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MCDF Level Structure and Isotope-Shift Calculations for Medium and Heavy Elements

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Outline

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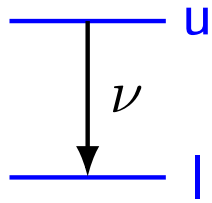
Isotope-Shift Theory

- Observed transition frequency isotope dependent
- Extraction of nuclear parameters
- Transition isotope shift parametrized by



$$\delta\nu^{AA'} = \left(M^{\mathrm{NMS}} + M^{\mathrm{SMS}}\right) \frac{A - A'}{AA'} + F\,\delta\left\langle r^2\right\rangle^{AA'} \qquad A > A'$$

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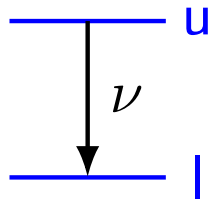

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- Field-shift due to change in charge distribution

$$\delta\nu^{\mathrm{FS}} = F\delta\left\langle r^2\right\rangle^{AA'}$$

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Isotope-Shift Theory

Mass Shift

- Transition isotope shift parametrized by

$$\delta\nu^{AA'} = \left(M^{\mathrm{NMS}} + M^{\mathrm{SMS}}\right)\frac{A - A'}{AA'} + F\delta\left\langle r^2\right\rangle^{AA'} \qquad A > A'$$

- Mass shift due to nuclear recoil

$$H = \frac{1}{2M}\sum_{ij} p_i p_j$$

- Separation into normal and specific mass shift
- Normal mass shift

$$H = \frac{1}{2M}\sum_{i} p_i^2 \qquad \delta\nu^{\mathrm{NMS}} \approx \nu^{\infty}\frac{m_e}{M}$$

- Two-electron contribution gives rise to specific mass shift

$$H = \frac{1}{2M}\sum_{i<j} p_i p_j$$

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Calculation of Isotope Shifts

- Mass Shift parameters

$$M_{\mathrm{NMS}} \propto \langle \psi \,|\, H_{\mathrm{NMS}} \,|\, \psi \rangle \qquad M_{\mathrm{SMS}} \propto \langle \psi \,|\, H_{\mathrm{NMS}} \,|\, \psi \rangle$$

- Estimate of field-shift parameter

$$F \propto \Delta \, |\psi(0)|^2$$

- Implemented in the GRASP2k package [1]

[1] C. Nazé et al., *CPC*, 184pp. 2187–2196

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Alternative approach:

- Calculation of $\delta\nu$ for several isotopes
- Solve system of equations, based on parametrization
- Variation between results interpreted as error estimate

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Multi-Configuration Dirac-Fock Method

General

- Multi-configuration expansion

$$\Psi(PJM) = \sum_{i=1}^{N} c_i \Phi(\gamma_i PJM) \qquad \sum_i |c_i|^2 = 1$$

- Configuration-state functions Φ are superpositions of Slater determinants
- Single-electron orbitals φ_i calculated by minimization of energy functional

$$E = \langle \Psi(PJM) | H_{\mathrm{DC}} | \Psi(PJM) \rangle \tag{1}$$

- Variation in c_i is called configuration interaction, leads to eigenvalue problem

$$\boldsymbol{H}\boldsymbol{c} = E\boldsymbol{c}$$

- Matrix Elements

$$H_{ij} = \langle \Phi_i | H_{\mathrm{DC}} + H' | \Phi_j \rangle$$

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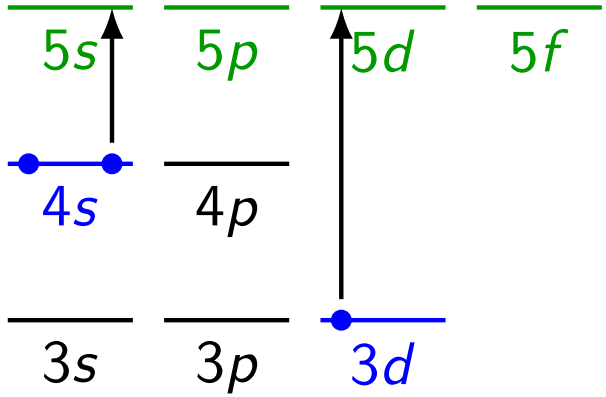
Multi-Configuration Dirac-Fock Method

Generation of basis sets

- Active-space method
- Configuration-state functions obtained by virtual excitations

