Community platform for Just Atomic Computations (JAC)

Interactive High-Level Language

JAC

Jena Atomic Calculator

A Julia implementation for atomic computations.

Open-source applications in physics, science and technology.

Stephan Fritzsche
Helmholtz-Institut Jena &
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23th November 2019

Atomic representations

- Configuration-based expansions
- Restricted active spaces (layer-by-layer)
- CI+perturbation theory; Gamov states
- Approximate Green functions, ...

Processes & properties

- Transition probabilities
- Excitation, ionization & recombination
- Auger, DR, Rayleigh-Compton, multi-γ
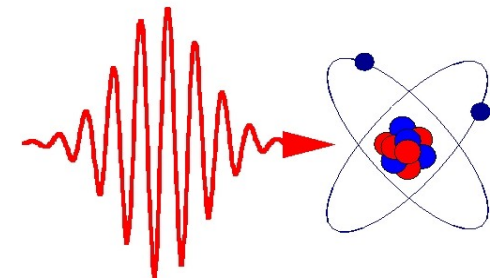- Hyperfine & Zeeman splitting; plasma
- Isotope shifts, Lande & form factors

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Atomic cascades

- Average singe-configuration approach
- Multiple-configuration approach
- Incorporation of shake-up & shake-off
- Ion & electron distributions, ...

Symbolic Racah algebra

- Wigner symbols, special values
- Symmetries & recursions
- Symbolic sum rule evaluation

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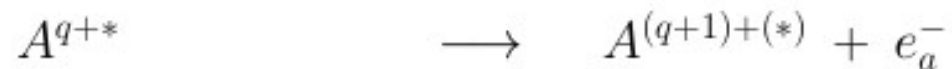
A few simple atomic processes:

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

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

$$A + \hbar\omega \longrightarrow A^{+*} + e_p^- \qquad \text{... (atomic) photoionization}$$

$$A^{q+*} \longrightarrow A^{(q+1)+(*)} + e_a^- \qquad \text{... Auger emission; autoionization}$$

$$e_s^- + A \longrightarrow A^* + e_s^{-'} \qquad \text{... electron} - \text{impact excitation}$$
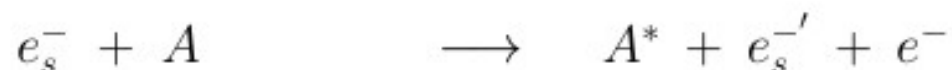
$$e_s^- + A \longrightarrow A^* + e_s^{-'} + e^- \qquad \text{... electron} - \text{impact ionization}$$

$$A + n\,\hbar\omega \longrightarrow A^* \qquad \text{... multi} - \text{photon excitation/decay}$$

Quiz: Atomic processes in a nutshell

-- for "intermediates" in atomic and plasma physics

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

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

$$A^{q+} + e_s^- \longrightarrow A^{(q-1)+} + \hbar\omega$$

$$A^{q+} + e_s^- \longrightarrow A^{(q-1)+*} \longrightarrow A^{(q-1)+(*)} + \hbar\omega$$

$$A + \hbar\omega \longrightarrow A^{(*)} + \hbar\omega'$$

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

$$A^{q+*} \longrightarrow A^{(q+2)+(*)} + (e_{a_1}^- + e_{a_2}^-)$$

$$A + \hbar\omega \longrightarrow A^* \longrightarrow A^{(*)} + \hbar\omega'$$

$$A + \hbar\omega \longrightarrow A^{+,*} + e_p^- \longrightarrow A^{(*)} + e_p^- + \hbar\omega'$$

$$A + Z_p \longrightarrow A^* + Z_p'$$

$$A^{(q+1)+} + Z_p \longrightarrow A^{(q+1)+(*)} + e^- + Z_p'$$

Quiz: Atomic processes in a nutshell

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

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

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

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

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

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

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

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

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

$$A + Z_p \longrightarrow A^* + Z_p' \qquad \dots \text{Coulomb excitation}$$

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

➭ 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 ?

