LIBPhys-UNL

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Bsc. in Physics Engineering

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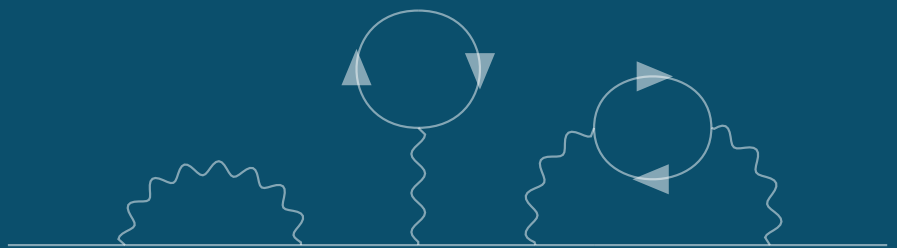
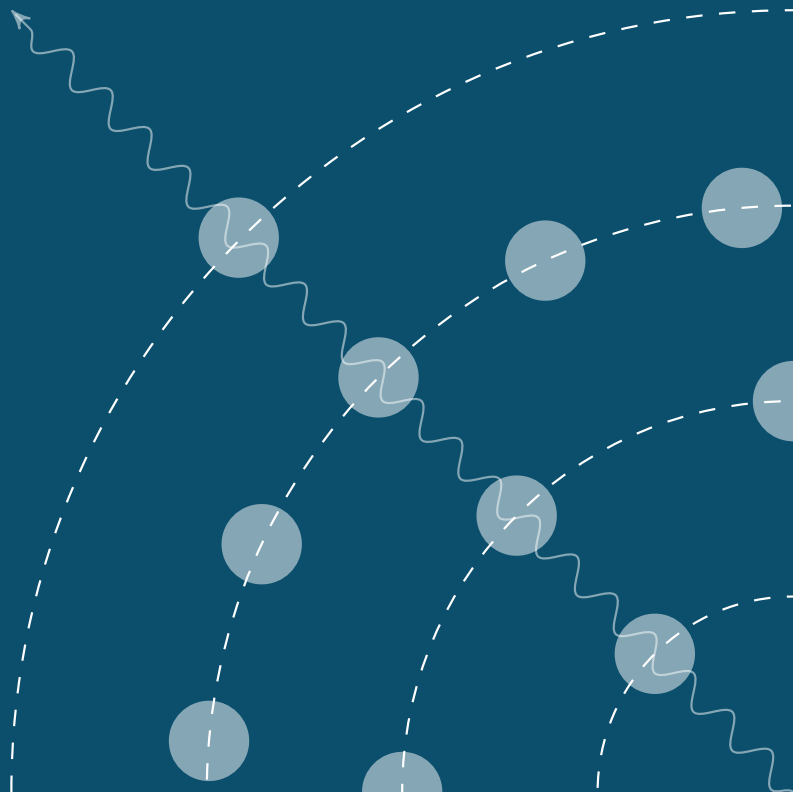
Advisor: Prof. Mauro Guerra
Co-Advisor: Prof. Jorge Machado

NOVA School of Science and Technology

X-ray Resonant Raman Scattering

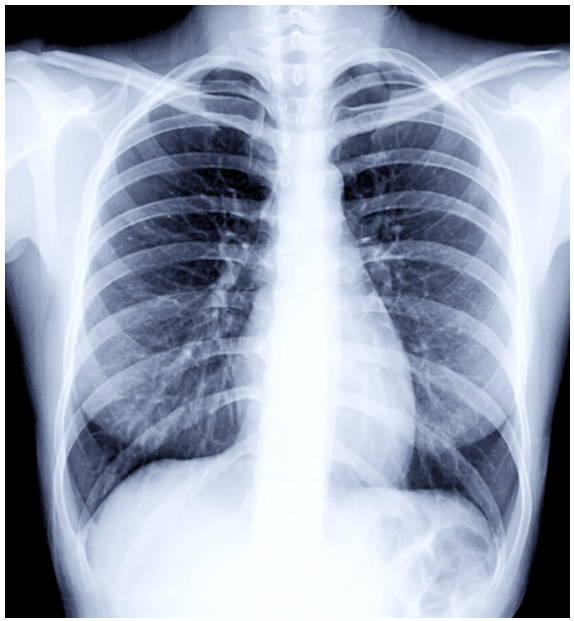
Spectra simulation from first principles for Copper below the ionization threshold using high-performance computing





Overview

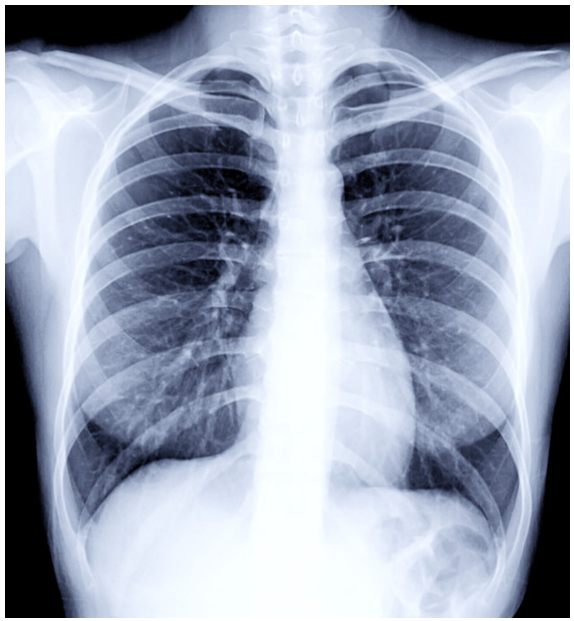
X-ray applications



(a) Imaging purposes (b) Sample quantification (c) Fundamental parameters

Figure: Application examples of x-ray radiation

X-ray applications



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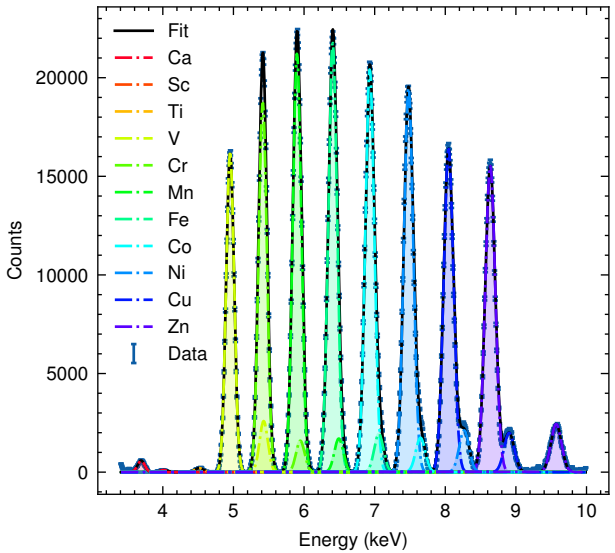

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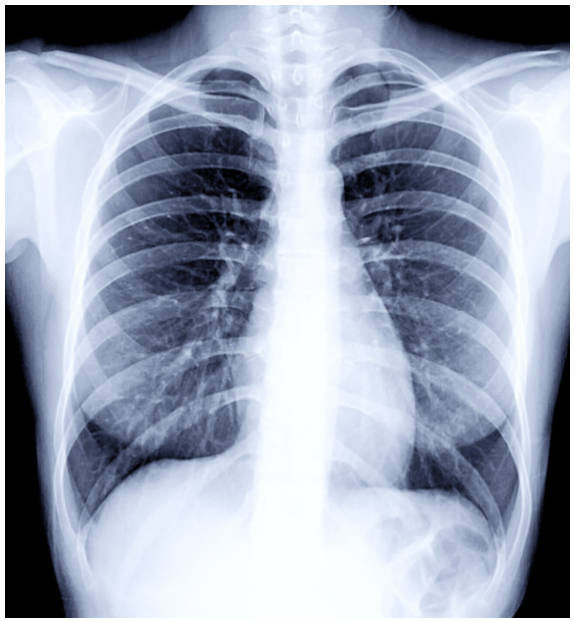

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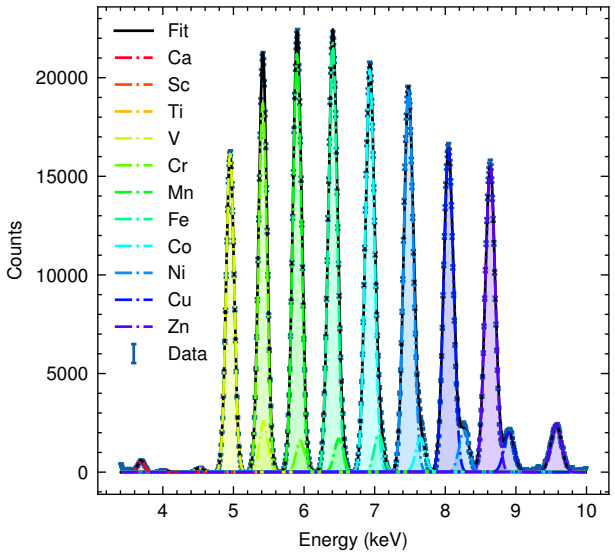