Example: Mn

Reference configuration: $3d^5 4s^2$



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Multi-Configuration Dirac-Fock Method

Generation of basis sets

- Active-space method
- Configuration-state functions obtained by virtual excitations
- Successive enlargement of active space: "correlation layer"
- Layer model allows to monitor convergence

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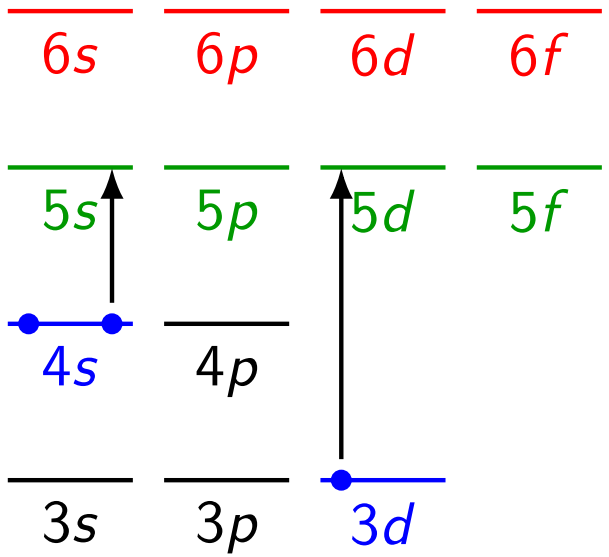

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Results

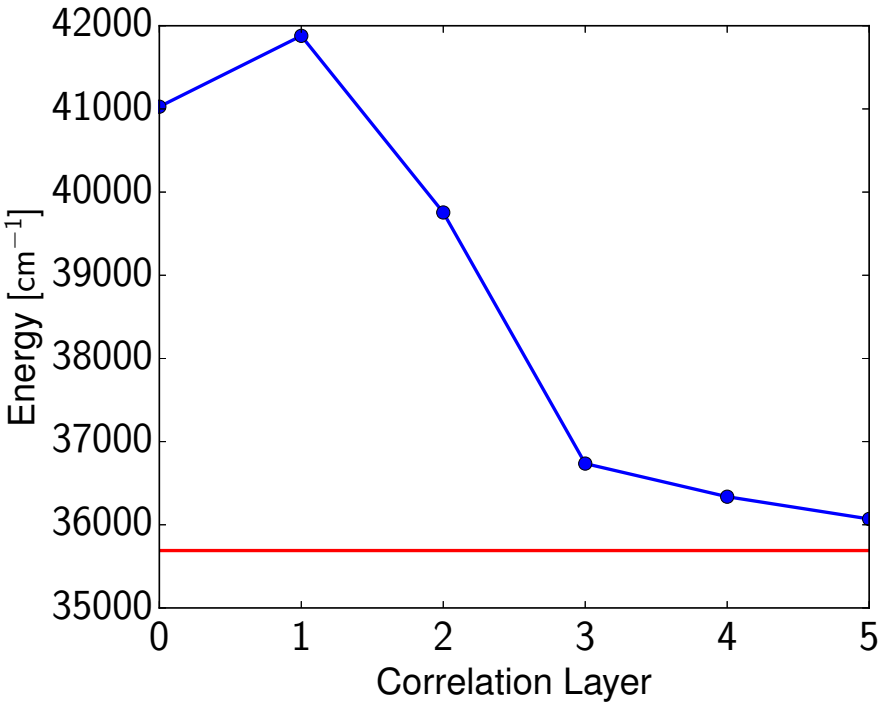
Manganese

- $3d^5 4s^2 \left(^6S_{5/2}\right) - 3d^5 4s4p \left(^6P^o_{3/2}\right)$, $\Delta E = 35\,690\,\mathrm{cm}^{-1}$
- Reference Configurations: $3d^5 \left(4s^2 + 4p^2\right)_{5/2}$, $\left(3d^5 4s4p + 3d^6 4p\right)_{3/2}$

Correlation Model

Layer	Exc.	Orbitals	N_{CSF}
0		3d 4s 4p	232
1	SDTQ	3d 4s 4p	8 295
2	SD	5s 5p 5d 5f	94 779
3	SD	6s 6p 6d 6f	243 621
4	SD	7s 7p 7d 7f	454 821
5	SD	8s 8p 8d 8f	728 379