Quiz: Atomic processes in a nutshell

-- for "intermediates" in atomic and plasma physics

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

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

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

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

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

$$A^{q+*} \longrightarrow A^{(q+2)+(*)} + (e_{a_1}^- + e^-)$$

$$A + \hbar\omega \longrightarrow A^* \longrightarrow \text{\,orescence}$$

$$A + \hbar\omega \longrightarrow \text{\& fluorescence}$$

$$A + Z_p \qquad \text{\,excitation}$$

$$A^{(q+1)+} + Z_p \qquad \text{... Coulomb ionization}$$

Accurate Atomic Amplitudes
$$\langle \Phi_\alpha \| V^L \| \Phi_\beta \rangle$$

➡ Indeed, ... processes occur in atomic, plasma and astro physics ... ous places elsewhere.

➡ How much ... can atomic theory provide ? -- Which tools are available ?

Demands from experiment

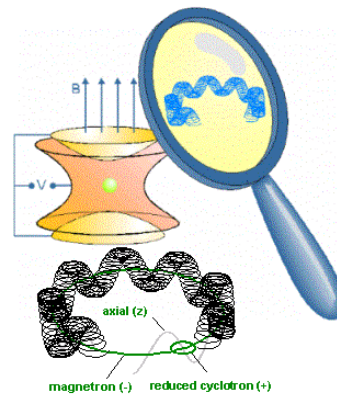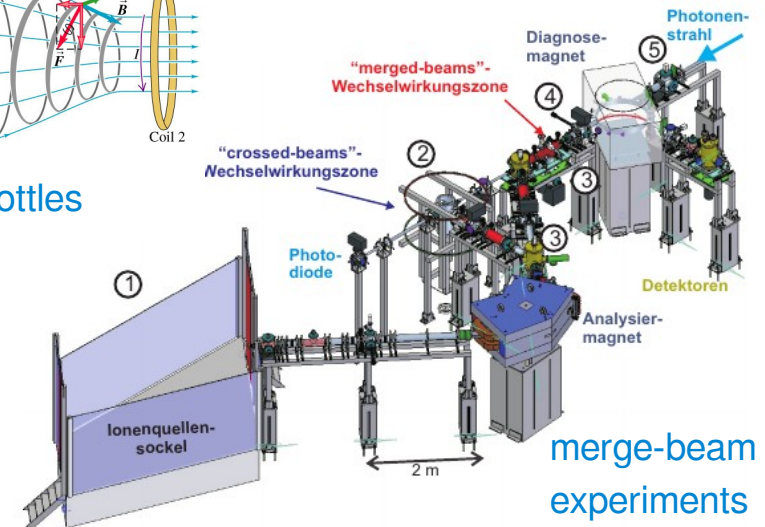### – owing to new large-scale facilities & detector developments
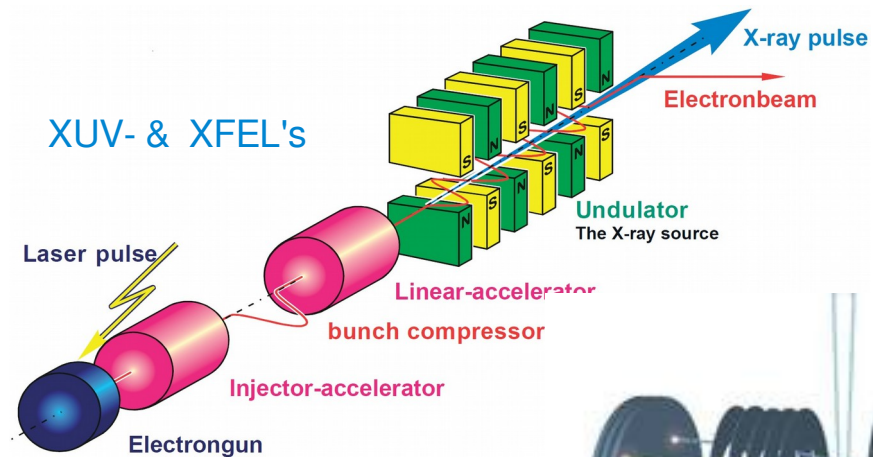
XUV- & XFEL's
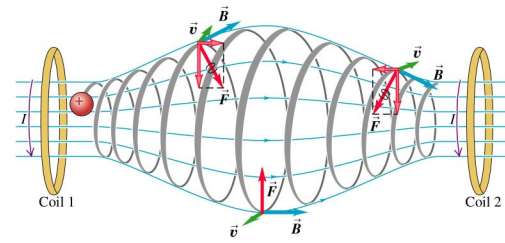
magnetic bottles