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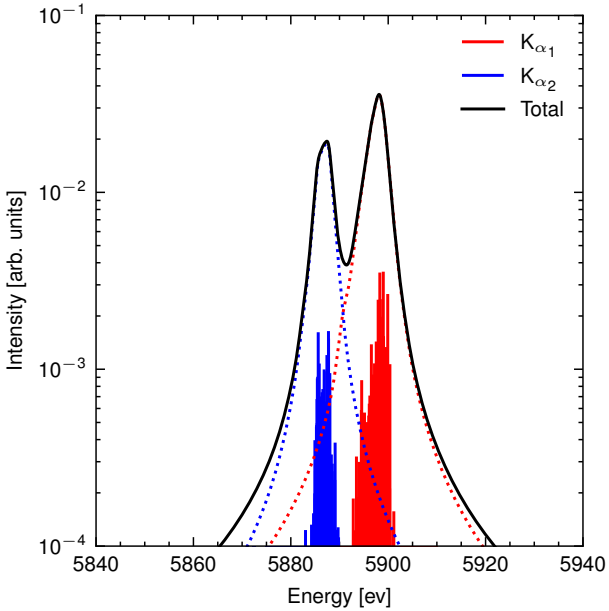

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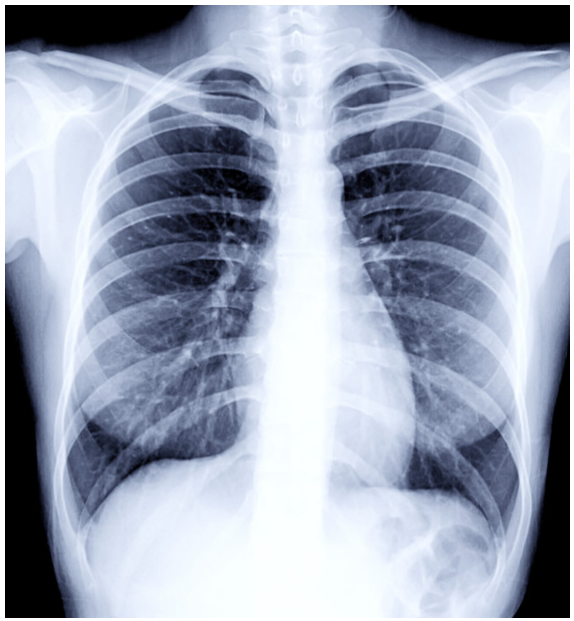

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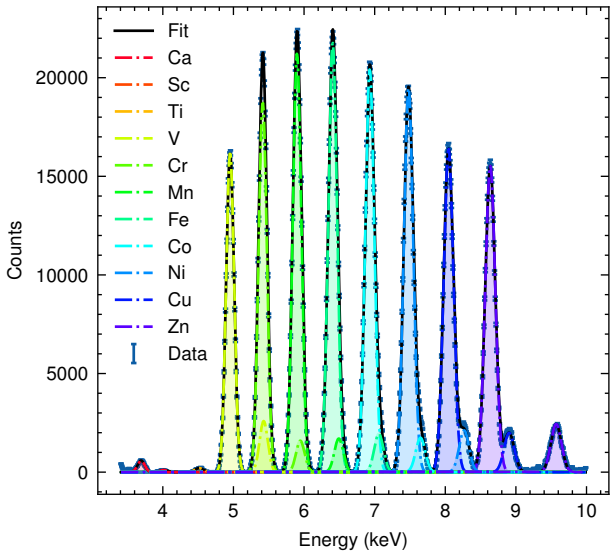

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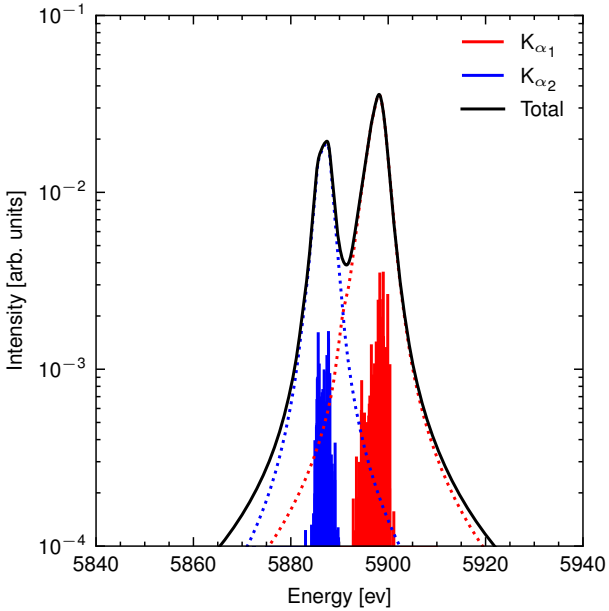

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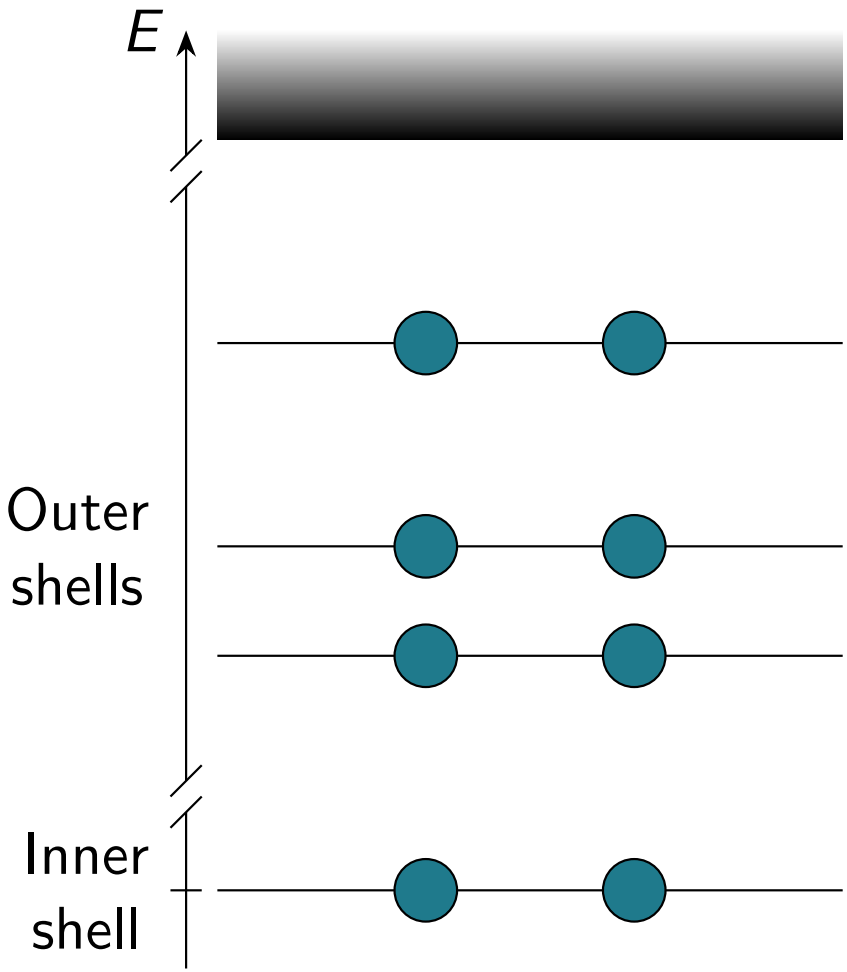

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- Energy transfer
- Ionization
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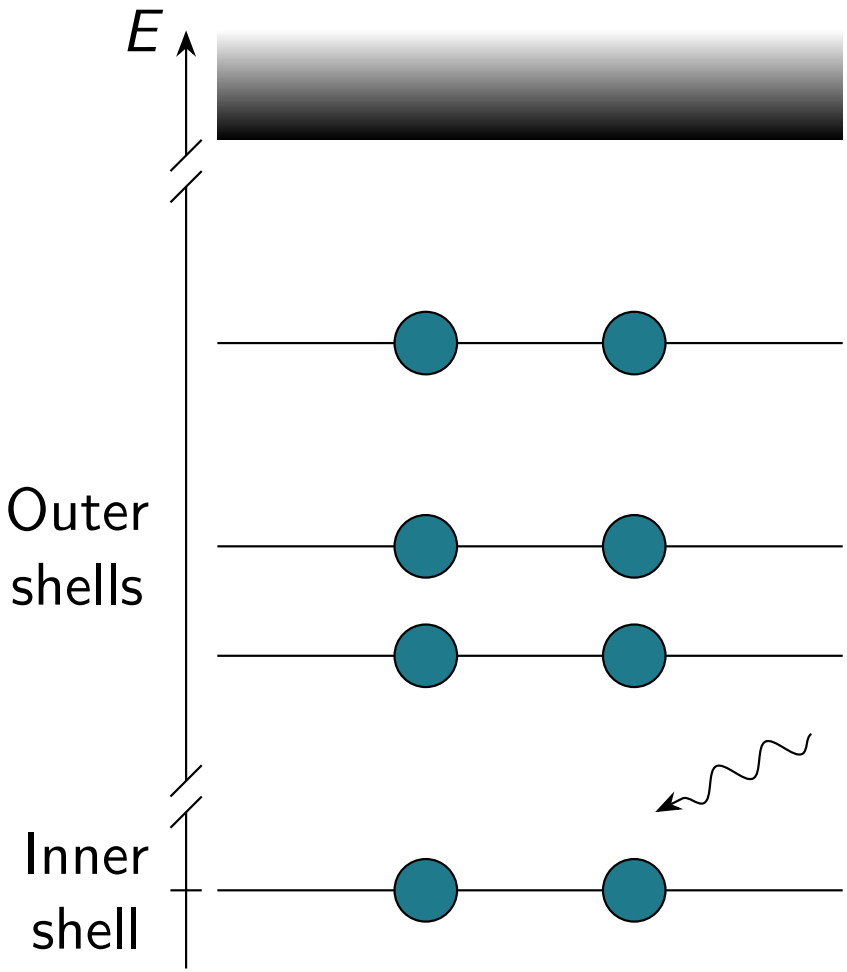