Transition energy



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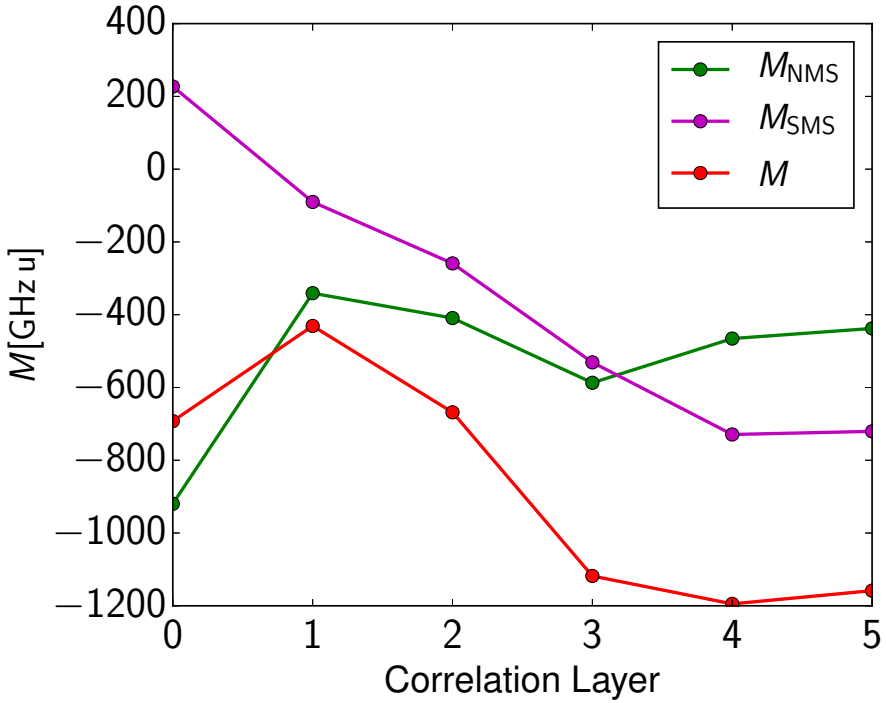
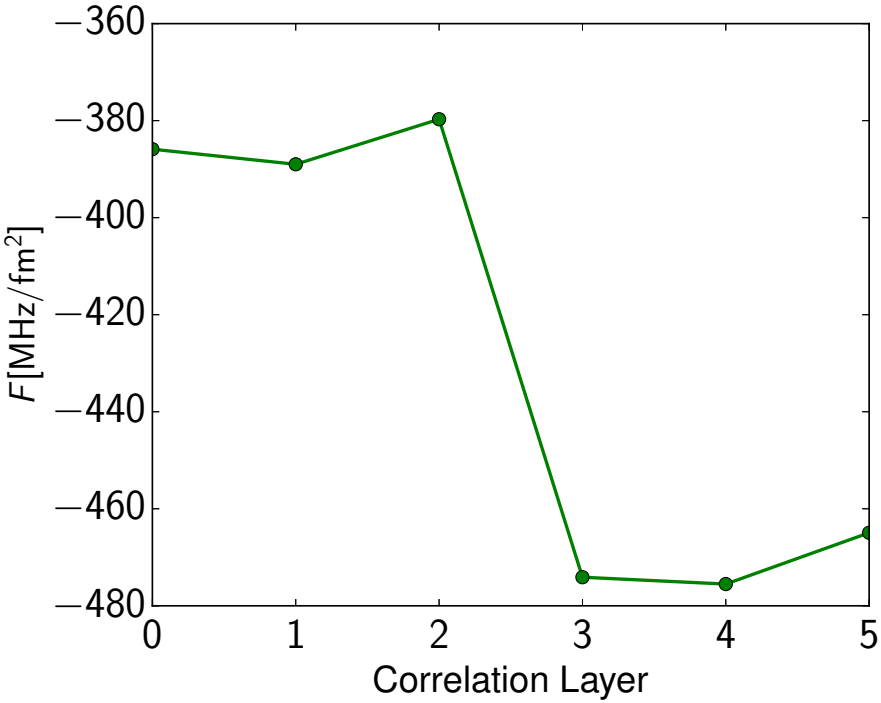
Mass-shift parameters



