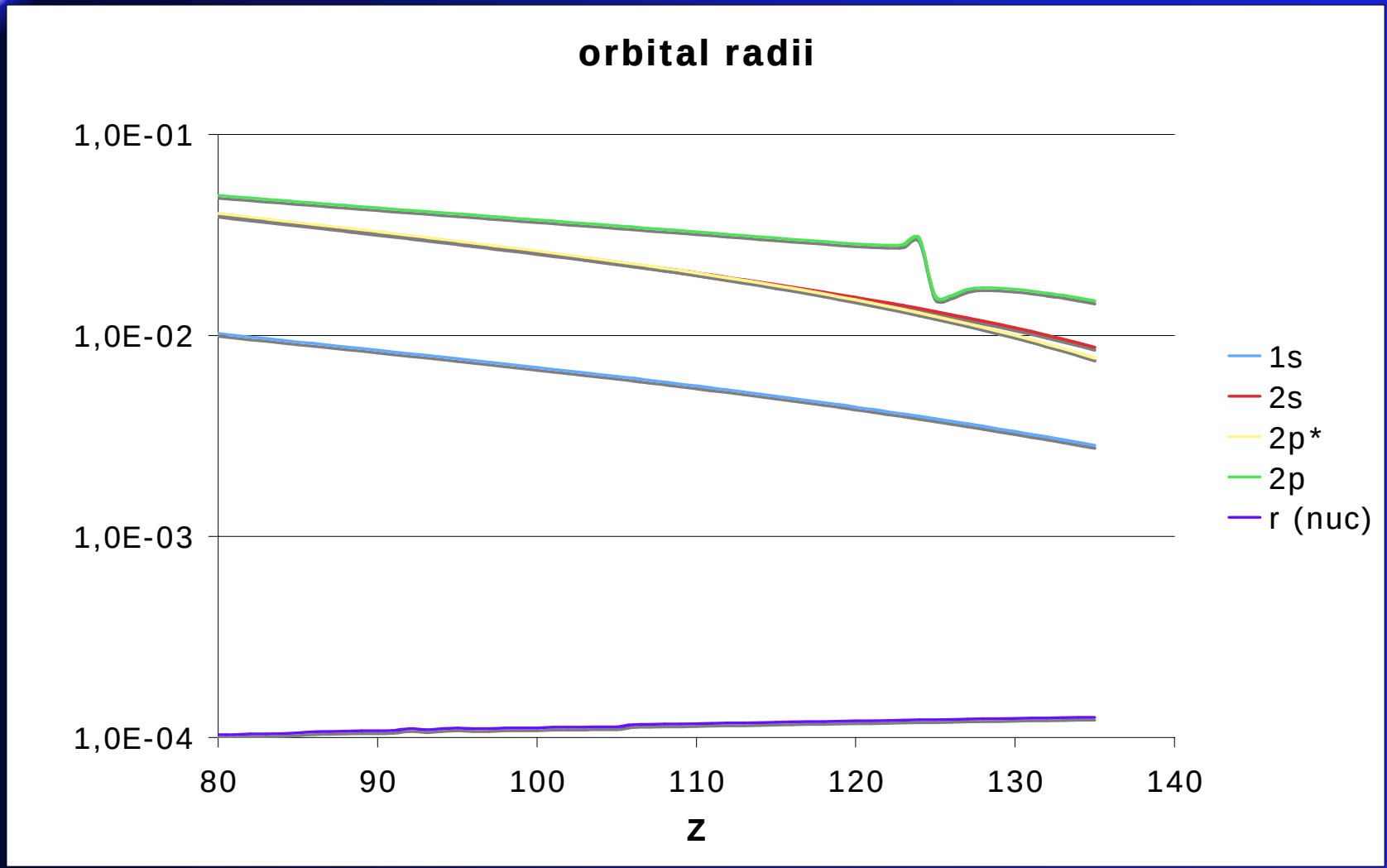
Summary

around Z=125:

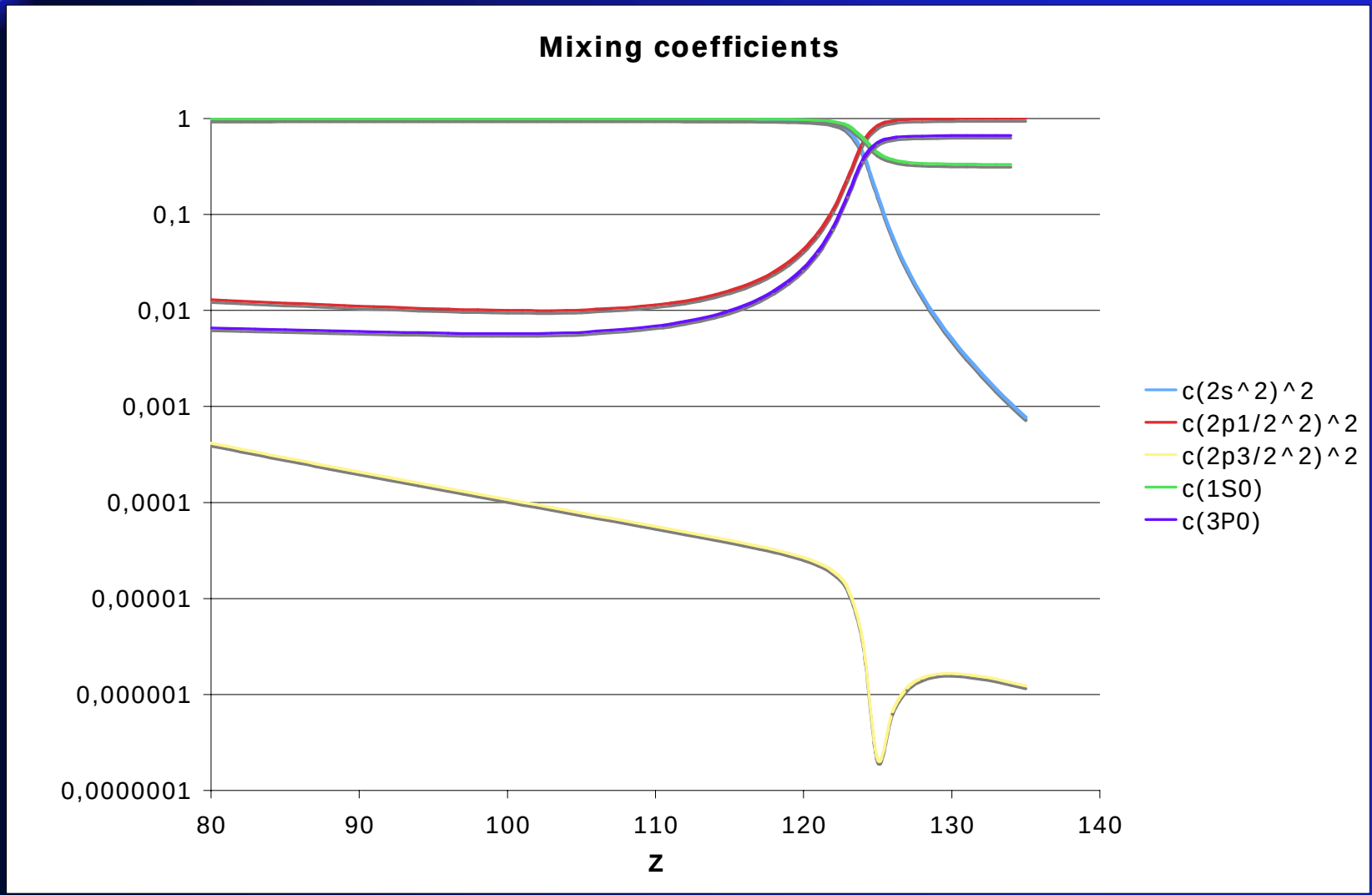
- Ground state becomes $^3P_0$
- Loop-after-loop Vacuum polarization has a strong enhancement
- Correlation becomes very strong

Other effects?