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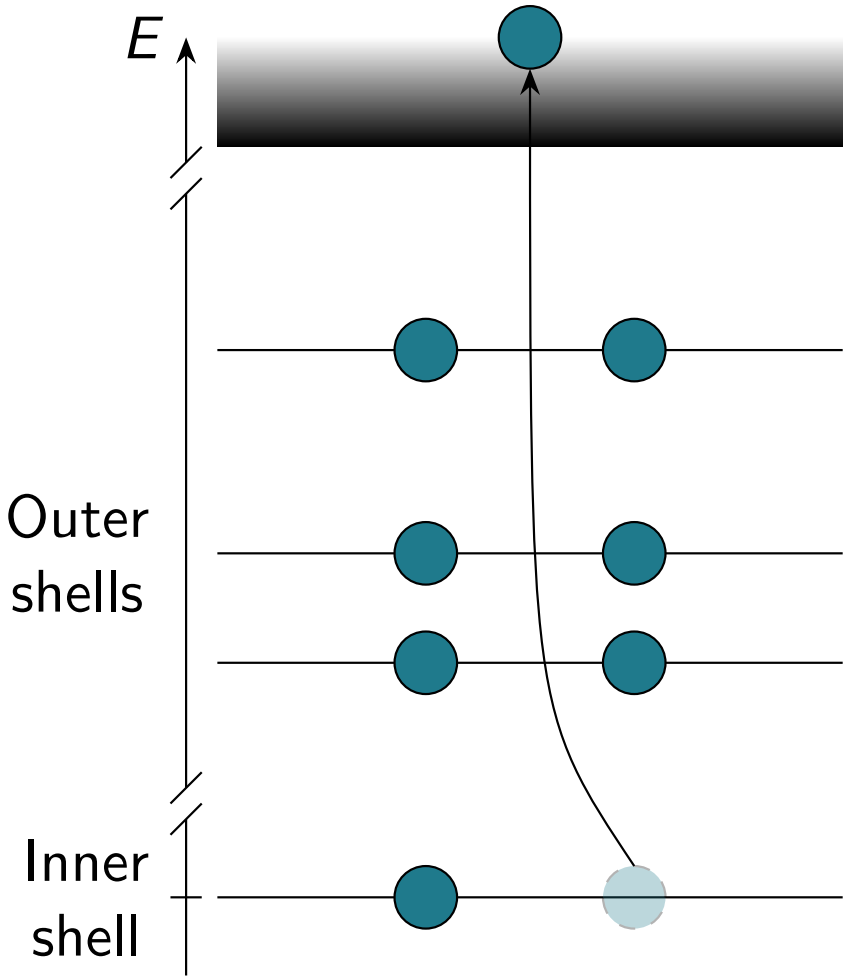

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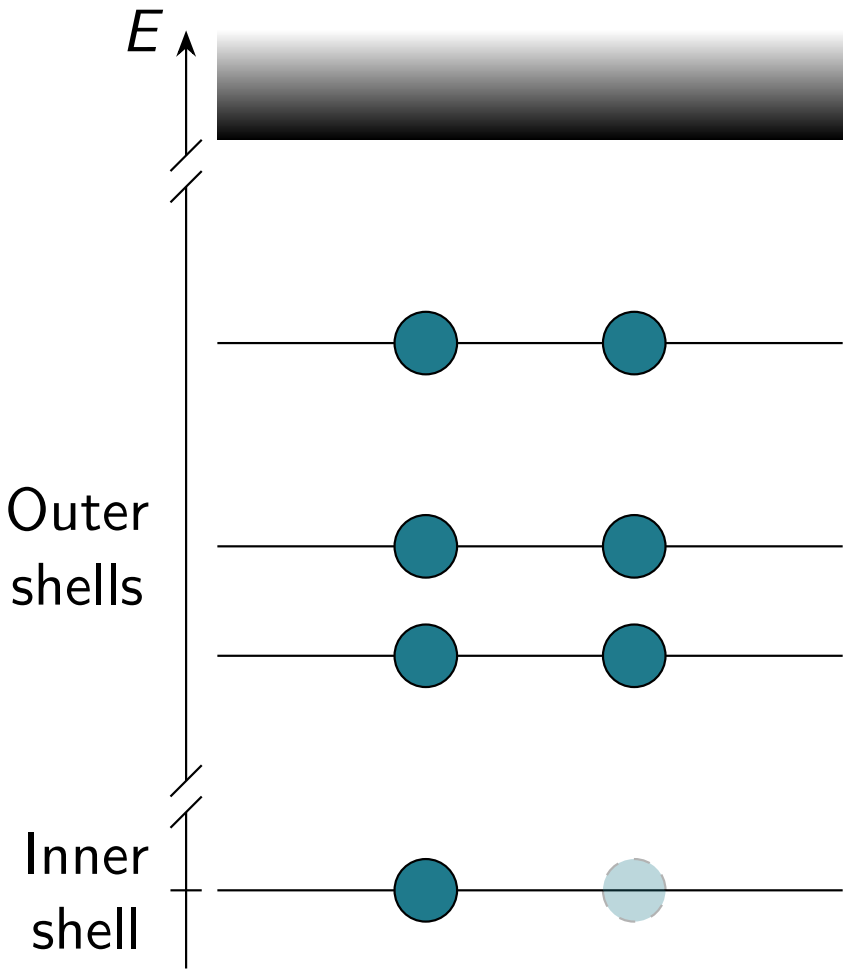

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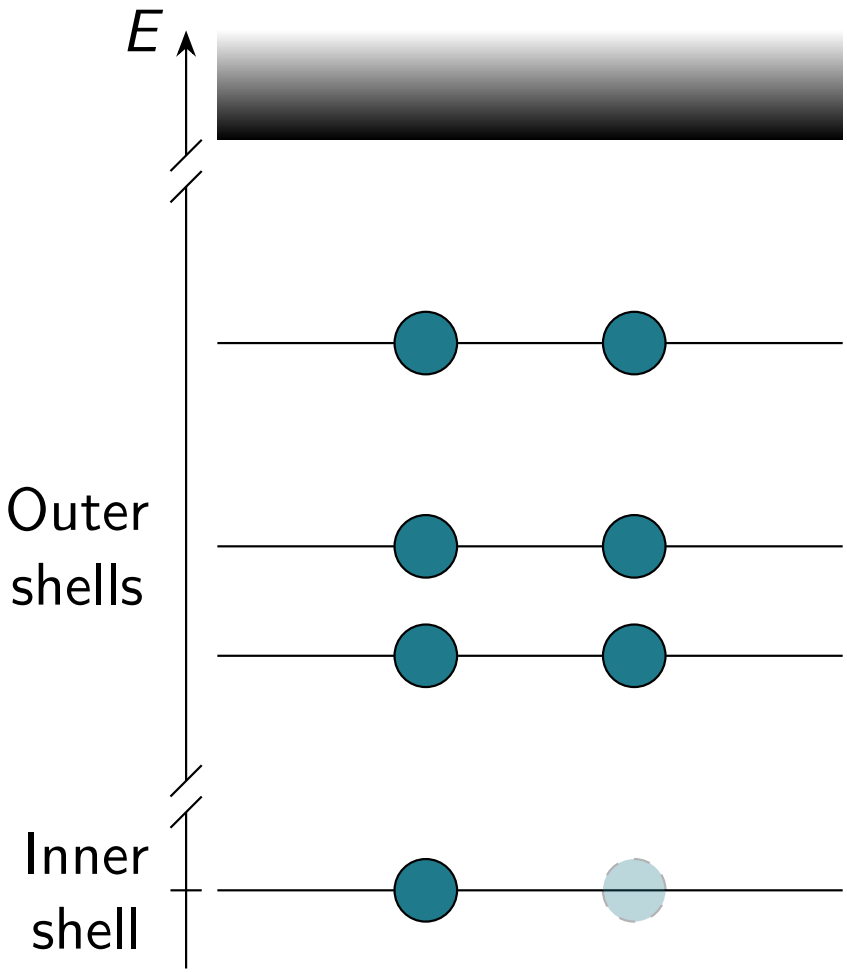