Field-shift parameter



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Atomic Physics Toolkit: JAC

General

- Package for atomic physics calculations
- Bound states and interaction with continuum states: Photo-ionization, auto-ionization, recombination...
- Many existing Tools in RATIP [2]
- Wave function generation using GRASP [3]
- Integrate existing software
- Data conversion and management

[2] S. Fritzsche, *CPC*, 183pp. 1525–1559

[3] P. Jönsson et al., *CPC*, 184pp. 2197–2203

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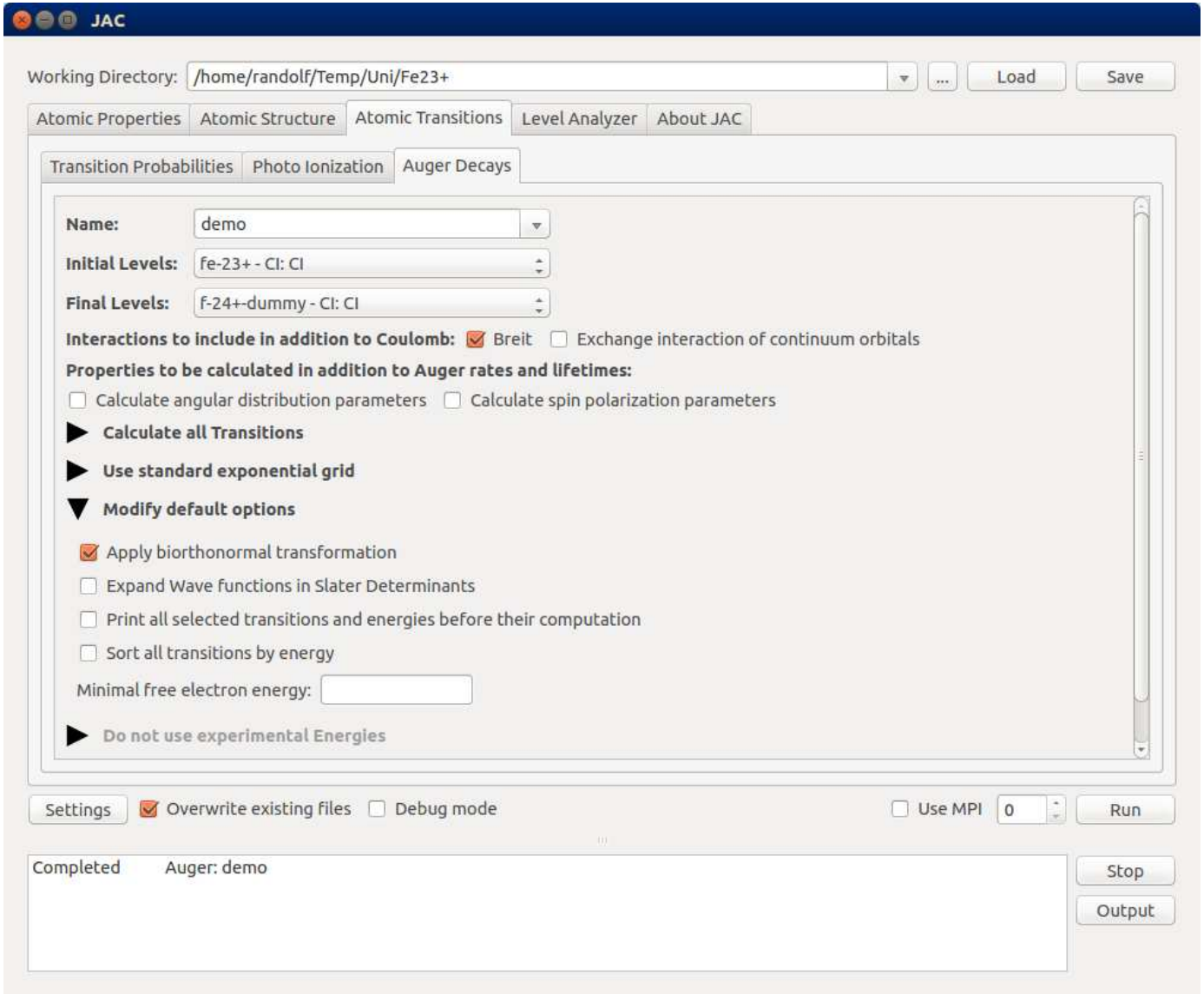

