https://www.github.com/OpenJAC/JAC.jl

Atomic Computations

JAC – A community approach to atomic structures, processes and cascades

Stephan Fritzsche
Helmholtz-Institut Jena &
Theoretisch-Physikalisches Institut Jena
14th March 2019

Hacky hours – **jDPG**

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Atomic Computations

JAC – A community approach to atomic structures, processes and cascades

Simple atomic processes:

$$A^* \longrightarrow A^{(*)} + \hbar\omega \quad \text{... photon emission}$$

$$A + \hbar\omega \longrightarrow A^* \quad \text{... photon excitation}$$

$$A + \hbar\omega \longrightarrow A^{+*} + e_p^-$$

$$A^{q+*} \longrightarrow A^{(q+1)+(*)} + e_a^-$$

$$e_s^- + A \longrightarrow A^* + e_s^{-\prime}$$

$$e_s^- + A \longrightarrow A^* + e_s^{-\prime} + e^-$$

$$A + n\,\hbar\omega \longrightarrow A^*$$

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Simple atomic processes:

A^*	$\longrightarrow$	$A^{(*)} + \hbar\omega$	... photon emission
$A + \hbar\omega$	$\longrightarrow$	A^*	... photon excitation
$A + \hbar\omega$	$\longrightarrow$	$A^{+*} + e_p^-$	... (atomic) photoionization
A^{q+*}	$\longrightarrow$	$A^{(q+1)+(*)} + e_a^-$	... Auger emission; autoionization
$e_s^- + A$	$\longrightarrow$	$A^* + e_s^{-\prime}$	... electron – impact excitation
$e_s^- + A$	$\longrightarrow$	$A^* + e_s^{-\prime} + e^-$	... electron – impact ionization
$A + n\,\hbar\omega$	$\longrightarrow$	A^*	... multi – photon excitation/decay

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Quiz: Atomic processes in a nutshell

-- for “intermediates” in atomic and plasma physics

$$A + n\,\hbar\omega \longrightarrow A^{+(*)} + e_p^- \quad \text{... multi-photon ionization}$$

$$A + n\,\hbar\omega \longrightarrow A^{+(*)} + (e_{p_1}^- + e_{p_2}^-) \quad \text{... multi-photon double ionization}$$

$$A^{q+} + e_s^- \longrightarrow A^{(q-1)+} + \hbar\omega \quad \text{... radiative recombination}$$

$$A^{q+} + e_s^- \longrightarrow A^{(q-1)+*} \longrightarrow A^{(q-1)+(*)} + \hbar\omega \quad \text{... dielectronic recombination}$$

$$A + \hbar\omega \longrightarrow A^{(*)} + \hbar\omega' \quad \text{... Rayleigh/Compton}$$

$$A^{q+*} \longrightarrow A^{(q+1)+(*)} + (e_a^- + \hbar\omega) \quad \text{... radiative Auger}$$

$$A^{q+*} \longrightarrow A^{(q+2)+(*)} + (e_{a_1}^- + e_{a_2}^-) \quad \text{... double Auger}$$

$$A + \hbar\omega \longrightarrow A^* \longrightarrow A^{(*)} + \hbar\omega' \quad \text{... photo-excitation \& fluorescence}$$

$$A + \hbar\omega \longrightarrow A^{+,*} + e_p^- \longrightarrow A^{(*)} + e_p^- + \hbar\omega' \quad \text{... photo-ionization \& fluorescence}$$

$$A + Z_p \longrightarrow A^* + Z_p' \quad \text{... Coulomb excitation}$$

$$A^{(q+1)+} + Z_p \longrightarrow A^{(q+1)+(*)} + e^- + Z_p' \quad \text{... Coulomb ionization}$$

- Indeed, these and many other processes occur in atomic, plasma and astro physics as well as at various places elsewhere.
- How much help can atomic theory provide ? -- Which tools are available ?

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Simple atomic processes:

A^*

$A + \hbar\omega$

$A + \hbar\omega$

A^{q+*}

$e_s^- + A$

$e_s^- + A$

$A + n\,\hbar\omega$

Plan of this tutorial

- Demands from theory & experiment: A short example
- Established structure codes: Strength and weaknesses
- JAC: A fresh approach and implementation
- Amplitudes, properties & processes
- First tutorial
- Atomic cascades
- Summary & conclusions

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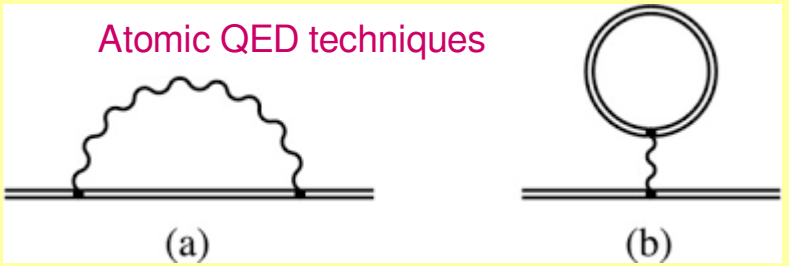
Atomic Computations

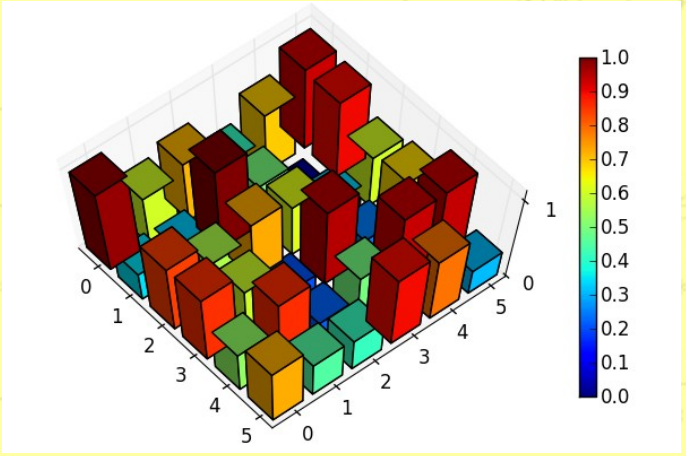
JAC – A community approach to atomic structures, processes and cascades

Dirac's equation

$$(\beta mc^2 + c\vec{\alpha}.\vec{p})\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

Atomic QED techniques





$$\left\{-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial r_m^2}-\frac{l_i(l_i+1)}{r_m^2}\right]+\sum_{\mathbf{R}_i}\frac{-Ze^2}{|\mathbf{r}_m-\mathbf{R}_i|}\right\}P_i(r_m)$$
$$+\left[\sum_j^{occ}\int dr_n P_j^\dagger(r_n)\frac{e^2}{|r_m-r_n|}P_j(r_n)\right]P_i(r_m)$$
$$-\left[\sum_j^{occ}\int dr_n P_j^\dagger(r_n)\frac{e^2}{|\mathbf{r}_m-\mathbf{r}_n|}P_i(r_n)\right]P_j(r_m)=\varepsilon_i P_i(r_m)$$