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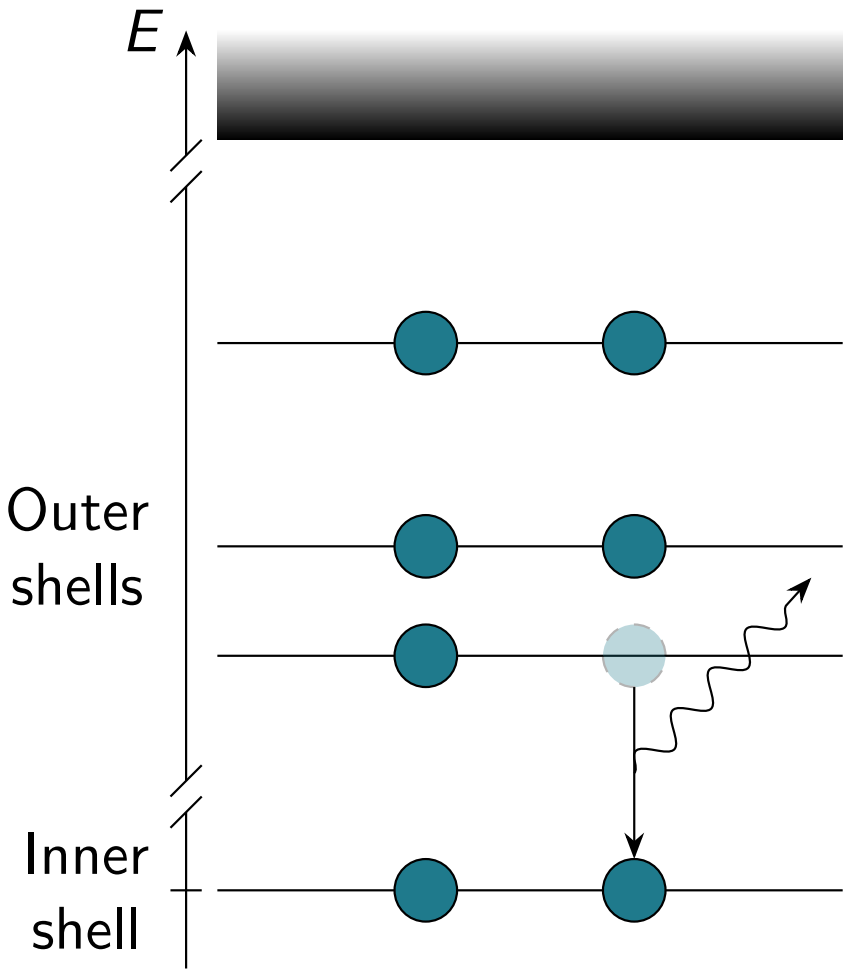

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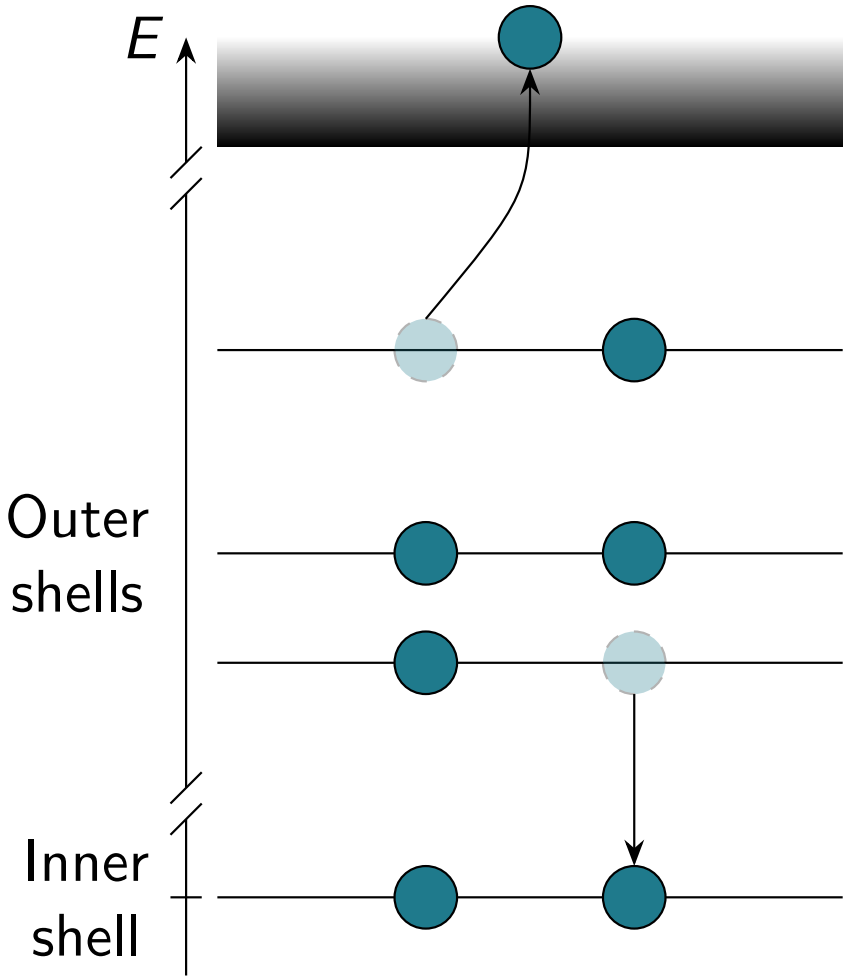

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Alternative processes

Shake processes

Post-ionization, the different number of particles in the system leads to a change in the Hamiltonian. This leads to the lack of orthogonality between non-equivalent states and free-wave wavefunctions in the initial and final configurations.

$$\langle 1s_i | 2s_f \rangle \neq 0 \qquad \langle 1s_i | e^-_{free} \rangle \neq 0$$

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Excitation of extra electron(s).

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The probability of these processes occurring is extremely dependent on the incident energy.
Since for this thesis, the energy ranges studied were below the ionization threshold, no shake processes were accounted for.

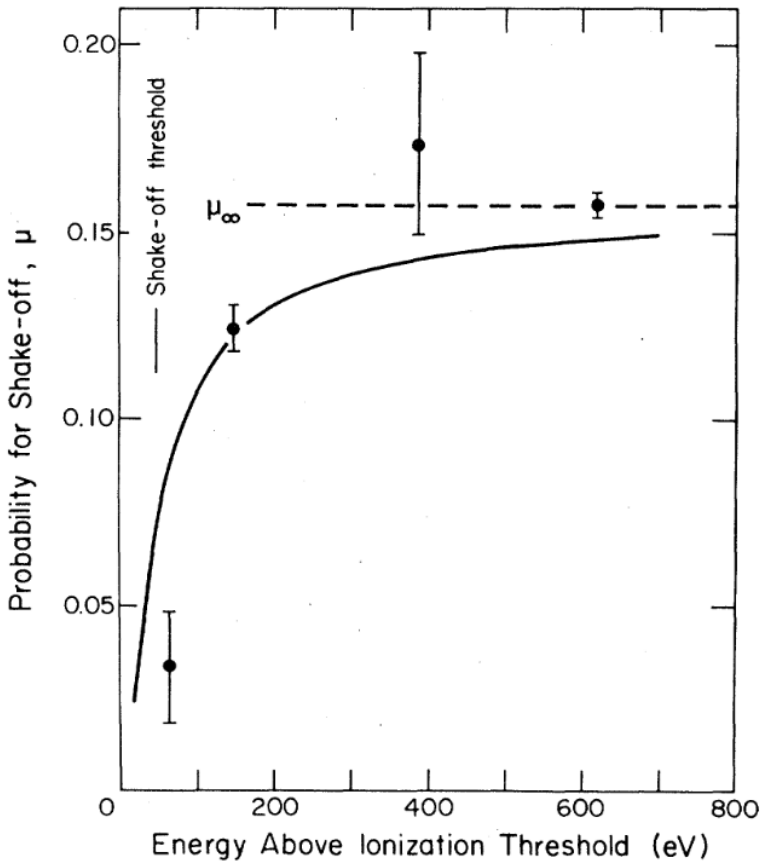

Figure: Thomas model for shake probability. [1]

Other processes

Photoexcitation

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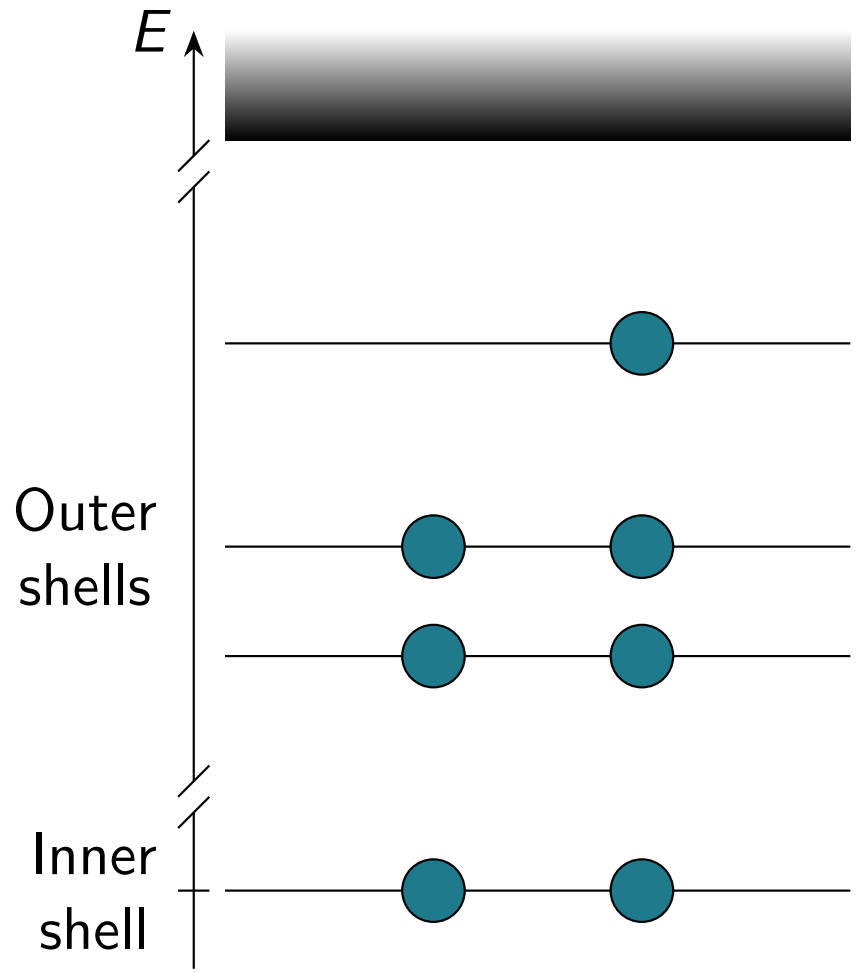