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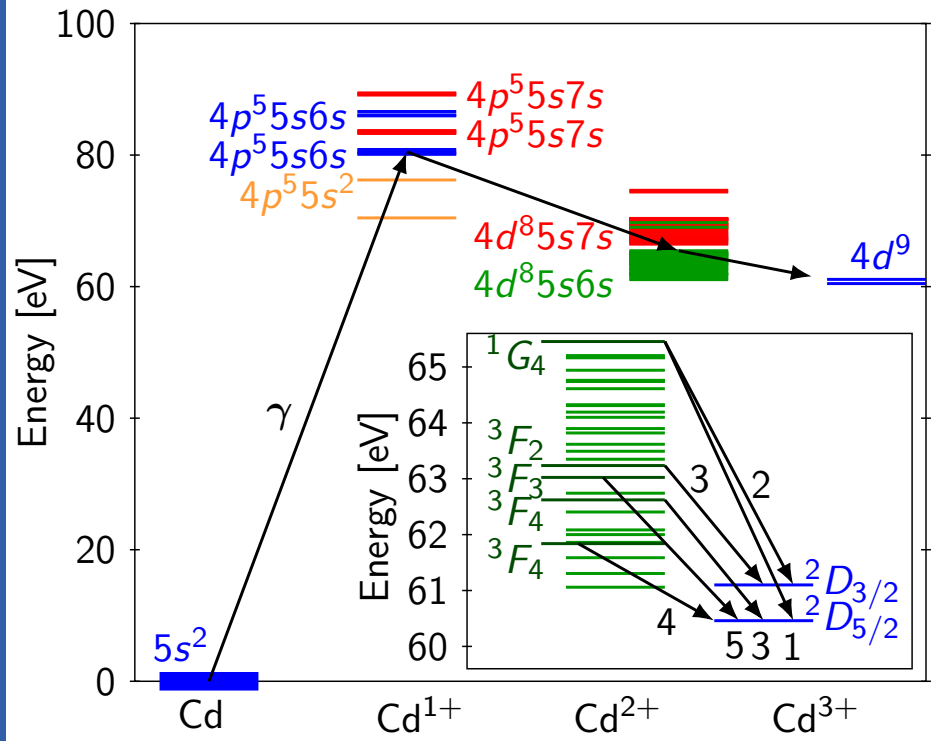
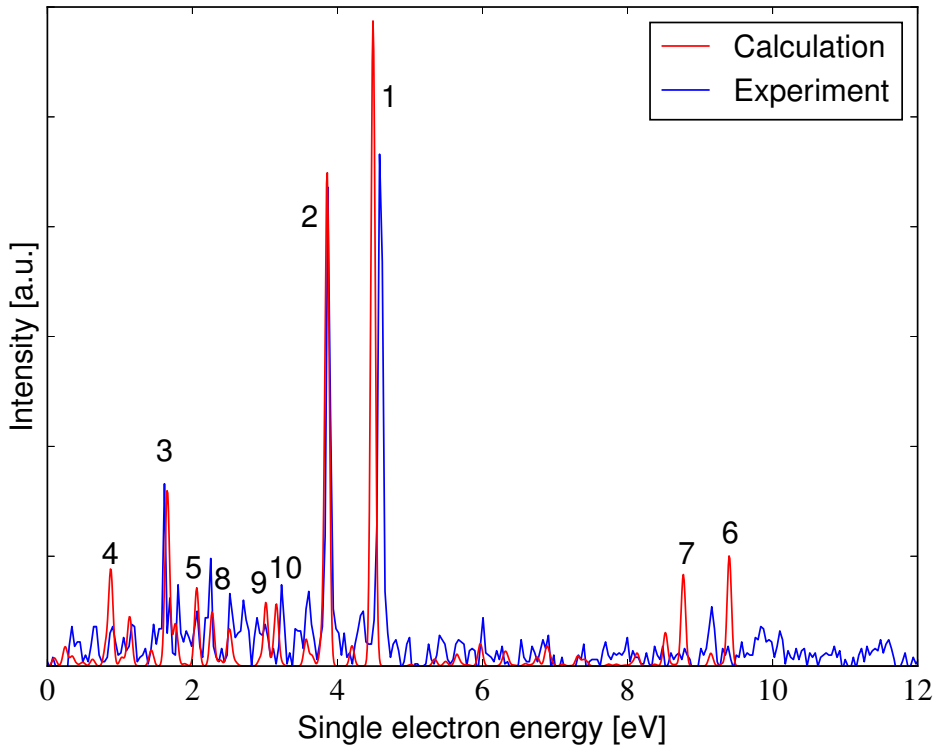
Double-Auger Cascades in Cadmium