Dirac-Fock & beyond

$e_s^- + A \longrightarrow A^* + e_s^{-\prime} + e^-$ ... electron – impact ionization

$A + n\,\hbar\omega \longrightarrow A^*$ ... multi – photon excitation/decay

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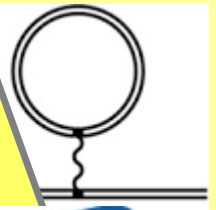


Accurate Atomic Amplitudes

$<\Phi_\alpha \| V^L \| \Phi_\beta>$

Approved

$$\left[\sum_j \int dr_n P_j^\dagger(r_n)\frac{e^2}{|r_m - r_n|}P_j(r_n)\right]P_i(r_m)$$

Dirac-Fock & beyond

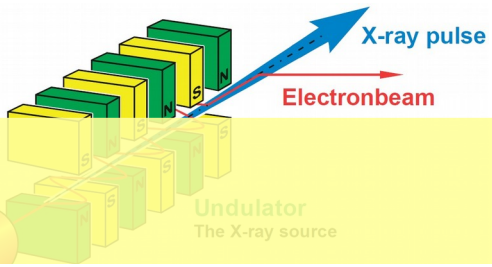
$$-\left[\sum_j^{occ} \int dr_n P_j^\dagger(r_n)\frac{e^2}{|\mathbf{r}_m - \mathbf{r}_n|}P_i(r_n)\right]P_j(r_m) = \varepsilon_i P_i(r_m)$$

$e_s^- + A \longrightarrow A^* + e_s^{-\prime} + e^-$ ... electron – impact ionization

$A + n\,\hbar\omega \longrightarrow A^*$ ... multi – photon excitation/decay

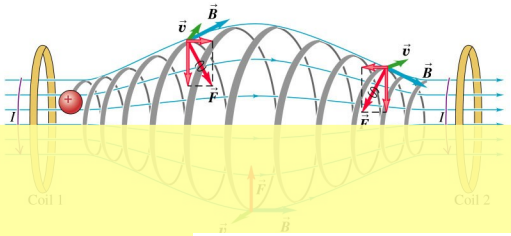
Demands from experiment

– owing to new large-scale facilities & detector developments



XUV- & XFEL's

Laser pulse



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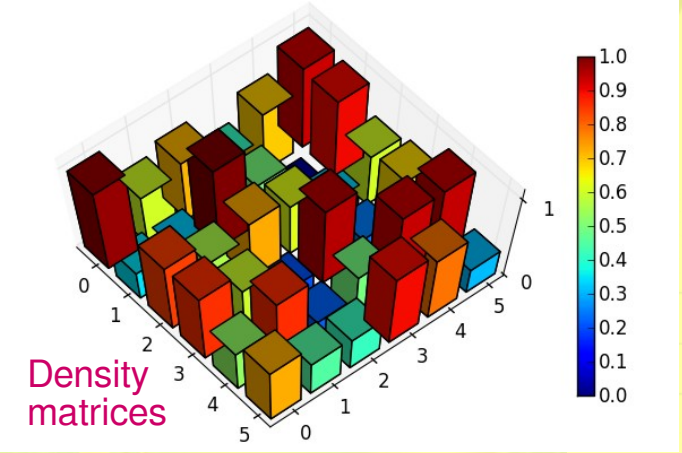


Density matrices

$$\left\{-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial r_m^2}-\frac{l_i(l_i+1)}{r_m^2}\right]+\sum_{\mathbf{R}_i}\frac{-Ze^2}{|\mathbf{r}_m-\mathbf{R}_i|}\right\}P_i(r_m)$$

$$+\left[\sum_j^{occ}\int dr_n P_j^{\dagger}(r_n)\frac{e^2}{|r_m-r_n|}P_j(r_n)\right]P_i(r_m)$$

Dirac-Fock & beyond

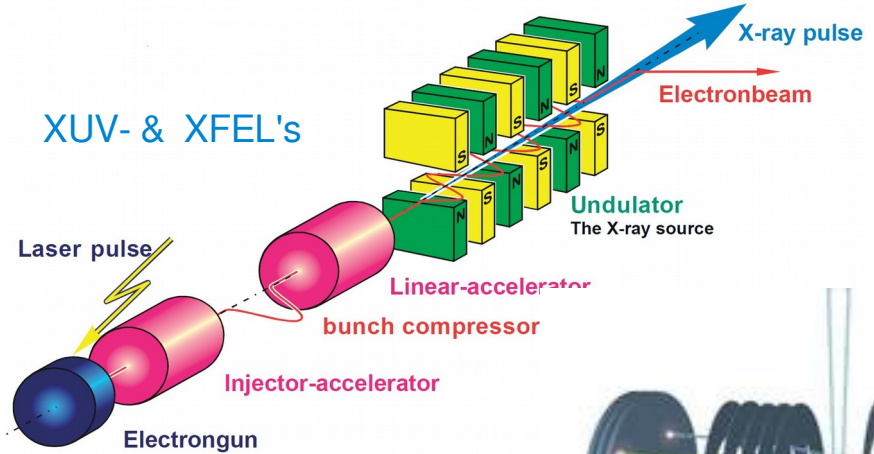
$$-\left[\sum_j^{occ}\int dr_n P_j^{\dagger}(r_n)\frac{e^2}{|\mathbf{r}_m-\mathbf{r}_n|}P_i(r_n)\right]P_j(r_m)=\varepsilon_i P_i(r_m)$$

merge-beam experiments

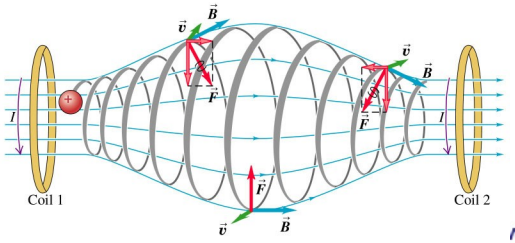
ion traps

Demands from experiment

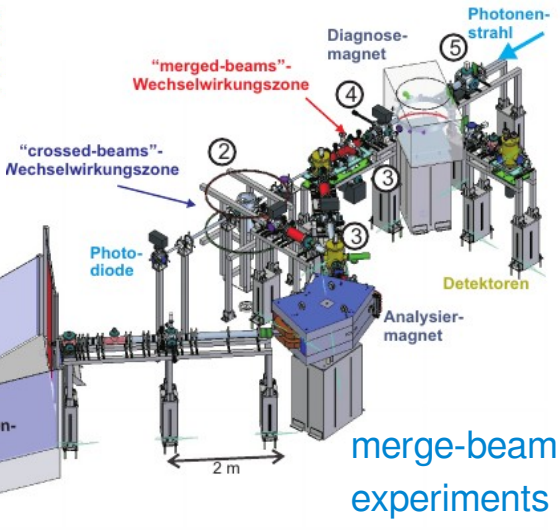
– owing to new large-scale facilities & detector developments