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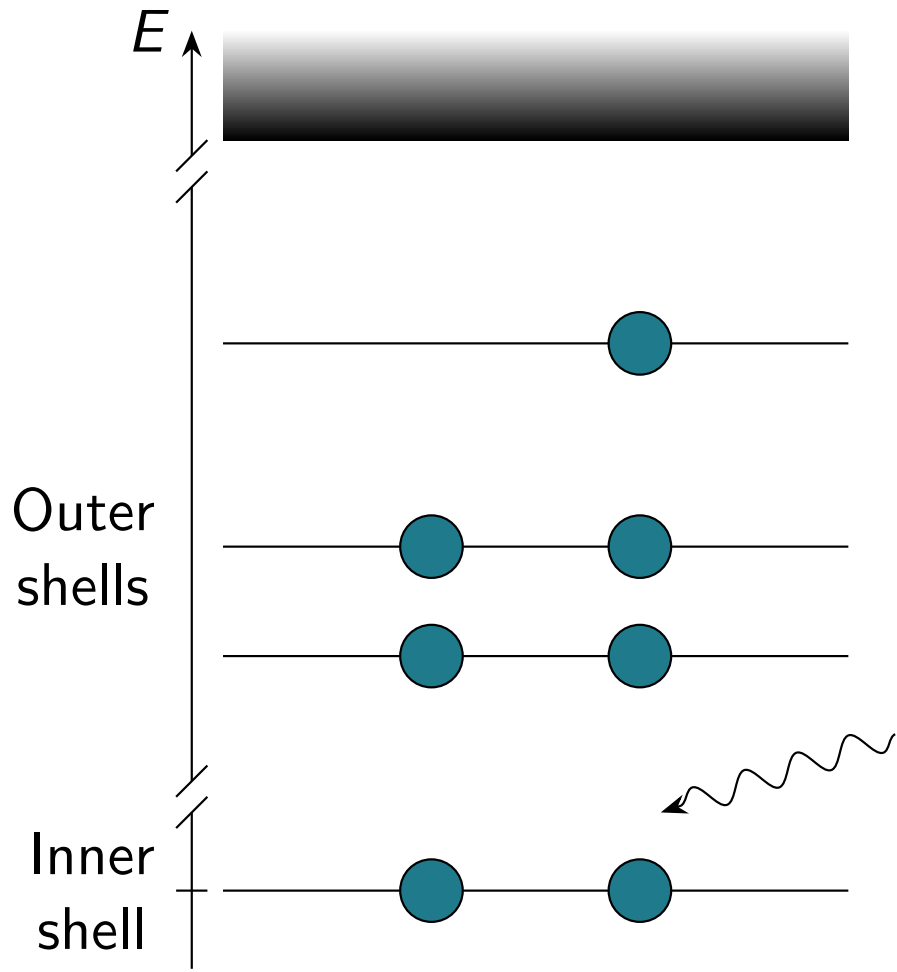

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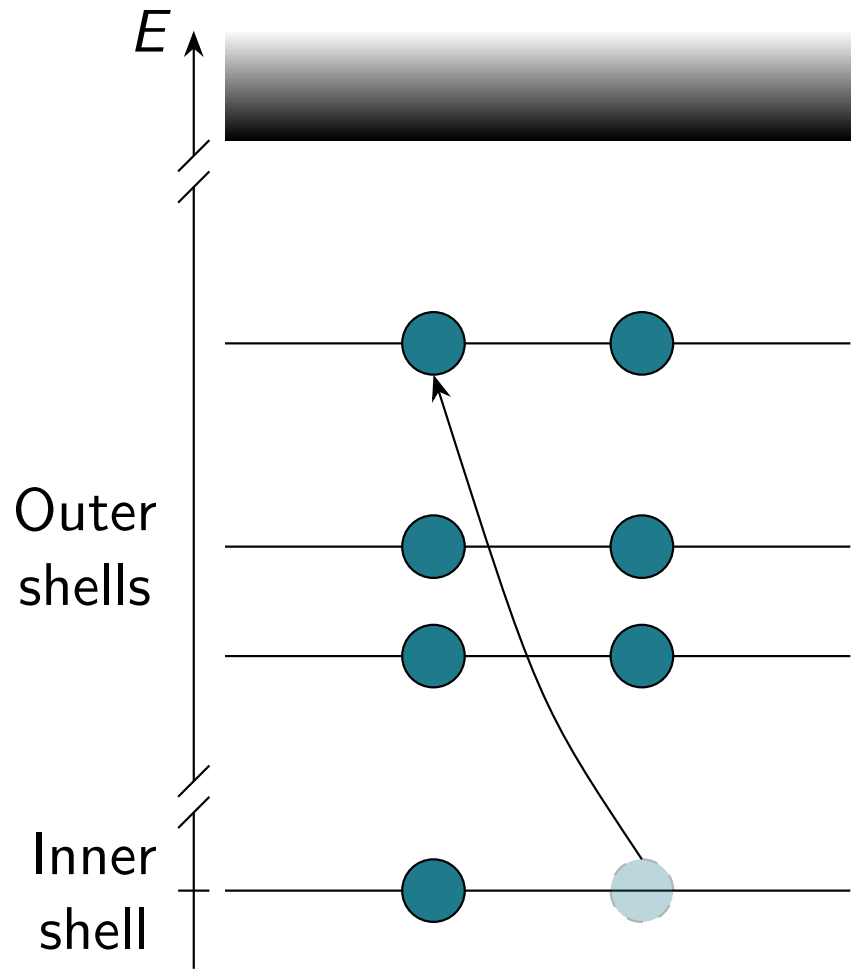

Schrödinger's Hamiltonian

In its most basic form, for a "classical" atom (nucleus + electrons), and when relativistic effects are not taken into account, the considered Hamiltonian follows the one use in Schrödinger's equation:

$$\hat{H} = \sum_{i}^{N} \frac{1}{2}\nabla_i^2 - \frac{Z}{r_i} + \sum_{j>i} \frac{1}{r_{ij}}$$

It incorporates:

- The kinetic energy of the electron.
- The potential energy of the electron-nucleus attraction.
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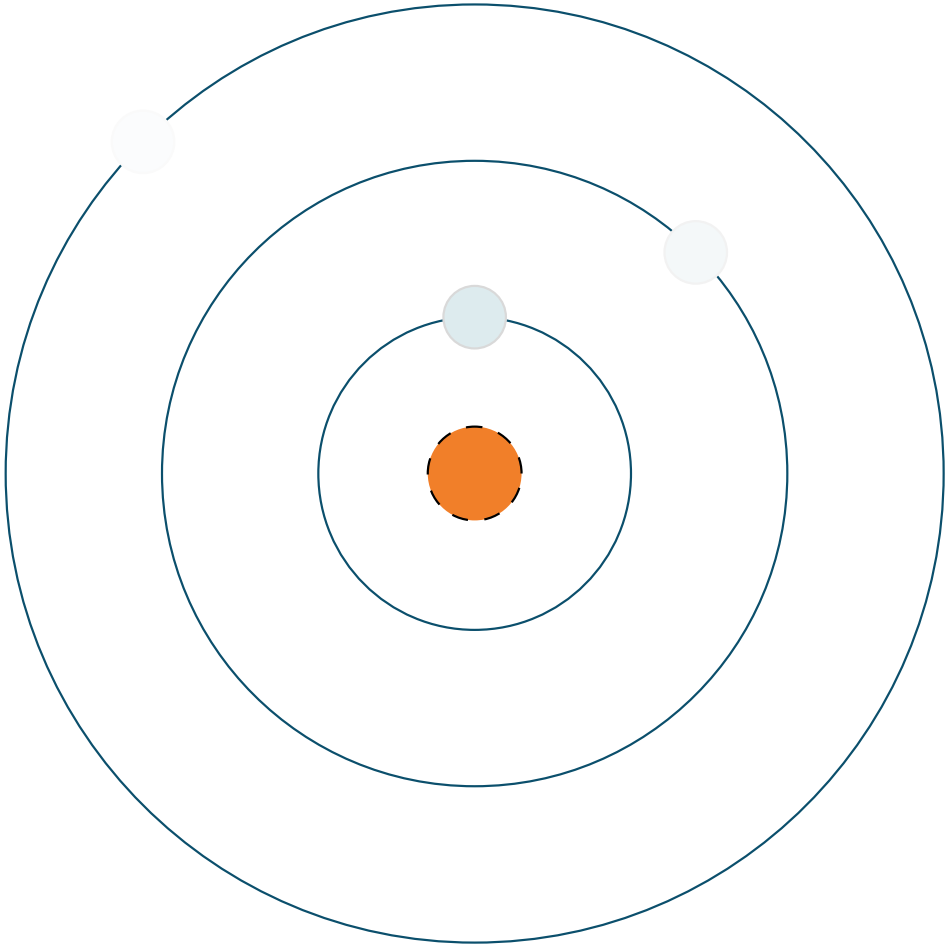
Solving the non-relativistic many-body problem

Due to the complexity introduced by the many bodies in the system, and their interactions, a numerical method needs to be employed as to obtain eigenfunctions for this Hamiltonian.