- Inner shell ionization is followed by multiple auger cascades
- Spectrum of emitted electrons calculated
- Process dominated by shake-up transitions 5s $\rightarrow$ 6s





[4] J. Andersson et al., *Phys. Rev. A*, 92p. 023414

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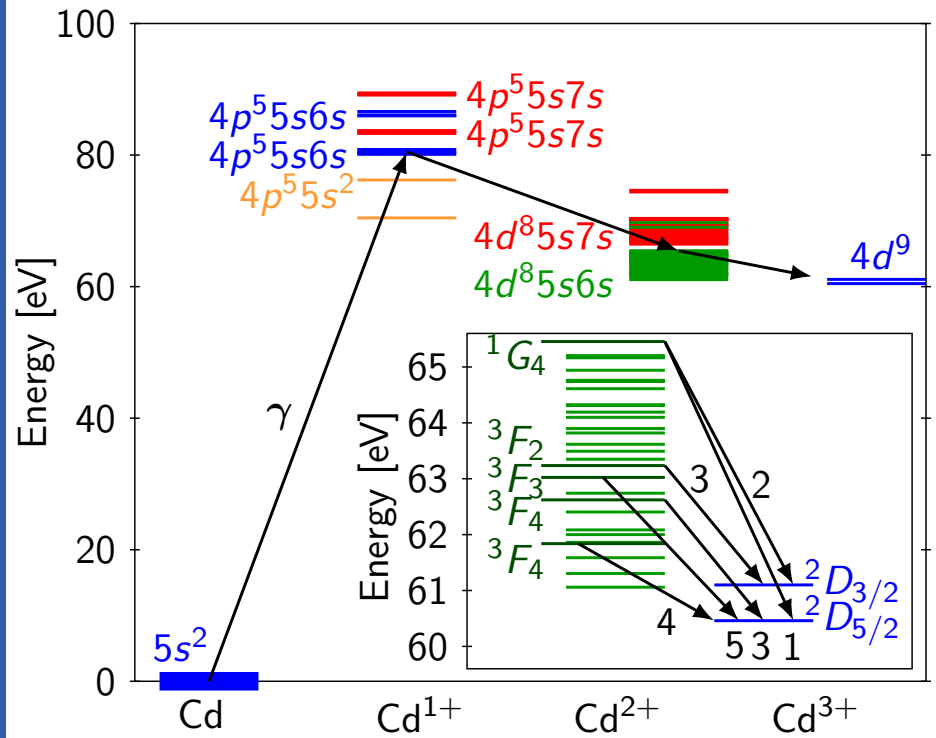
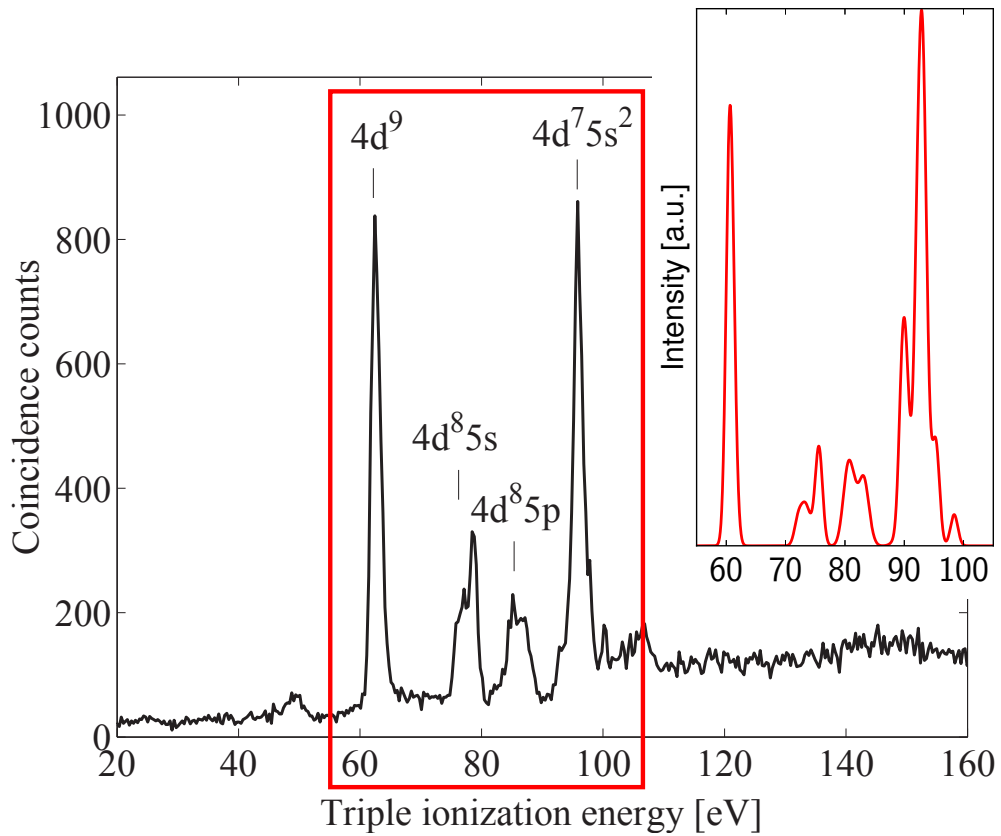