space missions
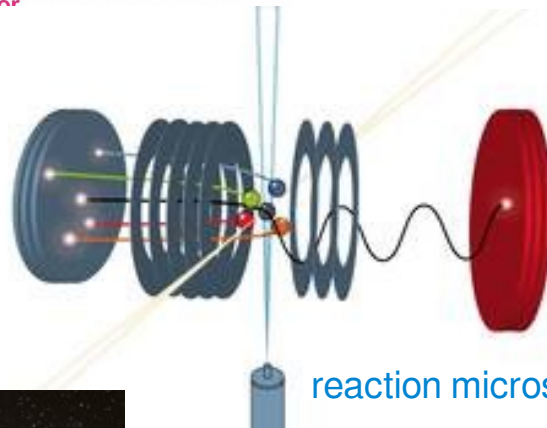
reaction microscopes

synchrotrons

merge-beam experiments

ion traps

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

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- Grasp/Ratip: Large

- FAC: Flexible

  ...as 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; coding is typically cumbersome. difficult to extent towards new processes,

Performance vs. productivity.

→ with applications in AMO physics, science & technology

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Atomic cascades

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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 ?

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.

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.

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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-- A fresh implementation in **Julia**

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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, ...

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. ... 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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- ➡ Generation of start orbitals
- ➡ Computation of angular coefficients (on fly)
- ➡ Self-Consistent-Field (SCF) iteration
- ➡ Set-up and diagonalization of Hamiltonian matrix
- ➡ Breit, QED, many-body corrections, ...
- ➡ Compute all (many-electron) transition amplitudes

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

Level-Level	J^P	J^P	(eV)			A (s^{-1})	gB (m^3 s^{-2} J^{-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	2.7710
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

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.
$\left\langle \alpha_f\mathbb{J}_f \left\| \mathbb{O}^{(\mathbb{M},\,\text{emission})} \right\| \alpha_i\mathbb{J}_i \right\rangle$	Radiative.amplitude()	Transition amplitude for the emission of a multipole ($\mathbb{M}$) photon.
$\left\langle \alpha_f\mathbb{J}_f \left\| \mathbb{O}^{(\mathbb{M},\,\text{absorption})} \right\| \alpha_i\mathbb{J}_i \right\rangle$	Radiative.amplitude()	Transition amplitude for the absorption of a multipole ($\mathbb{M}$) photon.
$\left\langle (\alpha_f\mathbb{J}_f,\,\varepsilon\,\kappa)\,\mathbb{J}_t \left\| \mathbb{O}^{(\mathbb{M},\,\text{photoionization})} \right\| \alpha_i\mathbb{J}_i \right\rangle$	PhotoIonization.amplitude()	Photoionization amplitude for the absorption of a multipole ($\mathbb{M}$) photon and the release of an electron in the partial wave $\left\vert \varepsilon\,\kappa \right\rangle$.
$\left\langle \alpha_f\mathbb{J}_f \left\| \mathbb{O}^{(\mathbb{M},\,\text{recombination})} \right\| (\alpha_i\mathbb{J}_i,\,\varepsilon\kappa)\mathbb{J}_t \right\rangle$	PhotoRecombination.amplitude()	Photorecombination amplitude for the emission of a multipole ($\mathbb{M}$) photon and the capture of an electron in the partial wave $\left\vert \varepsilon\,\kappa \right\rangle$.
$\left\langle (\alpha_f\mathbb{J}_f,\,\varepsilon\,\kappa)\,\mathbb{J}_t \left\| \mathbb{V}^{(\text{Auger})} \right\| \alpha_i\,\mathbb{J}_i \right\rangle$	Auger.amplitude()	Auger transition amplitude due to the electron-electron interaction and the release of an electron in the partial wave $\left\vert \varepsilon\,\kappa \right\rangle$.
$\left\langle \alpha_f\mathbb{J}_f \left\| \sum \exp i\,\mathbf{q}\cdot\mathbf{r}_i \right\| \alpha_i\mathbb{J}_i \right\rangle$	FormFactor.amplitude()	Amplitude for a momentrum transfer $\mathbf{q}$.
$\left\langle \alpha_f\mathbb{J}_f \left\| \mathbb{O}^{(\text{PNC})} \right\| \alpha_i\mathbb{J}_i \right\rangle$	PNC.amplitude()	Parity-nonconservation amplitude.