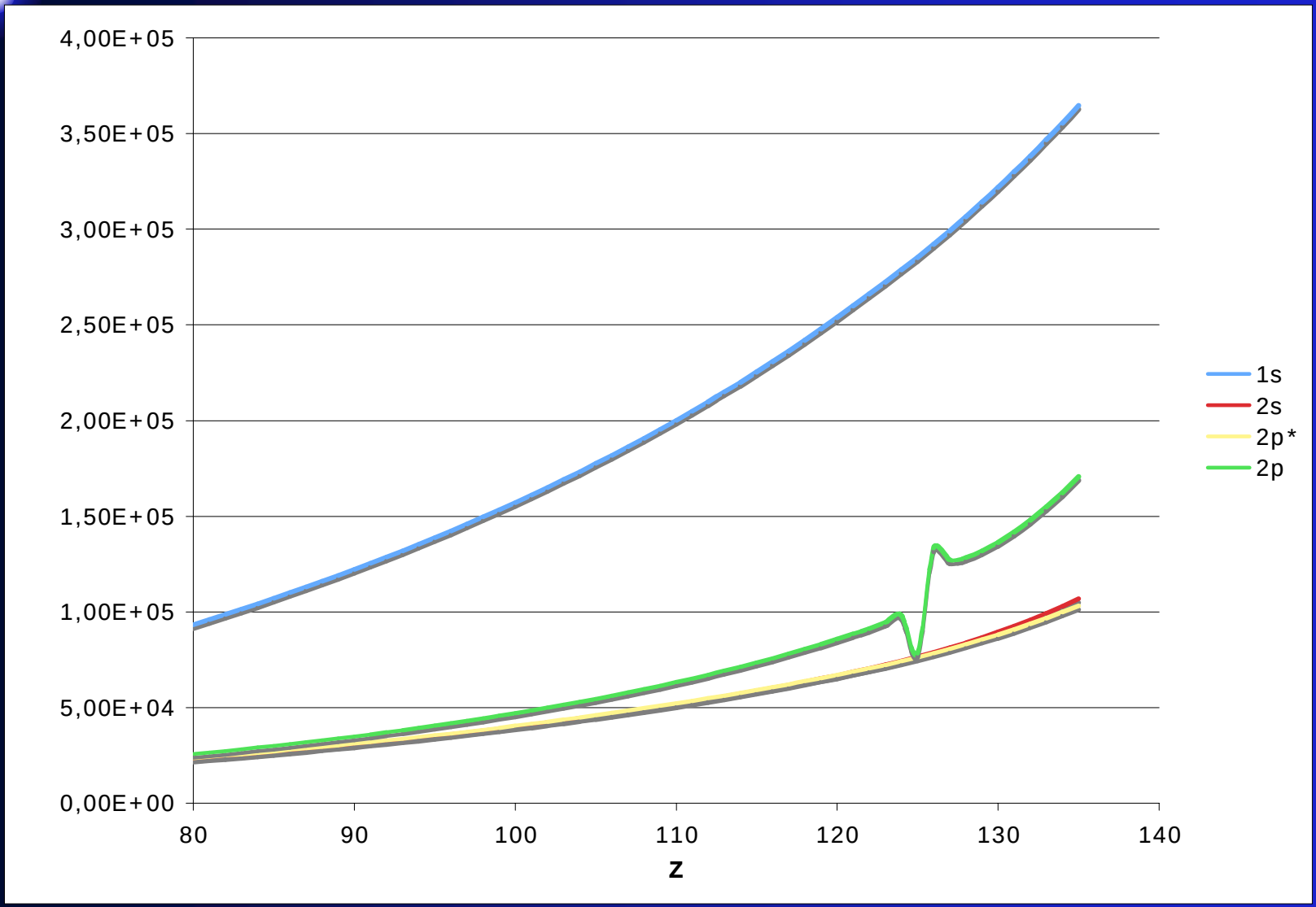
Be-like ions (4)