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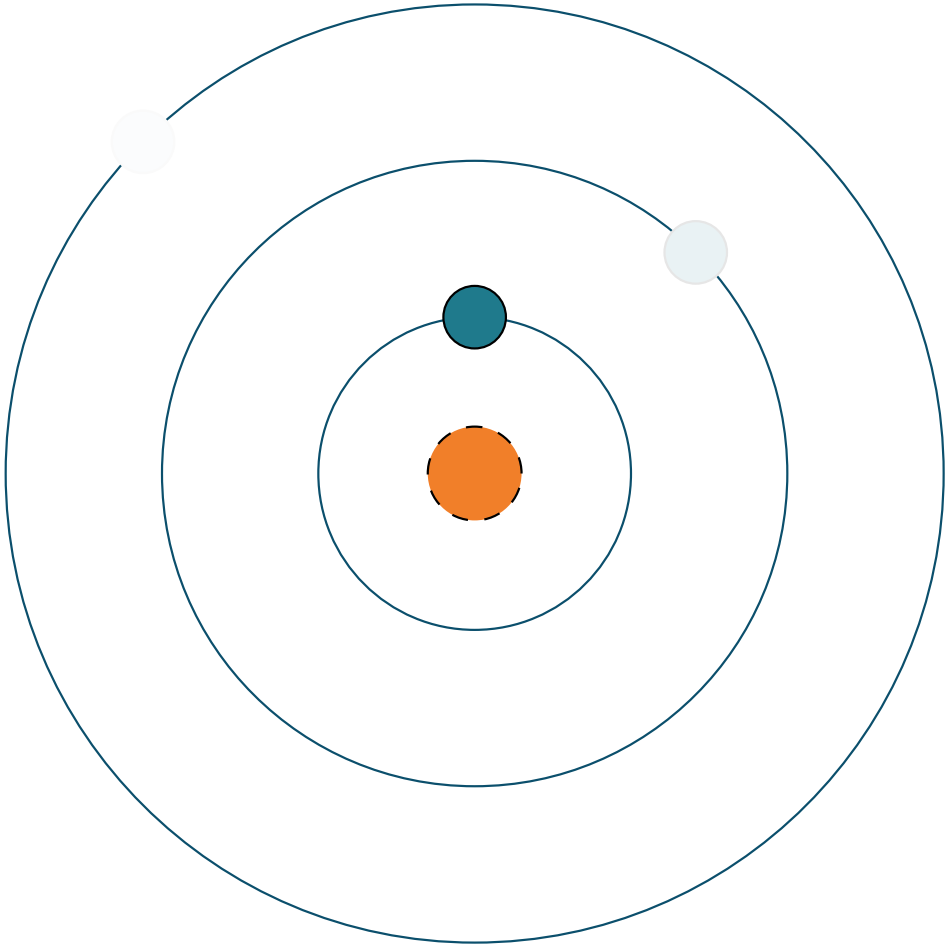

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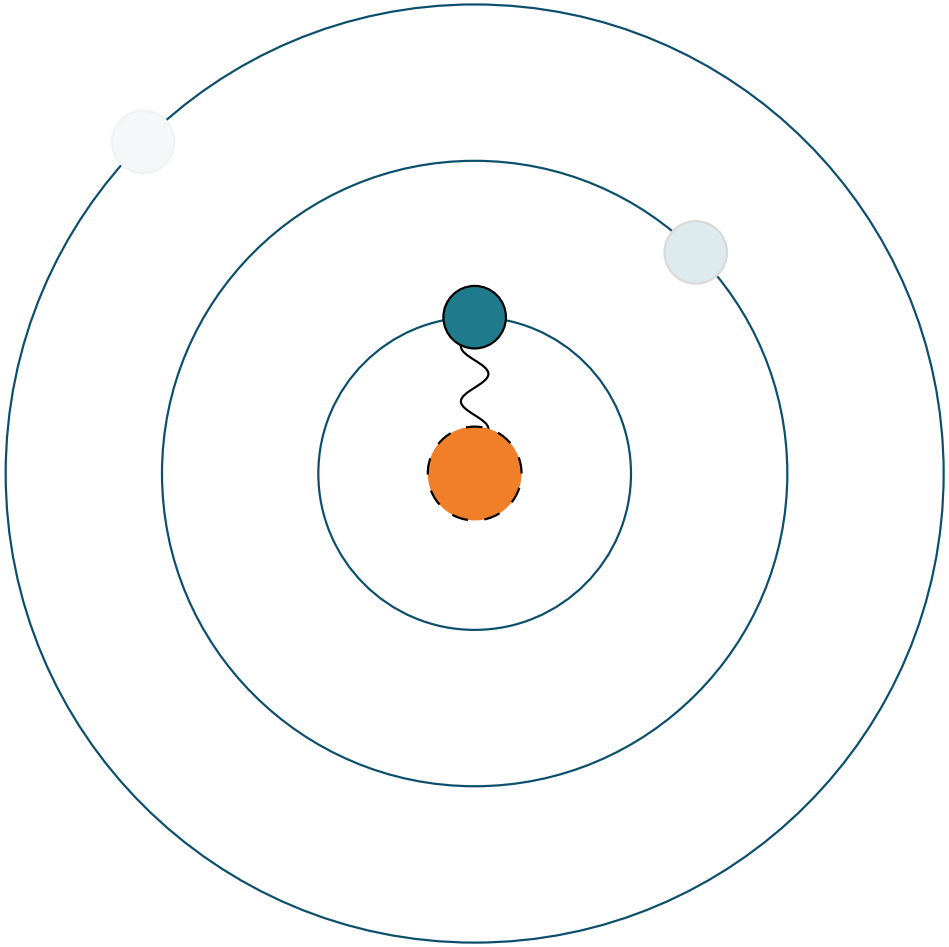

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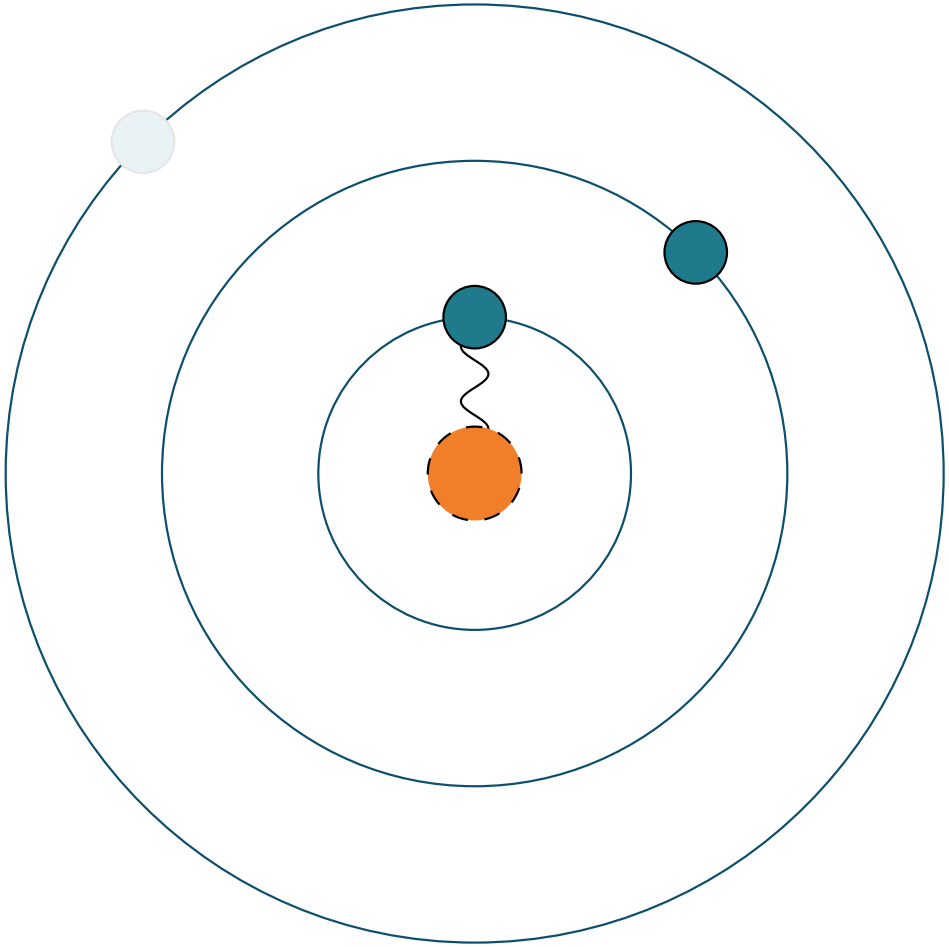