Jena Atomic Calculator (JAC)

2 atomic (level) **properties** implemented

Property	id	Brief explanation.
$\lvert \alpha \mathbb{J} \rangle \longrightarrow \lvert \alpha (J)\,\mathbb{F} \rangle$	HFS	Hyperfine splitting of an atomic level into hyperfine (sub-) levels with $F = \lvert I - J \rvert$, ..., $I + J - 1$, $I + J$; hyperfine A and B coefficients; hyperfine energies and interaction constants; representation of atomic hyperfine levels in a IJF-coupled basis.
$\lvert \alpha \mathbb{J} \rangle \longrightarrow \lvert \alpha \, \mathbb{J} M \rangle$	LandeJ	Zeeman splitting of an atomic level into Zeeman (sub-) levels; Lande $g_J =$ $g_F \equiv g(\alpha \mathbb{F})$ factors for the atomic and hyperfine levels.
$K^{(\mathrm{MS})}$, F	Isotope	Isotope shift of an atomic level for two isotopes with masses $E(\alpha \mathbb{J};\,A) - E(\alpha \mathbb{J};\,A')$; mass-shift parameter $K^{(\mathrm{MS})}$ and field
α-variations	AlphaX	Differential sensitivity parameter $\Delta q(\delta \alpha)$ of an atomic level; $\Delta q(\delta\alpha;\,\beta\mathbb{J})$, $K(\beta \mathbb{J})$.
$F(q;\,\alpha \mathbb{J})$	FormF	Standard and modified atomic form factor of an atomic level $\lvert \alpha \mathbb{J} \rangle$ 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.
$\lvert \alpha_i \mathbb{J}_i \rangle \longrightarrow \lvert \alpha_f \mathbb{J}_f \rangle + \hbar\omega$	EinsteinX [a]	Photon emission from an atom or ion; Einstein A and B coefficients and oscillator strength between levels $\lvert \alpha_i \mathbb{J}_i \rangle \rightarrow \lvert \alpha_f \mathbb{J}_f \rangle$ that belong to a single multiplet (representation).

GRASP (-like)

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 i... ions; energie-differential, partial and t... citation cross sections.

CURRENT FOCUS AREA

There are many other atomic processes and related entities.

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.
$A^{q+} + e^- \longrightarrow A^{(q-1)+} +$		
$A^{q+*} \longrightarrow A^{(q+1)+(*)} +$		
$A^{q+} + e^- \rightarrow A^{(q-1)+*} \rightarrow$		
$A + \hbar\omega_i \longrightarrow A^* \longrightarrow A^($		
$A + \hbar\omega \longrightarrow A^* \longrightarrow A^{(*}$		
$A + \hbar\omega_i \longrightarrow A^{(*)} + \hbar\omega$		
$A + n\,\hbar\omega \longrightarrow A^*$ or $A^* \longrightarrow A^* + n\,\hbar\omega$		
$A + Z_p \longrightarrow A^* + Z_p$		

There are many othe...