[4] J. Andersson et al., *Phys. Rev. A*, 92p. 023414

Shake-up Transitions: Biorthonormal transformation

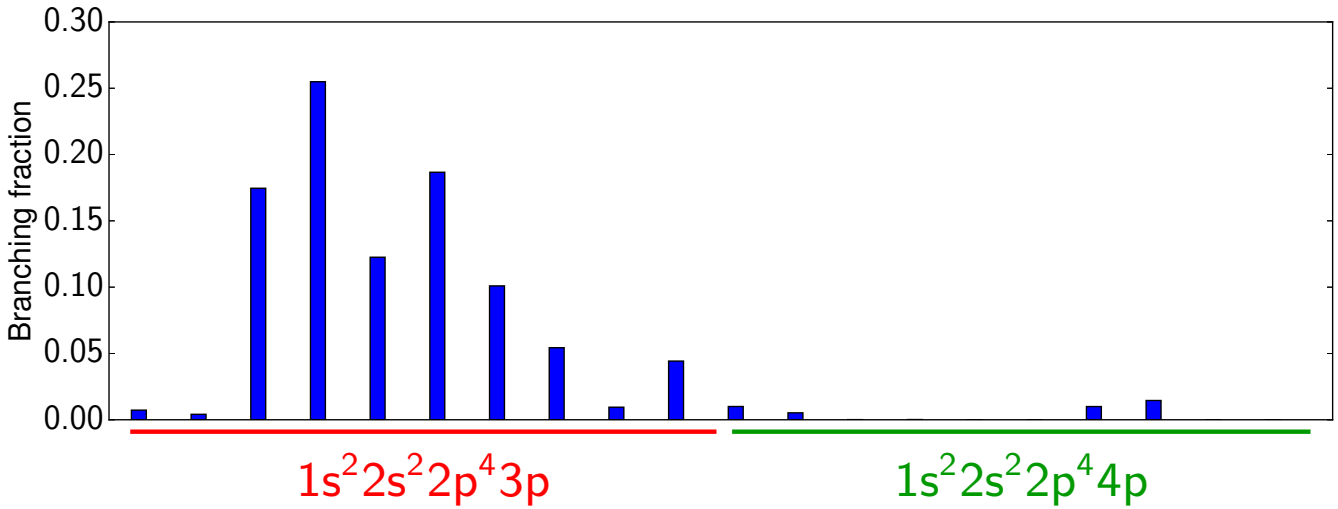
- Evaluation of transition amplitudes

$$A \propto \langle \psi \,|\, V \,|\, \psi' \rangle \qquad\qquad \langle \varphi_i \,|\, \varphi'_j \rangle = \delta_{ij}$$