Be-like ions (5)



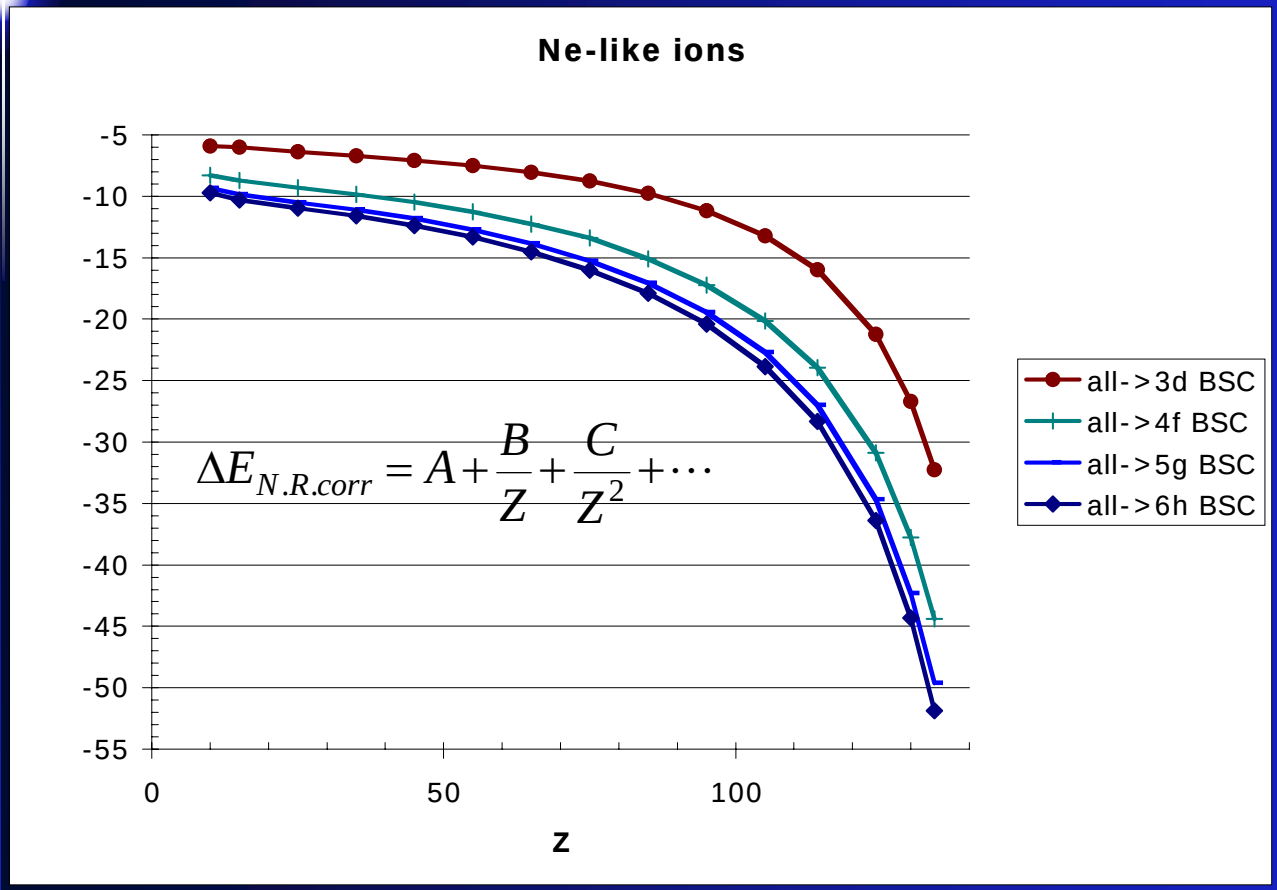
Be-like ions (6)