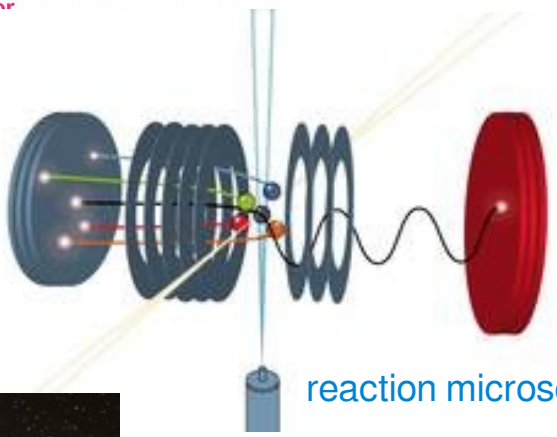
XUV- & XFEL's



magnetic bottles



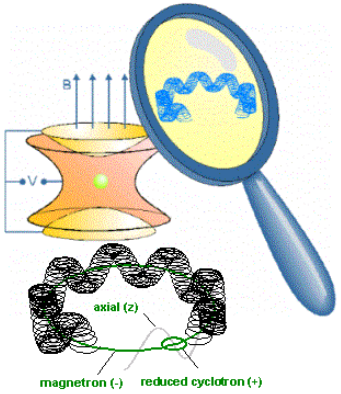
merge-beam experiments



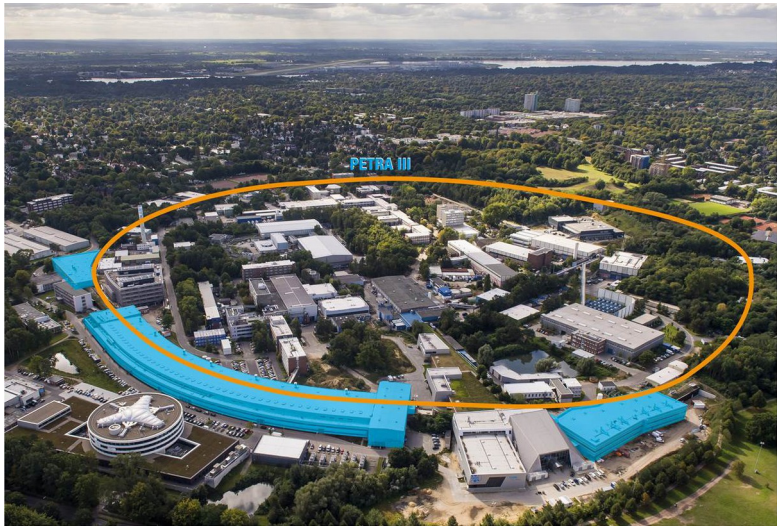
space missions

synchrotrons

reaction microscopes



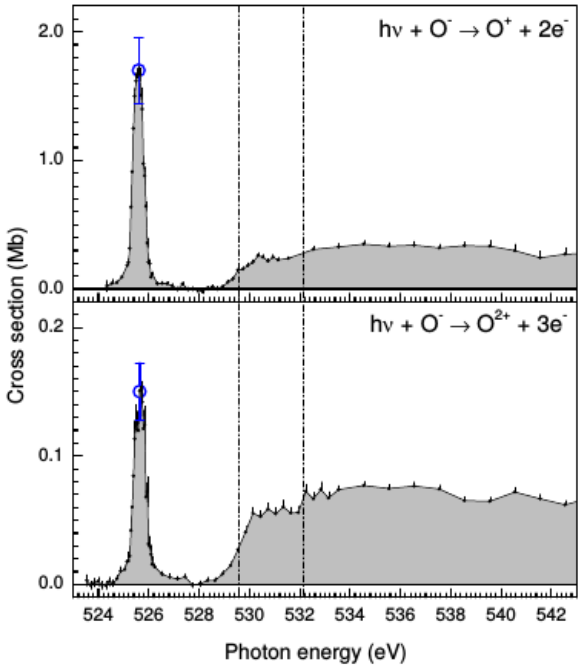
ion traps

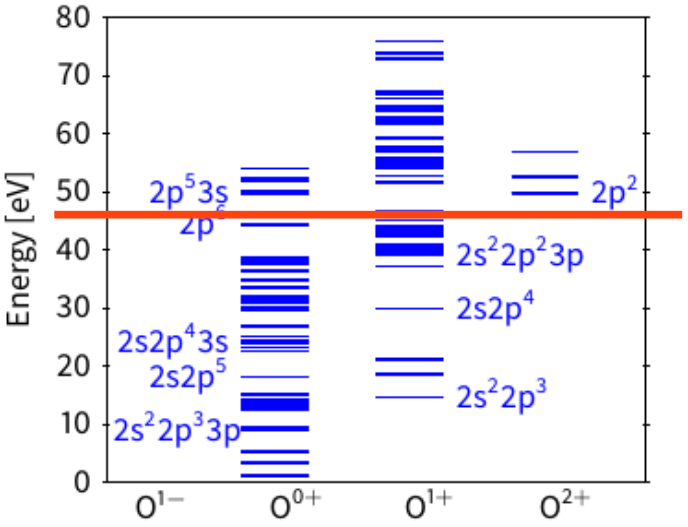


Ion & electron spectra after inner-shell excitations

– 1s-2p excitation of O^-, recorded at PIPE

$$O^-(1s^2\,2s^2\,2p^5) + \gamma \rightarrow O^-(1s\,2s^2\,2p^6\ {}^2S_{1/2}) \rightarrow O^{(m-1)+}(1s^2\,2l^{7-m}) + m\,e^-$$