- Shake-up transitions cannot be calculated in this approximation

Example: Neon 1s Auger decay

$1s2s^2 2p^6 3p \rightarrow 1s^2 2s^2 2p^4 \,(3p + 4p) + e^-$



[5] J. Olsen et al., *Phys. Rev. E*, 52pp. 4499–4508

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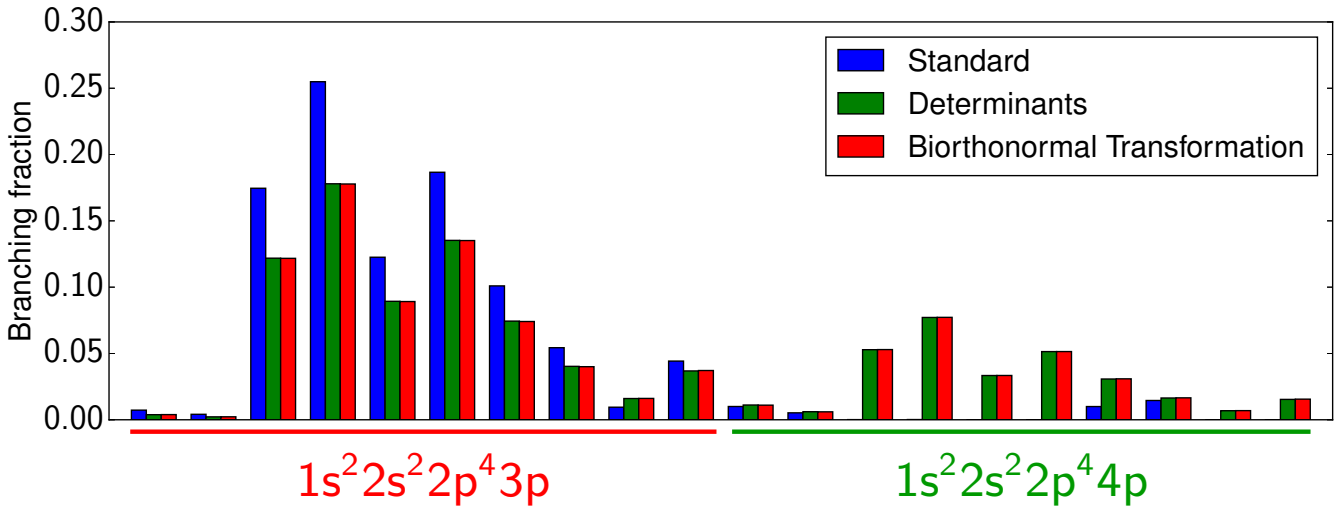
- Biorthonormal transformation [5] $\langle \varphi'_i | \varphi'_j \rangle = \delta_{ij},\ c_i \mapsto c'_i$



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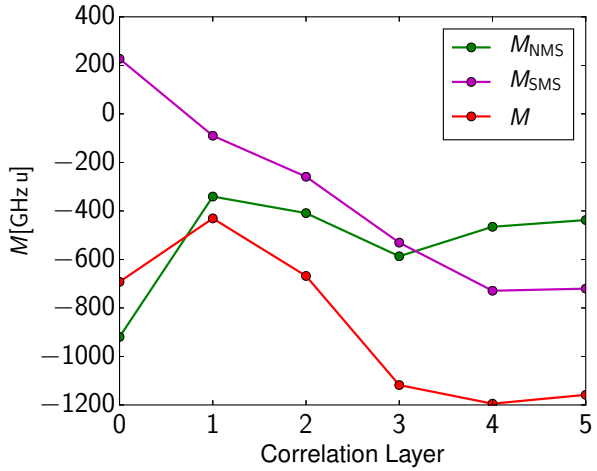
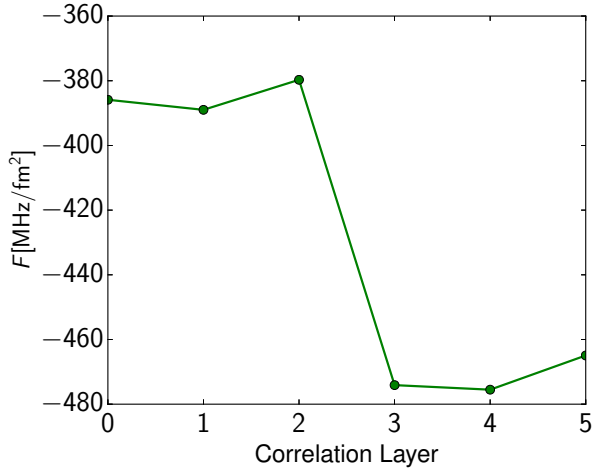
Conclusions

- Our strategy on calculation of isotope-shift parameters
- Some results on isotope-shift calculations: Manganese
- Glimpse on our new Atomic Physics Toolkit: JAC
- Example: Biorthonormal transformation applied to calculation of Auger transition rates





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