Be-like ions (summary)

- Variational calculations seems to disprove current wisdom
  - Perturbative QED may have a hard-time predicting such effects
  - Correlation does not become “negligible” at high-Z
- Is this general?
  - Check other cases with strong intra-shell correlation (Mg-like) No effect!
  - Generalize to complete correlation calculation of Be-like ions

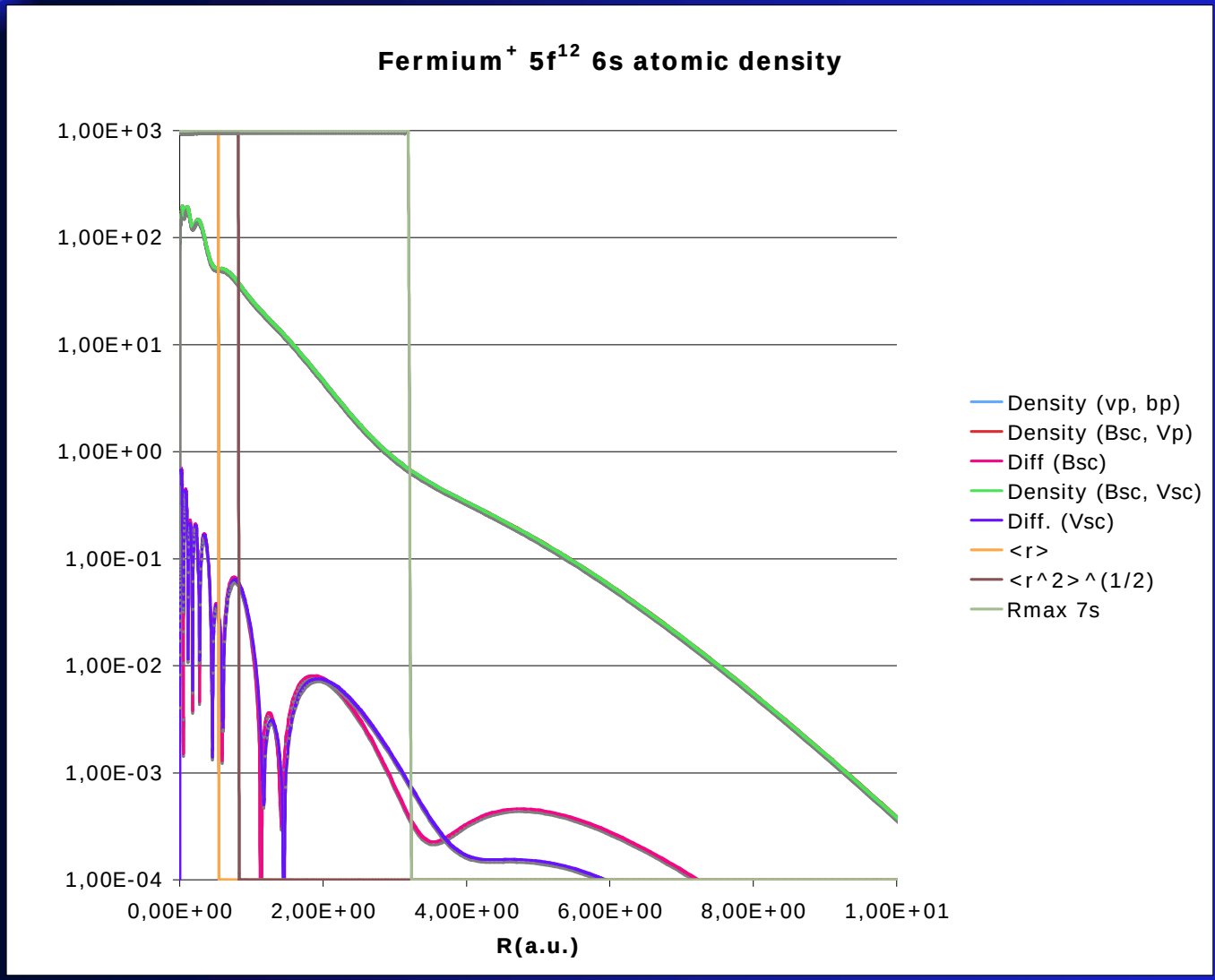
Total binding energy of Mg-like ions



Extension of the work below. Full Breit included. Projection operators included.
Includes all correlation within the n=1 to n=6 active space

J. P. Santos, G. C. Rodrigues, J. P. Marques, et al., Eur. Phys. J. D 37, 201 (2006).

QED effects on ion charge radii



Effect on operators: Fermium 1+ and 116 1+

Element 116^+	DF, Coul.	DF, Breit.	DF, Breit, VP
<r>	0,53928	0,53983	0,53979
<r^2>^(1/2)	0,82339	0,82425	0,82416
r $6d_{3/2}$	1,1816	1,1828	1,1829
r $6d_{5/2}$	1,2455	1,246	1,2461
r $7p_{1/2}$	1,9834	1,9894	1,9884
r $7p_{3/2}$	2,6644	2,6664	2,6674
r 7s	1,7601	1,7625	1,7605
r 1s	4,7699E-03	4,7835E-03	4,7646E-03
Total energy ($5f^{14}\ 6d^{10}\ 7s^2\ 7p^3\ {}^2P_{3/2}$)	-1416483,3	-1416496,1	-1416509,7