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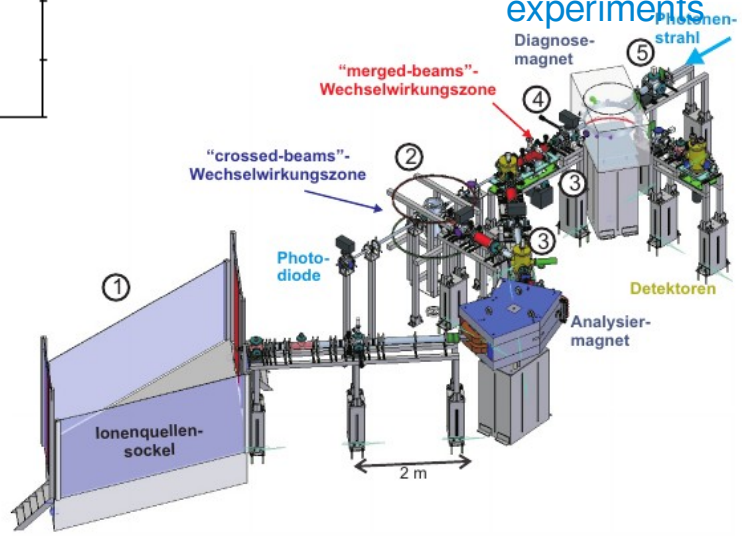

Double & triple detachments by Auger electron emission are energetically forbidden.

→ possible only due to shake-up

2s → 3s, 2p → 3p

PIPE – Photon-Ion spectrometer at PETRA III (Hamburg)

S. Schippers et al, PRA 94 (2016) 052412.

S. Schippers and coworkers, Gießen, Frankfurt, Hamburg collaboration (2015).

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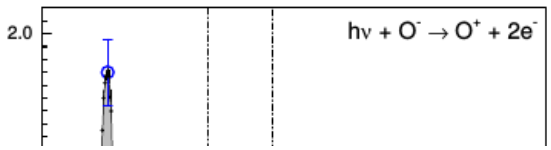

Model	Width [meV]	Branching Fraction O	Branching Fraction O^+	Branching Fraction O^{2+}	Ratio O^+/O^{2+}
Simple	133	0.77	0.23	0.0	—
$2s \rightarrow 3s + 2p \rightarrow 3p$	131	0.78	0.22	~ 0.0	—
$+ 2p^2 \rightarrow 3s^2 + 2p^2 \rightarrow 3p^2$	153	0.64	0.36	0.004	106
$+ 2s^2 \rightarrow 3s^2$	161	0.56	0.42	0.016	26
$+ 2s^2 \rightarrow 3p^2$	174	0.46	0.48	0.059	8.1
$+ 2p^2 \rightarrow 3d^2$	166	0.51	0.44	0.042	10.6
exp	164 ± 14	—	—	—	10.3

Established tools for atomic computations

-- including great physical insight & numerical expertise

- Clementi-Roetti: Roothan-Hartree-Fock wave functions with optimized exponents.
- Cowan's HFX: support & semi-empirical adjustment of level structures, transition probabilities & cross sections.
- ATSP: Breit-Pauli approximation, level energies & properties.
- Grasp/Ratip: Large-scale computations of individual energies, rates, ...
- FAC: Modelling and diagnostics of astro- & plasma processes.
  Flexible Atomic Code
- CI-MBPT: Combines CI and MBPT methods for bound-state properties.
- ...
- "Home-made": Large No. of tools for particular purposes.

→ huge number of applications in AMO physics, science & technology

Established tools for atomic computations

-- including great physical insight & numerical expertise

- Clementi-Roetti: Roothan-Hartree-Fock wave functions with optimized expon ts.
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  transition probabilities & cross secti
- ATSP: Breit-Pauli approximat
- Grasp/Ratip: Larg
- FAC: Flexi
  ds for bound-state properties.
- Large No. of tools for particular purposes.

Most often, Fortran (or C, C++) codes ... quite technical & with little use of the underlying 'physics language' as developed in atomic theory; difficult to extent towards new processes, coding is typically cumbersome.

Performance vs. productivity.

→ with applications in AMO physics, science & technology

https://www.github.com/OpenJAC/JAC.jl

Jena Atomic Calculator (JAC)

-- A fresh approach to the computation of atoms, ...

JAC ... Jena atomic calculator provides tools for performing atomic (structure) calculations at various degrees of complexity and sophistication.

Interactive High-Level Language

JAC

Jena's Atomic Calculator

A Julia implementation for atomic computations.

Open-source applications in physics, science and technology.

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-- A fresh approach to the computation of atoms, ...

JAC ... Jena atomic calculator provides tools for performing atomic (structure) calculations at various degrees of complexity and sophistication.

Central questions to any new implementation:

- Is a common (and community) platform for atomic computations desirable ?
- How can we benefit from a good 'core machinery' ?
- How simple and user-friendly can it be made ?
- How to combine productivity & performance in developing such a platform ?

Open-source applications in physics, science and technology.

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Jena Atomic Calculator (JAC)

-- A fresh approach to the computation of atoms, ...

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What do we need in atomic structure and collision theory ?

- Design of a high-level language with data types close to atomic physics.

  Shell, Subshell, Configuration, Orbital, Basis, Level, Multiplet, Cascade, Pulse, ...

- Implementation and comparison of different models & approximations.
- Simple to learn and apply.

  With a simplified control; standard vs. advanced computations, complete active spaces; atomic cascades; ...

- Simple access to graphical interfaces and representations.
- Support a coarse-grained decomposition of most computational steps.

  A pseudo-code description should allow summarizing the major problem.

- Framework for implementing future code ... and for modelling (even more) complex processes.
- Open-source, readily extentable. Encourage help, suggestions, requests & improvements to the code.

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Jena Atomic Calculator (JAC)

-- A fresh approach to the computation of atoms, ...

Struct	Brief explanation
`Atomic.CasComputation`	An individual or a series of systematically enlarged SCF computations.
`Atomic.CasStep`	Single-step of an (systematically enlarged) SCF calculation.
`Atomic.Computation`	An atomic computation of one or several multiplets, including the SCF and CI calculations, as well as of properties or processes.
`Basis`	(Relativistic) atomic basis, including the specification of the configuration space and radial orbitals.
`Cascade.Computation`	Specifies an atomic exciation/decay cascade, including the initial state, allowed processes and the depths of the cascade.
`Cascade.Simulation`	Specifies how a simulation of some cascade (data) has to be done.
`Cascade.Step`	An individual step of a Cascade.Computation that typically combines two ionization states of ions.
`Configuration`	(Non-relativistic) electron configuration as specified by its shell occupation.
`ConfigurationR`	(Relativistic) electron configuration as specified by its subshell occupation.
`EmMultipole`	A multipole (component) of the electro-magnetic field, specified by its parity and multipolarity.
`Level`	Atomic level in terms of its quantum numbers, symmetry, energy and its (possibly full) representation.
`Multiplet`	An ordered list of atomic levels.
`NuclearModel`	A nuclear model of an atom to keep all nuclear parameters together.
`Orbital`	(Relativistic) radial orbital function that appears as 'buildung block' in order to define the many-electron CSF; its is typically given on a (radial) grid and comprises as large and small component.
`Radial.Grid`	Radial grid to represent the (radial) orbitals and to perform all radial integrations.
`Radial.Potential`	Radial potential function.
`Radiative.Channel`	Radiative channel of well-defined multipolarity and gauge.
`Radiative.Line`	Radiative line between two given (initial- and final-state) levels, and along with all of its multipole channels.
`Radiative.Settings`	From the user specified settings for computing radiative lines.
`Shell`	Non-relativistic shell, such as $1s$, $2s$, $2p$, ...
`Subshell`	Relativistic subshell, such as $1s_{1/2}$, $2s_{1/2}$, $2p_{1/2}$, $2p_{3/2}$, ...
`Statistical.Tensor`	Statistical tensor of given rank k, projection q, and which typically depends on two atomic levels (resonances).