JAC as open-source

▶ Sizeable project: ~ 1100 functions/methods, > 30,000 lines

▶ Improve inline and web documentation.

▶ Further tests & tutorials.

▶ **Jac on git/Github:** https://www.github.com/OpenJAC/JAC.jl

▶ SF, CPC (2019); user guide & compendium.

▶ Welcomes support & collaboration.

▶ Incremental delivery; multiple approaches.

📖 **README.md**

`build passing` codecov

Jena Atomic Calculator (JAC) for the computation of atomic representations, 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 (atomic 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 forthcoming years, moreover, JAC will -- more and more -- facilitate also studies on atomic cascades, responses to external fields and particles, the time-evolution of atoms and ions as well as selected symbolic computations of expressions from Racah's algebra.

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 spectroscopists, 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 as well as features for integrated testing. In particular, many typical computations 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** or, in short, a **community platform for Just Atomic Computations**.

Remark: Although major efforts have been undertaken during the past two years, JAC is still in a very early state of its development and includes features that are only partly implemented or not yet tested in all detail. Despite of possible failures and deficiencies of the present code, however, I here annouce JAC and kindly ask potential users and developers for response, support and encouragement.

Kinds of computations

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

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 from a given multiplet. It also help compute **one** selected process at a time, if atomic levels from two or more multiplets are involved in some atomic transition.

2. **Atomic representations**: This kind concerns different representations of atomic wave functions; in particular, it includes systematically-enlarged restricted active-space (RAS) computations of atomic states and level energies due to a pre-specified active space of orbitals as well as due to the (number and/or kind of) virtual excitations that are taken to be into account. Such RAS computations are normally performed stepwise by making use of the (one-electron) orbital functions from some prior step. Other atomic representations refer to approximate atomic Green functions and, in the future, combined techniques with concepts from close-coupling, (exterior) complex scaling, DMRG or perturbation theory.

3. **Interactive computations**: Here, the (large set of) methods of the JAC program are applied interactively, either directly from the REPL or by using some short Julia script in order to compute and evaluate the desired observables (atomic parameters), such as energies, expansion coefficients, transition matrices and amplitudes, rates, cross sections, etc. An interactive computation typically first prepares and applies (certain instances of) JAC's data types, such as orbitals, configuration-state functions (CSF), atomic bases, levels, multiplets, and others. And like Julia, that is built on many (high-level) functions and methods, JAC then provides the required language elements for performing specific atomic computations at different degree of complexity and sophistication.

4. **Atomic cascade computations**: A cascade typically includes ions of an element in three or more charge states that are connected to each other by different atomic processes, such as photoionization, dielectronic recombination, Auger decay, radiative transitions, and where the relative level population of these charge states is determined by the set-up and geometry of the given experiment. Cascade computations are usually based on some predefined *(cascade) approach* that enables one to automatically select the state-space of the ions, to choose the atomic processes to be considered for the various steps of the cascade, and to specify perhaps additional restrictions in order to keep the computations feasible.

5. **Atomic responses**: With this kind, I wish to support in the future computations that help analyze the response of atoms to incident beams of light pulses and particles, such as field-induced ionization processes, high-harmonic generation and several others. For these responses, the detailed structure of the atoms and ions has often not yet been considered until today but will become relevant as more elaborate and accurate measurements will become feasible.