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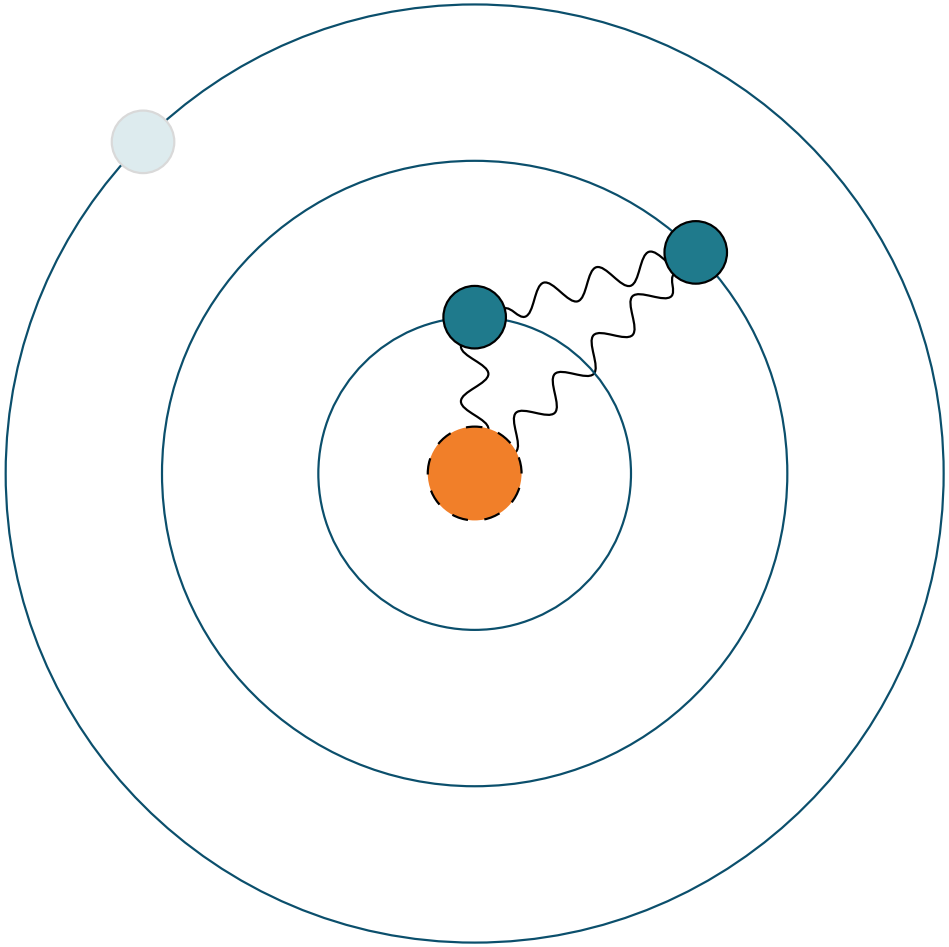

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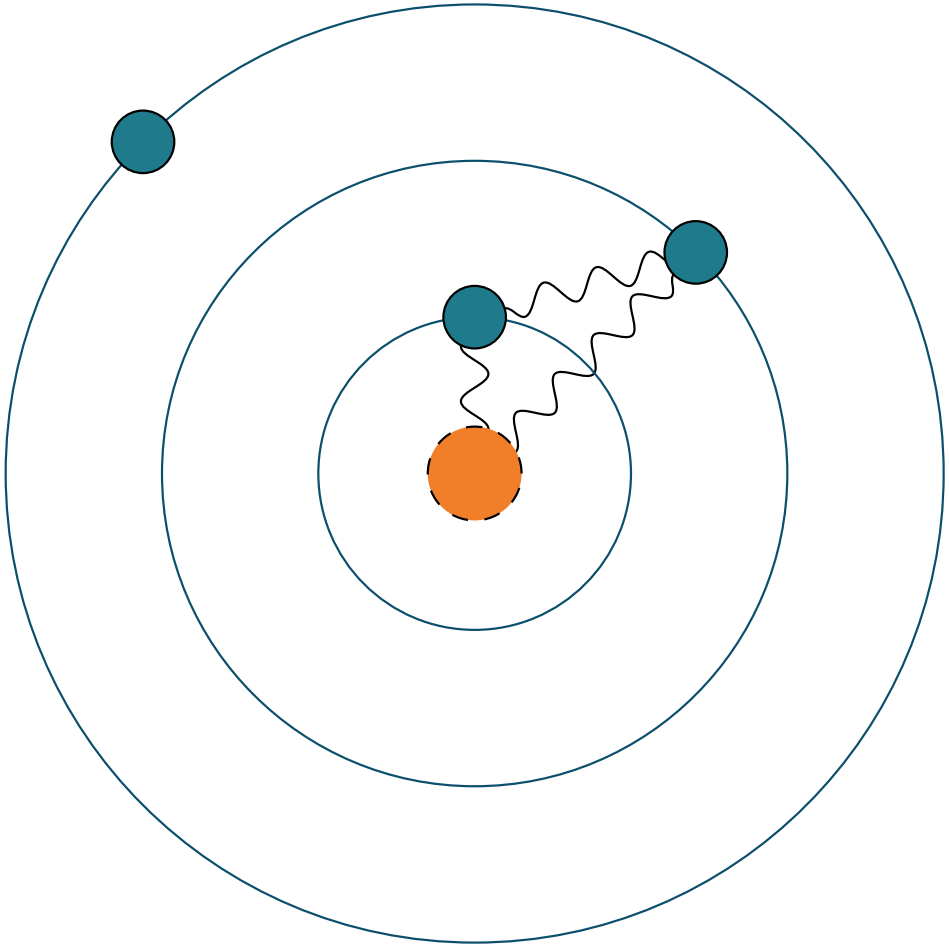

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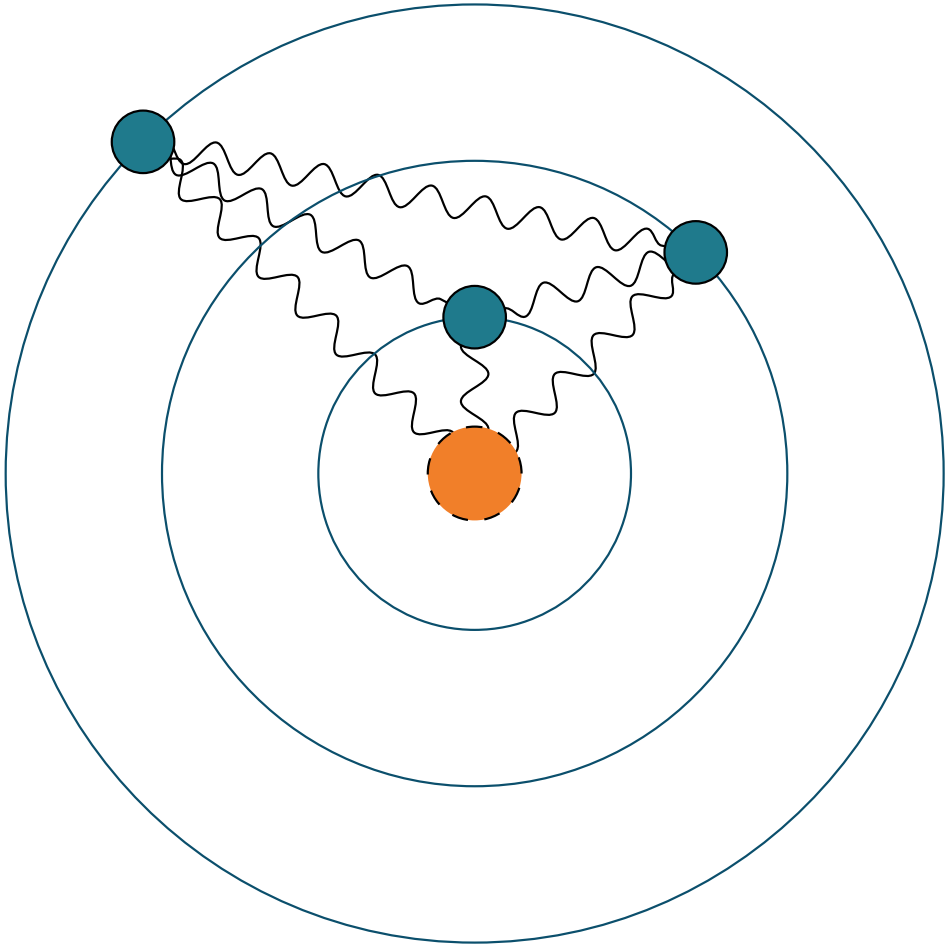


Solving the non-relativistic many-body problem

Each of the electrons' wavefunctions, u, are composed as a product of a spatial part, ψ, and one related to the electron's spin χ.