Landé factor	1,391236	1,392216	1,391890

Fermium$^+$	DF, Coul.	DF, Breit.	DF, Breit, VP
<r>	0,54496	0,54534	0,54531
<r^2>^(1/2)	0,82750	0,82800	0,82789
r $5f_{5/2}$	0,81710	0,81714	0,81719
r $5f_{7/2}$	0,83522	0,83478	0,83483
r 7s	3,2017	3,2054	3,2032
r 1s	6,9238E-03	6,9407E-03	6,9284E-03
Total energy ($5f^{11}\ 7s^2\ {}^4I_{15/2}$)	-946367,95	-946374,75	-946377,45
Total energy ($5f^{12}\ 7s\ {}^4I_{13/2}$)	-946367,96	-946374,76	-946377,46
Landé factor	1,226975	1,227150	1,227151

Breit and all-order VP have a large effect on total energy, but very small on radii and Landé g-factors

Fermium: ground state correlation

Contribution	Dirac-Foc	Dirac-Foc Breit	Correlation	Total
Coulomb	-948682,6593	2,4718	-3,3439	
Magnetic	1556,9048	-5,4744	0,0178	
Retardat.	-162,2941	0,5264	-0,0029	
Ret.>w2	-40,9350	0,2599	-0,0001	
Self-energy	1464,2558	0,0002	1,4679	
Screening	-134,1513	-6,1418	-1,4478	
Vac. Pol (Uehling)	-380,2252	1,6281		
Loop-a-loop Uehling	-1,1149	-1,5818		
Wichman&Kroll VP	20,7450	-0,0851		
Kallén&Sabry VP	-3,0095	0,0128		
Other 2nd Order	-12,1723			
Recoil	0,3100			
Total	-946374,3459	-8,3839	-3,3090	-946386,0388