6. **Atomic time-evolution of statistical tensors**: We here wish to simulate the population and coherences of (atomic) levels using the *Liouville equation*, when atoms and ions are irradiated by (intense) light pulses. For these computations,

Quickstart

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

A very **simple example** has been discussed in the CPC reference above and just 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 by an instance of an `Atomic.Computation`, together with the specifier `process=Radiative`. 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 = Radiative,
            processSettings = Radiative.Settings([E1, M1, E2, M2], [UseCoulomb, UseBabushkin] )
    perform(comp::Atomic.Computation)
```

This example is discussed also in one of the tutorials below.

Tutorials

The following IJulia/Jupyter notebooks introduce the reader to JAC and demonstrate several 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 *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 estimates for hydrogenic atoms and ions
- Specifying nuclear models and potentials
- Selection and use of atomic potentials
- Self-Consistent-Field (and CI) computations for carbon

(I) Examples using JAC

-- SCF + CI computations; QED estimates, ...

Example: Low-lying levels of [Ne] 3p 3d2
           ... together with QED corrections and jj → LS transformation

```
> wa = Atomic.Computation("QED estimate + jj-LS level transformation",  Nuclear.Model(26.);
            configs=[Configuration("[Ne] 3p 3d^2")],
            asfSettings=AsfSettings(true, false, "meanDFS", "hydrogenic", ..., [1],  0, 1.0e-6,
                            Subshell[],  true, false, Petersburg(), LSjjSettings(true),
                            false, [1,2,3,4], false, LevelSymmetry[] ) )


> perform(wa)

  ... in perform('computation: SCF', ...)
```

(I) Examples using JAC

-- SCF + CI computations; QED estimates, ...

Example: Low-lying levels of [Ne] 3p 3d2
          ... together with QED corrections and jj → LS transformation

```
Energy of each level relative to lowest level:

Level  J Parity          Hartrees                        eV                       [eV]

  2    7/2 -       3.339411435945294e-03       9.087001366310990e-02      9.087001366310990e-02
  3    9/2 -       8.914068369904271e-03       2.425641554221373e-01      2.425641554221373e-01
```

```
LSjj.expandLevelsIntoLS():: Relativistic basis with 45 CsfR will be transformed into a nonrelativistic basis with 45 CsfNR.

LS-expansion of selected atomic levels:

 Level   1      5/2 -   -3.15900127e+04  [eV]  has weight 1.0000e+00 of 1s^2 2s^2 2p^6 3p^1 3d^2
     1)  9.9631e-01   of      ^4G_5/2
     2)  2.4092e-03   of      ^4F_5/2
     3)  1.2089e-03   of      ^2F_5/2

 Level   2      7/2 -   -3.15899218e+04  [eV]  has weight 1.0000e+00 of 1s^2 2s^2 2p^6 3p^1 3d^2
     1)  9.9327e-01   of      ^4G_7/2
     2)  4.6786e-03   of      ^4F_7/2
     3)  1.1071e-03   of      ^2G_7/2

 Level   3      9/2 -   -3.15897701e+04  [eV]  has weight 1.0000e+00 of 1s^2 2s^2 2p^6 3p^1 3d^2
     1)  9.9289e-01   of      ^4G_9/2
     2)  5.1819e-03   of      ^4F_9/2
     3)  1.5459e-03   of      ^2G_9/2

 Level   4     11/2 -   -3.15895197e+04  [eV]  has weight 1.0000e+00 of 1s^2 2s^2 2p^6 3p^1 3d^2
     1)  9.9980e-01   of      ^4G_11/2
     2)  2.0174e-04   of      ^2H_11/2
```

(II) Examples using JAC

-- perform a 3-layer RAS computation

Example: Beryllium ground level $1s^2\ 2s^2\ {}^1S_0$ + SD {1s, 2s, 2p, ... 4f}

```
> name        = "Beryllium 1s^2 2s^2 ^1S_0 ground state"
> refConfigs  = [Configuration("[He] 2s^2")]
> rasSettings = RasSettings([1], 24, 1.0e-6, false, true, [1,2,3] )
> from        = [Shell("2s")]
> frozen      = [Shell("1s")]
> to          = [Shell("2s"), Shell("2p")]
> step1       = RasStep(seFrom=from, seTo=to, deFrom=from, deTo=to, frozen=frozen)