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Jena Atomic Calculator (JAC)

-- A fresh implementation in **Julia**

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  With a simplified cont
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- Support a coarse-g
  A pseudo-code descr
- Framework for imp
- open-source, readil

Why Julia ?

- (Very) fast, high-level language (from MIT, since ~ 2012).
- Combines productivity and performance.
- Multiple dispatch ... to distinguish generic code, still dynamic.
- Just in-time (JIT) compilation, fast loops.
- Rapid code development: no linkage; in-built benchmarking.
- Most code & macros are written in Julia.
- Extensive list of packages.
- No storage management, little declaration; type stability.
- Easy documentation, ...

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Jena Atomic Calculator (JAC)

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JAC ... Jena atomic calculator provides tools for performing atomic (structure) calculations at various degrees of complexity and sophistication. ... JAC also facilitates interactive computations, the simulation of atomic cascades, the time-evolution of statistical tensors as well as various semi-empirical estimates of atomic properties. In addition, the Jac module supports the graphical representation of level energies, electron and photon spectra, radial orbitals and others.

Example: Einstein A and B coefficients for the Fe X spectrum;

$$Fe^{9+}\ \ [Ne]\ 3s^2\ 3p^5 \rightarrow\ [Ne]\ 3s\ 3p^6\ +\ 3s^2\ 3p^4\ 3d$$

```
> wa = Atomic.Computation("Fe X: Einstein",  NuclearModel(26.), ...,
            [Configuration("[Ne] 3s^2 p^5")], ...,
            [Configuration("[Ne ] 3s 3p^6"), Configuration("[Ne] 3s^2 3p^4 3d") ], ...,
            Radiative, Radiative.Settings([E1, M2], [UseCoulomb, UseBabushkin], false, false, ...  )
> perform(wa)

   ... in perform('computation: SCF', ...)
   Compute CI matrix of dimension 1 x 1 for the symmetry 1/2^+ ...   done.
   Compute CI matrix of dimension 1 x 1 for the symmetry 3/2^+ ...   done.
   ...
```

GUI ?
(graphical user interface)

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Example: Einstein A and B coefficients for the Fe X spectrum;

			(eV)			A (s^{-1})	gB (m s^{3} J^{-2} s^{-1})	strength GF	(eV
1 - 2	1/2 +	1/2 -	3.39446D+01	E1	Babushkin	1.35358D+09	7.92148D+18	5.41457D-02	8.9094
1 - 2	1/2 +	1/2 -	3.39446D+01	E1	Coulomb	1.29696D+09	7.59015D+18	5.18810D-02	8.5367
1 - 1	1/2 +	3/2 -	3.58795D+01	E1	Babushkin	2.94707D+09	1.46045D+19	1.05516D-01	1.9398
1 - 1	1/2 +	3/2 -	3.58795D+01	E1	Coulomb	2.65412D+09	1.31527D+19	9.50275D-02	1.7469
2 - 2	1/2 +	1/2 -	4.66937D+01	E1	Babushkin	5.99420D+06	1.34769D+16	1.26717D-04	3.9454
2 - 2	1/2 +	1/2 -	4.66937D+01	E1	Coulomb	7.32071D+06	1.64593D+16	1.54759D-04	4.8185
2 - 1	1/2 +	3/2 -	4.86286D+01	E1	Babushkin	3.51480D+06	6.99614D+15	6.85074D-05	2.3134
2 - 1	1/2 +	3/2 -	4.86286D+01	E1	Coulomb	4.20990D+06	8.37972D+15	8.20557D-05	2.7716
3 - 2	1/2 +	1/2 -	5.03941D+01	E1	Babushkin	1.70893D+08	3.05647D+17	3.10161D-03	1.1248
3 - 2	1/2 +	1/2 -	5.03941D+01	E1	Coulomb	1.81643D+08	3.24872D+17	3.29670D-03	1.1955

https://www.github.com/OpenJAC/JAC.jl

Jena Atomic Calculator (JAC)

-- currently supports seven types of computations

JAC ... Jena atomic calculator provides tools for performing atomic (structure) calculations at various degrees of complexity and sophistication. ... JAC also facilitates interactive computations, the simulation of atomic cascades, the time-evolution of statistical tensors as well as various semi-empirical estimates of atomic properties. In addition, the Jac module supports the graphical representation of level energies, electron and photon spectra, radial orbitals and others.

Types of computations:

- Atomic computations of amplitudes, properties and processes.
  - ... based on explicitly specified levels and/or electron configurations; many-electron amplitudes from a given list of (level) properties and atomic processes.
- Restricted active-space computations (RAS).
  - ... systematic enlargement of the CSF basis due to virtual excitations from reference conf.
- Interactive computations
  - ... making use of JAC's high-level atomic language.
- Simulation of atomic cascades following inner-shell excitations.
- Computation of atomic responses.
- Time evolution of statistical tensors in (intense) light pulses.
- Semi-empirical estimates of atomic properties, cross sections, etc.
  - ... Lotz formula, asymptotic behaviour of cross sections, etc.