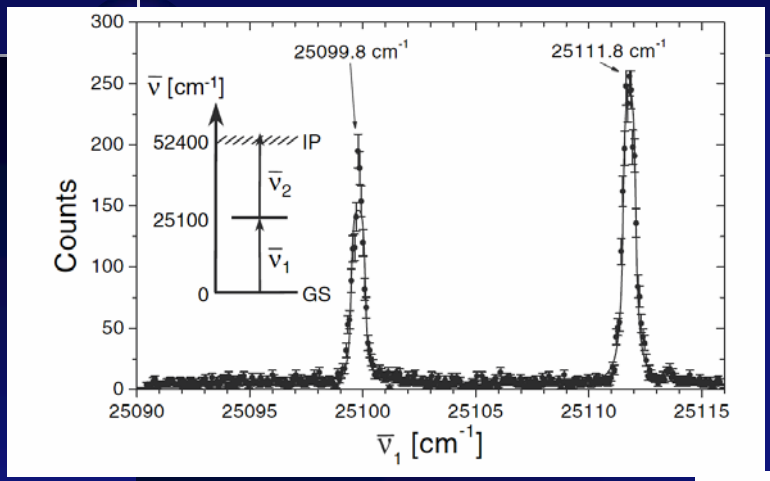
- Even at the Dirac-Fock level all order Breit has a very large effect
- Crossed QED-Breit terms are large.
- All numbers in eV

Transitions…

Contribution	Dirac-Foc	Dirac-Foc Breit	Total
Coulomb	10787,6	0,0	10787,6
Magnetic	23,0	0,1	23,1
Retardat.	-4,0	0,0	-4,0
Ret.>w2	-5,4	0,1	-5,3
Self-energy	-12613,7	0,0	-12613,7
Screening	12479,7	0,2	12479,9
Vac. Pol (Uehling)	42,3	-0,3	41,9
Loop-a-loop Uehling	1,0	-0,8	0,2
Wichman&Kroll VP	-2,0	0,0	-2,0
Kallén&Sabry VP	0,3	0,0	0,3
Other 2nd Order	0,0	0,0	0,0
Recoil	-6,3	0,0	-6,3
Total	10702,5	-0,8	10701,7

Effects that are large on total energy, are mostly negligible on transition energy
Correlation is the dominant effect by far…
Values in cm^{-1}

Comparison with experiment



M. Sewtz, H. Backe, A. Dretzke, et a
Rev. Lett. 90, 163002 (2003).

S. Fritzsche, using GRASP

Table I. Results of MCDF calculations. Listed are wave number $\bar{\nu}$, total angular momentum quantum number J, transition rate A_{ki}, configuration in the LS coupling scheme with largest expansion coefficient c, term assignment and $|c|^2$. Taken from [4, 7].

No.	$\bar{\nu}$ [cm^{-1}]	J	A_{ki} [1/s]	Config.	Term	$\lvert c\rvert^2$
0	0	6	0	$5f^{12}7s^2$	$^3H^e_6$	0.96
1	25,226	6	$1.89 \cdot 10^6$	$5f^{12}7s7p$	$^5I^o_6$	0.46
2	25,471	5	$1.28 \cdot 10^6$	$5f^{12}7s7p$	$^5G^o_5$	0.34
3	27,394	6	$2.43 \cdot 10^8$	$5f^{12}7s7p$	$^3H^o_6$	0.62
4	27,633	5	$1.98 \cdot 10^8$	$5f^{12}7s7p$	$^3G^o_5$	0.60
5	27,802	7	$3.67 \cdot 10^8$	$5f^{12}7s7p$	$^3I^o_7$	0.66
6	28,540	5	$2.82 \cdot 10^5$			
7	29,359	5	$3.58 \cdot 10^7$			

Conclusion and perspectives

- QED and relativistic many-body effects in SHE are deeply mixed
- Screening of the self-energy almost completely cancel self-energy for quasi-neutral systems.
- All-order Breit contributions very significant
- Strongly non-perturbative effects for highly-ionized system wash out when going to neutral systems
- All-order calculations with vacuum polarization, as a model of all order QED, do not show unexpected behavior when $Z\,\alpha \rightarrow 1$