> append!(frozen, [Shell("2s"), Shell("2p")])
> append!(to,     [Shell("3s"), Shell("3p"), Shell("3d")])
> step2       = RasStep(seFrom=from, seTo=to, deFrom=from, deTo=to, frozen=frozen)

> append!(frozen, [Shell("3s"), Shell("3p"), Shell("3d")])
> append!(to,     [Shell("4s"), Shell("4p"), Shell("4d"), Shell("4f")])
> step3       = RasStep(seFrom=from, seTo=to, deFrom=from, deTo=to, frozen=frozen)
>
> wa   = RasComputation(name, Nuclear.Model(4.), Radial.Grid("grid: exponential"), refConfigs,
                        LevelSymmetry(0, Basics.plus), 4, [step1, step2, step3], rasSettings)

> wb = perform(wa, output=true)
```

(II) Examples using JAC

-- perform a 3-layer RAS computation

Example: Beryllium ground level $1s^2\, 2s^2\ {}^1S_0$ + SD {1s, 2s, 2p, ... 4f}

```
++ Compute the orbitals, orbitals and multiplet for step 3 ...
--------------------------------------------------------------------
>> include Configuration: 1s^2 2s^2
>> include Configuration: 1s^2 2s^1 2p^1
>> include Configuration: 1s^2 2s^1 3s^1
>> include Configuration: 1s^2 2s^1 3p^1
>> include Configuration: 1s^2 2s^1 3d^1
>> include Configuration: 1s^2 2s^1 4s^1
```

```
>> include Configuration: 1s^2 4f^2
(Re-) Define a new standard subshell list.
Construct a basis with 26 CSF for J^P = 0 + with 16 subshells: 1s_1/2  2s_1/2 ...  4f_5/2  4f_7/2
>> Start orbital 1s_1/2 is taken from prior basis
>> Start orbital 2s_1/2 is taken from prior basis
>> Start orbital 2p_1/2 is taken from prior basis
>> Start orbital 2p_3/2 is taken from prior basis
>> Start orbital 3s_1/2 is taken from prior basis
>> Start orbital 3p_1/2 is taken from prior basis
>> Start orbital 3p_3/2 is taken from prior basis
>> Start orbital 3d_3/2 is taken from prior basis
>> Start orbital 3d_5/2 is taken from prior basis
>> Start orbital 4s_1/2 is taken from hydrogenic orbitals
```

```
... in perform['computation: SCF for RAS step'] ...
(Re-) Define the standard grid with 390 grid points.
(Re-) Define a storage array for various B-spline matrices:

Iteration 1 for symmetries ...
  4s_1/2::  en [a.u.] = -3.5737567e-03;    self-cons'cy = 9.8581e-01  [1.0000e+02 for sym-block kappa = -1]
  4p_1/2::  en [a.u.] = -4.8807579e-03;    self-cons'cy = 9.8067e-01  [1.0000e+02 for sym-block kappa = 1]
  4p_3/2::  en [a.u.] = -8.9716778e-03;    self-cons'cy = 9.6475e-01  [1.0000e+02 for sym-block kappa = -2]
  4d_3/2::  en [a.u.] = -7.1004657e-03;    self-cons'cy = 9.7200e-01  [1.0000e+02 for sym-block kappa = 2]
  4d_5/2::  en [a.u.] = -9.6912201e-03;    self-cons'cy = 9.6198e-01  [1.0000e+02 for sym-block kappa = -3]
```

(II) Examples using JAC

-- perform a 3-layer RAS computation

Example: Beryllium ground level $1s^2\ 2s^2\ {}^1S_0$ + SD {1s, 2s, 2p, ... 4f}