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Not yet implemented (fully); external help & contributions are very welcome.

https://www.github.com/OpenJAC/JAC.jl

Jena Atomic Calculator (JAC)

1 atomic **amplitudes** implemented

Amplitude	Call within JAC	Brief explanation.
$\left\langle \alpha \mathbb{J} \left\| \mathbb{T}^{(1)} \right\| \beta \mathbb{J}' \right\rangle$, $\left\langle \alpha \mathbb{J} \left\| \mathbb{T}^{(2)} \right\| \beta \mathbb{J}' \right\rangle$	Hfs.amplitude()	Amplitude for the hyperfine ineraction with the magnetic-dipole and electric-quadrupole field of the nucleus.
$\left\langle \alpha \mathbb{J} \left\| \mathbb{N}^{(1)} \right\| \beta \mathbb{J}' \right\rangle$	LandeZeeman.amplitude()	Amplitude for the ineraction with an external magnetic field.
$\left\langle \alpha_f \mathbb{J}_f \left\| \mathbb{O}^{(\mathrm{M,\ emission})} \right\| \alpha_i \mathbb{J}_i \right\rangle$	Radiative.amplitude()	Transition amplitude for the emission of a multipole ($\mathbb{M}$) photon.
$\left\langle \alpha_f \mathbb{J}_f \left\| \mathbb{O}^{(\mathrm{M,\ absorption})} \right\| \alpha_i \mathbb{J}_i \right\rangle$	Radiative.amplitude()	Transition amplitude for the absorption of a multipole ($\mathbb{M}$) photon.
$\left\langle (\alpha_f \mathbb{J}_f, \varepsilon\, \kappa)\, \mathbb{J}_t \left\| \mathbb{O}^{(\mathrm{M,\ photoionization})} \right\| \alpha_i \mathbb{J}_i \right\rangle$	PhotoIonization.amplitude()	Photoionization amplitude for the absorption of a multipole ($\mathbb{M}$) photon and the release of an electron in the partial wave $\|\varepsilon\, \kappa\rangle$.
$\left\langle \alpha_f \mathbb{J}_f \left\| \mathbb{O}^{(\mathrm{M,\ recombination})} \right\| (\alpha_i \mathbb{J}_i, \varepsilon\kappa) \mathbb{J}_t \right\rangle$	PhotoRecombination.amplitude()	Photorecombination amplitude for the emission of a multipole ($\mathbb{M}$) photon and the capture of an electron in the partial wave $\|\varepsilon\, \kappa\rangle$.
$\left\langle (\alpha_f \mathbb{J}_f,\ \varepsilon\, \kappa)\, \mathbb{J}_t \left\| \mathbb{V}^{(\mathrm{Auger})} \right\| \alpha_i\, \mathbb{J}_i \right\rangle$	Auger.amplitude()	Auger transition amplitude due to the electron-electron interaction and the release of an electron in the partial wave $\|\varepsilon\, \kappa\rangle$.
$\langle \alpha_f \mathbb{J}_f \| \sum \exp i\, \mathbf{q} \cdot \mathbf{r}_i \| \alpha_i \mathbb{J}_i \rangle$	FormFactor.amplitude()	Amplitude for a momentrum transfer $\mathbf{q}$.
$\left\langle \alpha_f \mathbb{J}_f \left\| \mathbb{O}^{(\mathrm{PNC})} \right\| \alpha_i \mathbb{J}_i \right\rangle$	PNC.amplitude()	Parity-nonconservation amplitude.

... Lotz formula, asymptotic behaviour of cross sections, etc.

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Jena Atomic Calculator (JAC)

2 atomic (level) **properties** implemented

JAC ... Jena atomic calculator provides tools for performing atomic (structure) calculations at various degrees of complexity and sophistication. ... JAC also facilitates interactive computations, the simulation of atomic cascades, the time-evolution of statistical tensors as well as various semi-empirical estimates of atomic properties. In addition, the Jac module supports the graphical representation of level energies, electron and photon spectra, radial orbitals and others.

Property	id	Brief explanation.
$\|\alpha\mathbb{J}\rangle \longrightarrow \|\alpha(J)\,\mathbb{F}\rangle$	HFS	Hyperfine splitting of an atomic level into hyperfine (sub-) levels with $F = \|I-J\|, \ldots, I+J-1, I+J$; hyperfine A and B coefficients; hyperfine energies and interaction constants; representation of atomic hyperfine levels in a IJF-coupled basis.
$\|\alpha\mathbb{J}\rangle \longrightarrow \|\alpha\,\mathbb{J}M\rangle$	LandeJ	Zeeman splitting of an atomic level into Zeeman (sub-) levels; Lande $g_J \equiv g(\alpha\mathbb{J})$ and $g_F \equiv g(\alpha\mathbb{F})$ factors for the atomic and hyperfine levels.
$K^{(\mathrm{MS})},\ F$	Isotope	Isotope shift of an atomic level for two isotopes with masses $A,\ A'$: $\Delta E^{AA'} = E(\alpha\mathbb{J};\ A) - E(\alpha\mathbb{J};\ A')$; mass-shift parameter $K^{(\mathrm{MS})}$ and field-shift parameter F.
α-variations	AlphaX	Differential sensitivity parameter $\Delta q(\delta\alpha)$ of an atomic level; $\Delta E(\delta\alpha;\ \beta\mathbb{J})$, $\Delta q(\delta\alpha;\ \beta\mathbb{J})$, $K(\beta\mathbb{J})$.
$F(q;\ \alpha\,\mathbb{J})$	FormF	Standard and modified atomic form factor of an atomic level $\|\alpha\mathbb{J}\rangle$ with a spherical-symmetric charge distribution.
$\omega(\alpha\mathbb{J}) + a(\alpha\mathbb{J}) = 1$	Yields	Fluorescence & Auger decay yields of an atomic level.
$\alpha^{(\mathrm{M})}(L,\omega)$		Static and dynamic (ac, multipolar) polarizibilities.
$E(\alpha\mathbb{J};$ plasma model$)$	Plasma	Plasma shift of an atomic level as obtained for different but still simple plasma models.
$\|\alpha_i\mathbb{J}_i\rangle \longrightarrow \|\alpha_f\mathbb{J}_f\rangle + \hbar\omega$	EinsteinX [a]	Photon emission from an atom or ion; Einstein A and B coefficients and oscillator strength between levels $\|\alpha_i\mathbb{J}_i\rangle \rightarrow \|\alpha_f\mathbb{J}_f\rangle$ that belong to a single multiplet (representation).

https://www.github.com/OpenJAC/JAC.jl

3 Atomic **processes** in JAC

– combining often (bound) levels with a different No. of electrons

Process	id	Brief explanation.
$A^* \longrightarrow A^{(*)} + \hbar\omega$	RadiativeX	Photon emission from an atom or ion; transition probabilities; oscillator strengths; angular distributions.
$A + \hbar\omega \longrightarrow A^*$	PhotoExc	Photoexcitation of an atom or ion; alignment parameters; statistical tensors.
$A + \hbar\omega \longrightarrow A^{+*} + e_p^-$	PhotoIon	Photoionization of an atom or ion; cross sections; angular parameters; statistical tensors.
$A^{q+} + e^- \longrightarrow A^{(q-1)+} + \hbar\omega$	Rec	Photorecombination of an atom or ion; recombination cross sections; angular parameters.
$A^{q+*} \longrightarrow A^{(q+1)+(*)} + e_a^-$	AugerX	Auger emission (autoionization) of an atom or ion; rates; angular and polarization parameters.
$A^{q+} + e^- \rightarrow A^{(q-1)+*} \rightarrow A^{(q-1)+(*)} + \hbar\omega$	Dierec	Dielectronic recombination (DR) of an atom or ion; resonance strengths.
$A + \hbar\omega_i \longrightarrow A^* \longrightarrow A^{(*)} + \hbar\omega_f$	PhotoExcFluor	Photoexcitation of an atom or ion with subsequent fluorescence emission.
$A + \hbar\omega \longrightarrow A^* \longrightarrow A^{(*)} + e_a^-$	PhotoExcAuto	Photoexcitation & autoionization of an atom or ion.
$A + \hbar\omega_i \longrightarrow A^{(*)} + \hbar\omega_f$	Compton	Rayleigh or Compton scattering of photons at an atom or ion; angle-differential and total cross sections.
$A + n\,\hbar\omega \longrightarrow A^*$ or $A^* \longrightarrow A^* + n\,\hbar\omega$	MultiPhoton	Multi-photon (de-) excitation of an at… ing two-photon decay, etc.
$A + Z_p \longrightarrow A^* + Z_p$	CoulExc	Coulomb excitation of an atom or ic… ions; energie-differential, partial and t… citation cross sections.

There are many other atomic processes and related entities.

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Jena Atomic Calculator (JAC)

-- currently supports six types of computations

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Types of computa

- Atomic computat
  ... based on explici
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  ... systematic enlarg
- Interactive comp
  ... making use of th
- Simulation of ato
- Time evolution o
- Semi-empirical e
  ... Lotz formula, asy

JAC as open-source

- Sizeable project: ~ 900 functions/methods, > 30,000 lines
- Improve inline and web documentation.
- Further tests & tutorials.
- **Jac on git/Github:** https://www.github.com/fritzsche/JAC
- Reference hopefully soon; extended manual & compendium.
- Welcomes support & collaboration.
- Incremental delivery; multiple approaches.

https://www.github.com/OpenJAC/JAC.jl

README.md

Jena Atomic Calculator (JAC) for the computation of atomic structures, processes and cascades

What is JAC?

We here provide a first public version of *JAC*, the Jena Atomic Calculator and an open-source Julia package for doing atomic computations. JAC is a (relativistic) electronic structure code for the computation of (many-electron) interaction amplitudes, properties as well as a large number of excitation and decay processes for open-shell atoms and ions across the whole periodic table. In the future, moreover, JAC will -- more and more -- facilitate also studies on atomic cascades, responses as well as the time-evolution of atoms and ions.

A primary guiding philosophy of JAC was to develop a **general and easy-to-use toolbox for the atomic physics community**, including an interface that is equally accessible for working spectroscopiest, theoreticians and code developers. Beside of its simple use, however, I also wish to provide a modern code design, a reasonable detailed documentation of the code and features for integrated testing. In particular, most typical calculations and the handling of atomic data should appear within the code similar to how they would appear in spoken or written language. Shortly speaking, JAC aims to provide a powerful **platform for daily use and to extent atomic theory towards new applications**.

Kinds of computations

In some more detail, JAC distinguishes and aims to support (partly still in the future) **seven kinds of computations** which can be summarized as follows:

1. **Atomic computations**, based on explicitly specified electron configurations: This kind refers to the computation of level energies, atomic state representations and to either one or several atomic properties for selected levels of a given multiplet. It also help compute *one* selected process at a time, if atomic levels from two or more multiplets are involved in atomic transitions.
2. **Restricted active-space computations (RAS)**: This kind concerns systematically-enlarged calculations of atomic states

Quickstart

The numerous features of JAC can be easily understood by following the tutorials that are distributed together with the code. Further details can then be found from the Manual, Compendium & Theoretical Background to JAC. Make use the index or a full-text search to find selected items in this (.pdf) manual.

A very first **simple example** has been discussed in the reference above and refers to the low-lying level structure and the Einstein A and B coefficients of the 3s 3p^6 + 3s^2 3p^4 3d → 3s^2 3p^5 transition array for Fe^9+ ions, also known as the spectrum Fe X. To perform such a computation within the framework of JAC, one needs to specify the initial- and final-state configurations in an instance of an `Atomic.Computation`, together with the specifier `process=RadiativeX`. We here also provide a title (line), the multipoles (default E1) and the gauge forms for the coupling of the radiation field that are to be applied in these calculations:

```
comp = Atomic.Computation("Energies and Einstein coefficients for the spectrum Fe X",  Nuclear.Model(26.);
                initialConfigs = [Configuration("[Ne] 3s 3p^6"), Configuration("[Ne] 3s^2 3p^4 3d")],
                finalConfigs   = [Configuration("[Ne] 3s^2 3p^5")],
                process = RadiativeX,
                processSettings = Radiative.Settings([E1, M1, E2, M2], [UseCoulomb, UseBabushkin] )
perform(comp::Atomic.Computation)
```

This example is discussed also in the tutorial.

Tutorials

The following IJulia/Jupyter notebooks introduce the reader to JAC and demonstrate various features of this toolbox.
They can be explored statically at GitHub or can be run locally after the software repository has been cloned and installed. In order to modify the cell-output of the notebooks and to better print the *wide tables*, you can create or modify the file ~/.jupyter /custom/custom.css in your home directory and add the line: div.output_area pre { font-size: 7pt;} .

- Getting started
- Simple hydrogenic estimates
- Nuclear models and potentials
- Atomic potentials
- SCF + CI computations for carbon
- Einstein coefficients for Fe X