```
++ Compute the orbitals, orbitals and multiplet for step 3 ...
-------------------------------------------------------------
>> include Configuration: 1s^2 2s^2
>> include Configuration: 1s^2 2s^1 2p^1
>> include Configuration: 1s^2 2s^1 3s^1
>> include Configuration: 1s^2 2s^1 3p^1
>> include Configuration: 1s^2 2s^1 3d^1
>> include Configuration: 1s^2 2s^1 4s^1
```

```
Iteration 24 for symmetries ...
  4s_1/2::  en [a.u.] = -2.6797841e-02;   self-cons'cy = 4.7926e-10   [3.5897e-06 for sym-block kappa = -1]
  4p_1/2::  en [a.u.] = -1.8224737e-02;   self-cons'cy = 5.1515e-10   [1.0847e-06 for sym-block kappa = 1]
  4p_3/2::  en [a.u.] = -1.8226522e-02;   self-cons'cy = 4.9805e-10   [2.5561e-07 for sym-block kappa = -2]
  4d_3/2::  en [a.u.] = -1.1395165e-02;   self-cons'cy = 4.6992e-10   [6.4048e-07 for sym-block kappa = 2]
  4d_5/2::  en [a.u.] = -1.1427393e-02;   self-cons'cy = 2.5511e-10   [7.0632e-07 for sym-block kappa = -3]
  4f_5/2::  en [a.u.] = -4.6790493e-03;   self-cons'cy = 2.1881e-09   [4.5994e-07 for sym-block kappa = 3]
  4f_7/2::  en [a.u.] = -2.6981071e-02;   self-cons'cy = 9.4701e-09   [1.2018e-06 for sym-block kappa = -4]
Maximum number of SCF iterations = 24 is reached ... computations proceed.
Compute CI matrix of dimension 26 x 26 for the symmetry 0^+ ...    ... done.

  Eigenenergies:

  Level  J Parity          Hartrees                    eV                        [eV]

     1     0 +      -1.461679119136138e+01    -3.977431474818703e+02    -3.977431474818703e+02
     2     0 +      -1.436293253130269e+01    -3.908353014884933e+02    -3.908353014884933e+02
     3     0 +      -1.434689228820103e+01    -3.903988242415993e+02    -3.903988242415993e+02
```

```
Dict{String,Any} with 4 entries:
  "reference multiplet" => name:         Reference multiplet:   …
  "step2"                   => name:     Multiplet:   …
  "step3"                   => name:     Multiplet:   …
  "step1"                   => name:     Multiplet:   …
```

Atomic representations

- Configuration-based expansions
- Restricted active spaces (layer-by-layer)
- CI+perturbation theory; Gamov states
- Approximate Green functions, ...

Processes & properties

- Transition probabilities
- Excitation, ionization & recombination
- Auger, DR, Rayleigh-Compton, multi-γ
- Hyperfine & Zeeman splitting; plasma
- Isotope shifts, Lande & form factors

Atomic cascades

- Average singe-configuration approach
- Multiple-configuration approach
- Incorporation of shake-up & shake-off
- Ion & electron distributions, ...

Symbolic Racah algebra

- Wigner symbols, special values
- Symmetries & recursions
- Symbolic sum rule evaluation

Interactive High-Level Language

JAC

Jena Atomic Calculator

A Julia implementation for atomic computations.

Open-source applications in physics, science and technology.

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Time evolution

- Liouville equation for statistical tensors & atomic density matrices
- Atoms in intense light pulses
- Angle & polarization-dep. observables

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Open-source applications in physics, science and technology.

Atomic descriptors

- Feature transform. & machine learning
- Bi-spectra of electronic densities
- Subshell & coupling descriptors
- Atomic fragments & effective charges

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Jena Atomic Calculator

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- Hyperfine & Zeeman ...

Time evolution

- Liouville equation for statistical tensors & atomic density matrices

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 available with us.

technology.

Symbolic Racah algebra

- Wigner symbols, special values
- Symmetries & recursions
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