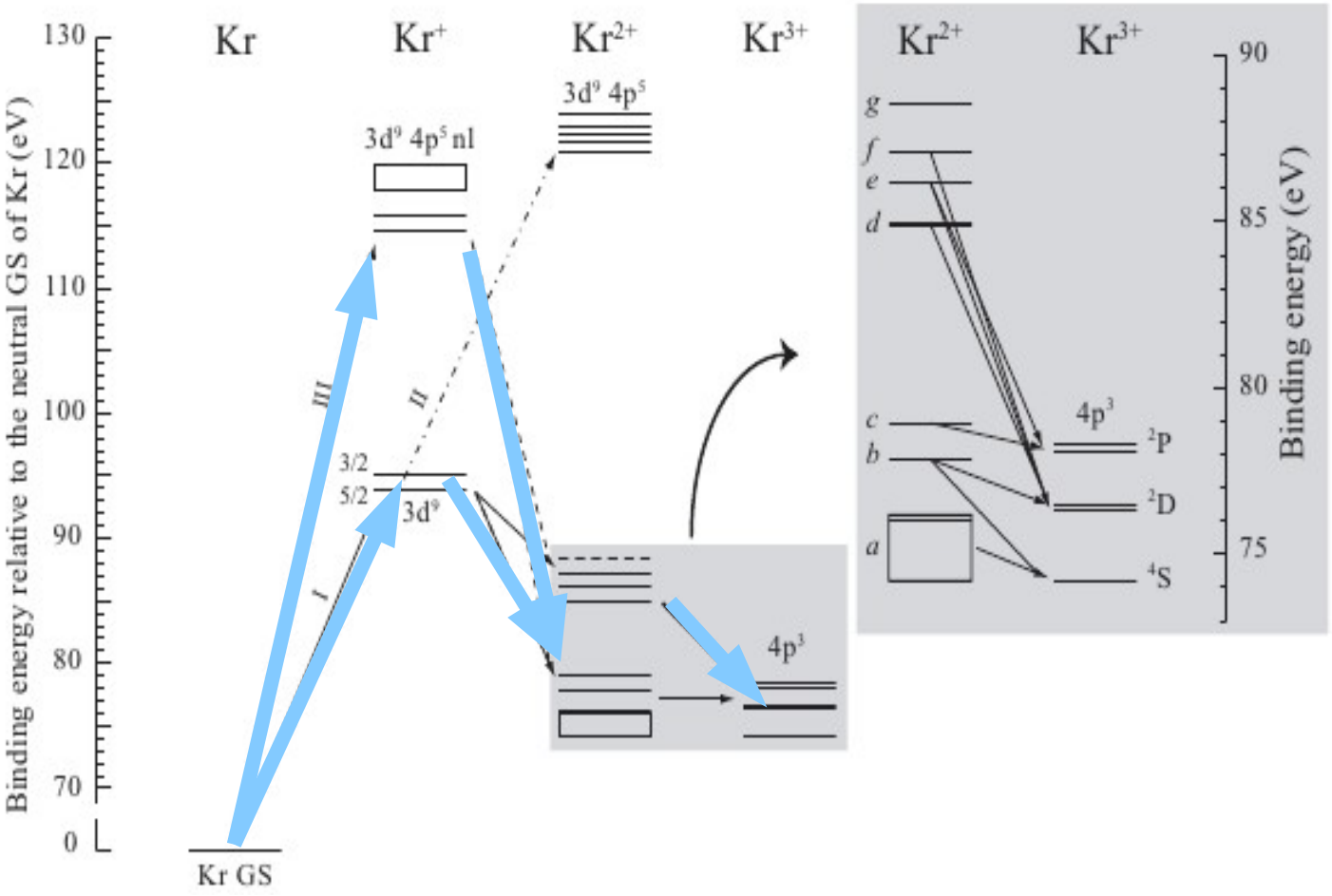
4 Atomic cascades in JAC

– coincidence techniques using a magnetic bottle

Kr → Kr^{3+}

Double Auger decay of 3d-ionized krypton

- Coincidence on 3d photo electron as first arrival electron.
- Six stripes arise from combination of 3d hole states and the ^4S, ^2D and ^2P finals states of Kr^{3+} $4p^{-3}$
- Dark spots refer to Auger lines.



Calculations are needed and helped identify new levels & decay pathes in the sequential (auto-) ionization.

E. Andersson et al, PRA 82 (2010) 043418.

4 Atomic cascades in JAC

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$Kr \rightarrow Kr^{3+}$

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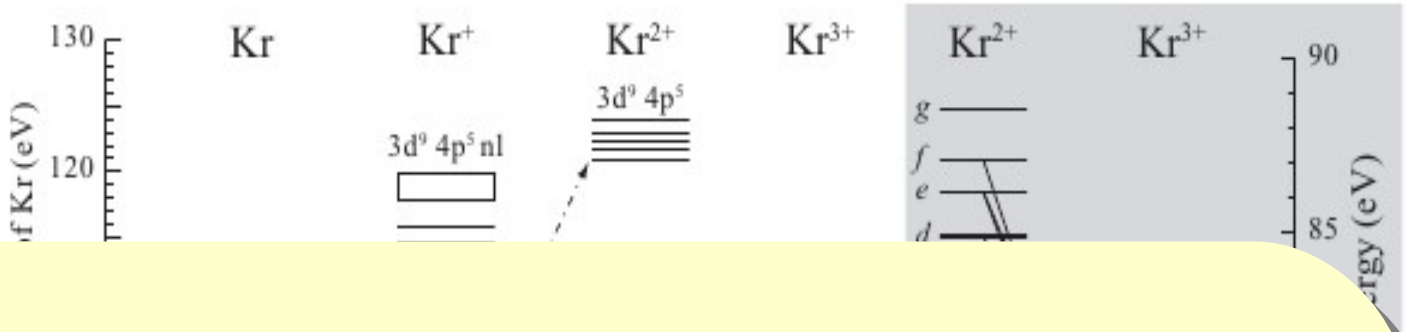
3d-ionized krypton



Four approaches to deal with cascades:

- Average singe-configuration approach (averageSCA).

  ... 'common set of orbitals' for all ionization stage; 'configuration-averaged' data throughout all simulations

- Singe-configuration approach (SCA).

  ... all fine-structure transitions amplitudes are calculated explicitly; still simplified continuum.

- Multiple-configuration approach (MCA).
- Multiple-configuration-shake approach (shakeMCA)

  ... incorporates e-e correlations by configuration mixing & shake-transitio

Not yet implemented.

https://www.github.com/OpenJAC/JAC.jl

Summary and outlook

Atomic properties
- Hyperfine splitting & representation
- Zeeman splitting; Lande factors
- Isotope shifts, atomic for factors
- Plasma shifts, α-variations
- Approximate Greens function, ...

Atomic processes
- Photon emission & transition probabilities
- Photoexcitation, ionization & recombinat.
- Auger emission & di-electr. recombination
- Rayleigh-Compton scattering
- Multiphoton (de-) excitation, ...

Interactive High-Level Language

JAC

Jena Atomic Calculator

A Julia implementation for atomic computations.

Atomic responses
- Field-induced processes & ionization
- High-harmonic generation
- Particle-impact processes

Atomic time-evolution
- Liouville equation for statistical tensors & atomic density matrices
- Atoms in intense light pulses
- Angle- & polarization-dependent observables

Collaboration & support:

- encourage contributions from the atomic physics community;
- Including both, incremental improvements and multiple approaches for algorithms and modules
- PhD and “post-doc” positions with us available.