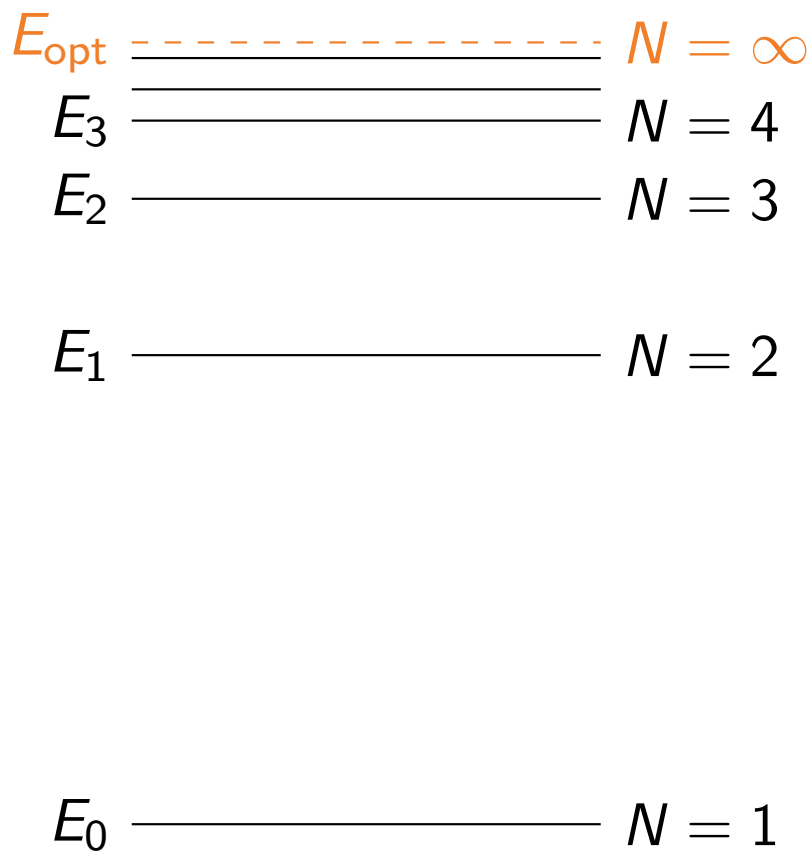
$$u = \psi\chi$$

The system's wavefunction should then be written as a Slater determinant as to account for anti-symetry and the fermionic nature of the electrons.

$$\frac{1}{\sqrt{N!}} \begin{vmatrix} u_1(x_1) & u_2(x_1) & \dots & u_N(x_1) \\ u_1(x_2) & u_2(x_2) & \dots & u_N(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ u_1(x_N) & u_2(x_N) & \dots & u_N(x_N) \end{vmatrix}$$

Solving the non-relativistic many-body problem

Through a self-consistent field approach, the method solves, for each cycle, a set of integro-differential equations as a way to compute new wavefunctions and the new energy for the system.



Solving the non-relativistic many-body problem

This process is then repeated up until the energy difference in-between two steps is under a pre-defined benchmark value, as to assure the computation has converged.

METER DIAGRAMA DE BLOCOS

Limitations of the non-relativistic approach

While Schrödinger's equation may be quite accurate for low energy systems (e.g. Hydrogen), where the speed of the surrounding electrons is not comparable to that of light, such is not the case for more complex and heavier systems.

Speed of 1s electrons in ground state configurations (% of c)

Hydrogen:	0.516%
Copper:	14.751%
Uranium:	49.211%

$$E_k = mc^2 \left(\frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} - 1 \right)$$

Relativistic approaches

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- Incorporates the relativistic energy-mass relation.
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- Accounts for spin interactions.
- Yields two-component solutions, for positive and negative energies.
- The "Dirac sea" originated the talks about the possible existence of anti-particles.

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Field retardation effects:

Necessary to account for Breit's corrections:

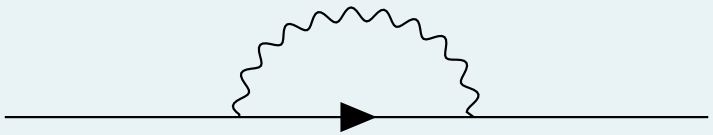
$$H_B = \sum_{i>j} \frac{e^2}{r_{ij}} - e^2 \left(\frac{\boldsymbol{\alpha}_i \boldsymbol{\alpha}_j}{r_{ij}} + \frac{(\boldsymbol{\alpha}_i \boldsymbol{\nabla}_i)(\boldsymbol{\alpha}_j \boldsymbol{\nabla}_j) r_{ij}}{2} \right),$$

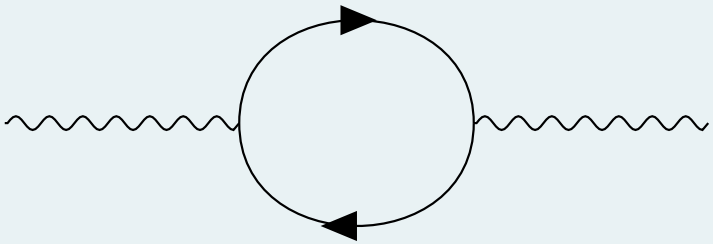
So, what is missing?

$$H = H_D + H_B$$

Field quantization effects (QED):

Necessary to account for effects from Quantum Electrodynamics, such as Self-energy and Vacuum Polarization.





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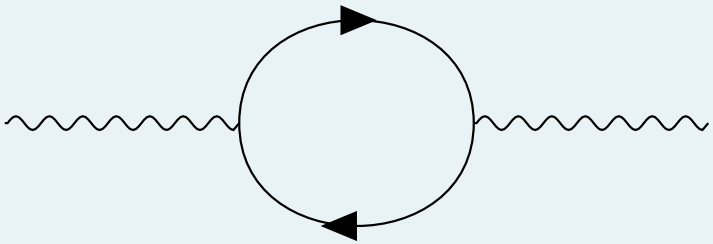

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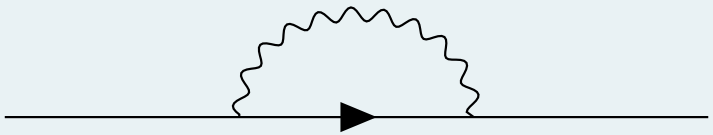

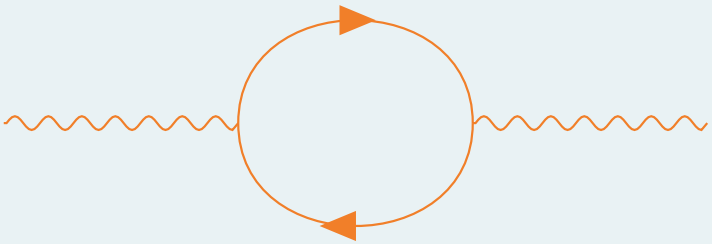

The state-of-the-art

Reasons for this study

- Copper is a dominant element in today's technological progress.
- A great deal of studies has been performed on its emission spectrum.
- Most studies note a skewness in the K_α transition lines, being mostly attributed to satellite lines, but leaving open the possibility of its cause coming from photoexcited states.
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mcdfgme (Multi Configuration Dirac-Fock General Matrix Elements)

This code is a novel computational implementation, based on the Hatree-Fock method, capable of calculating a plethora of atomic parameters, while incorporating all previously mentioned necessary considerations.
It has proven time and time again to have excellent accuracy and precision when performing calculations for the most varied systems.

Overview

The considered excitations

As previously stated, the focal point of this work is that of computing radiative relaxation spectra for excited Copper.

Ground State: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 3d^{10}\ 4s^1$

Excitations of any one of the consituent electrons to orbitals:

$4s$	$4p$	$4d$	$4f$		
$5s$	$5p$	$5d$	$5f$	$5g$	
$6s$	$6p$	$6d$	$6f$	$6g$	$6h$
$7p$	$8p$	$9p$			

The calculated configurations

In order to account to all possible decay possibilities, it was necessary to perform calculations for two different sets of configurations.

1-hole configurations

Related to the initial and final states of radiative transitions.
Obtained by running a hole through all orbitals in the base-configurations.

2-holes configurations

Related to the final states of Auger transitions.
Obtained by running a combination of two holes through all orbitals in the base-configurations.

The level manifold

It is now necessary to compute all possible levels the studied atomic system can be in. As it will be shown, this is no simple task...

The level manifold

Besides the original configuration, three other sets of quantum numbers are necessary for defining a level:

- The hole orbital labels: $(n\ l_j)$
- The total angular momentum number: J
- The eigenvalue/Lagrange multiplier: ϵ

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Here, we know two base things:

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Let us analyse an excitation from $2p$.

This leads to the possibility of the electron having come from:

- $1s$
- $2s$
- $2p$
- $3s$
- $3p$
- $3d$
- $4s$

The level manifold- an example: $2p \rightarrow 4p$ excited Copper

For this configuration, three subshells are open: $2p$, $4s$, and $4p$.

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Possibilities for J values follow:

2p		4s		4p		Total/J
M_l	M_s	M_l	M_s	M_l	M_s	$M_l + M_s$
1	$-1/2$	0	$-1/2$	1	$-1/2$	$1/2$
1	$1/2$	0	$-1/2$	1	$-1/2$	$3/2$
1	$1/2$	0	$1/2$	1	$-1/2$	$5/2$
1	$1/2$	0	$1/2$	1	$1/2$	$7/2$

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1	$1/2$	0	$1/2$	1	$1/2$	$7/2$

The level manifold- an example: $2p \rightarrow 4p$, $J = {}^{5}/_{2}$

Even for this **very** specific example, the branching-out continues:

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There are many possibilities for achieving this certain combination of a given configuration and J value. Each, is represented by the respective ϵ.

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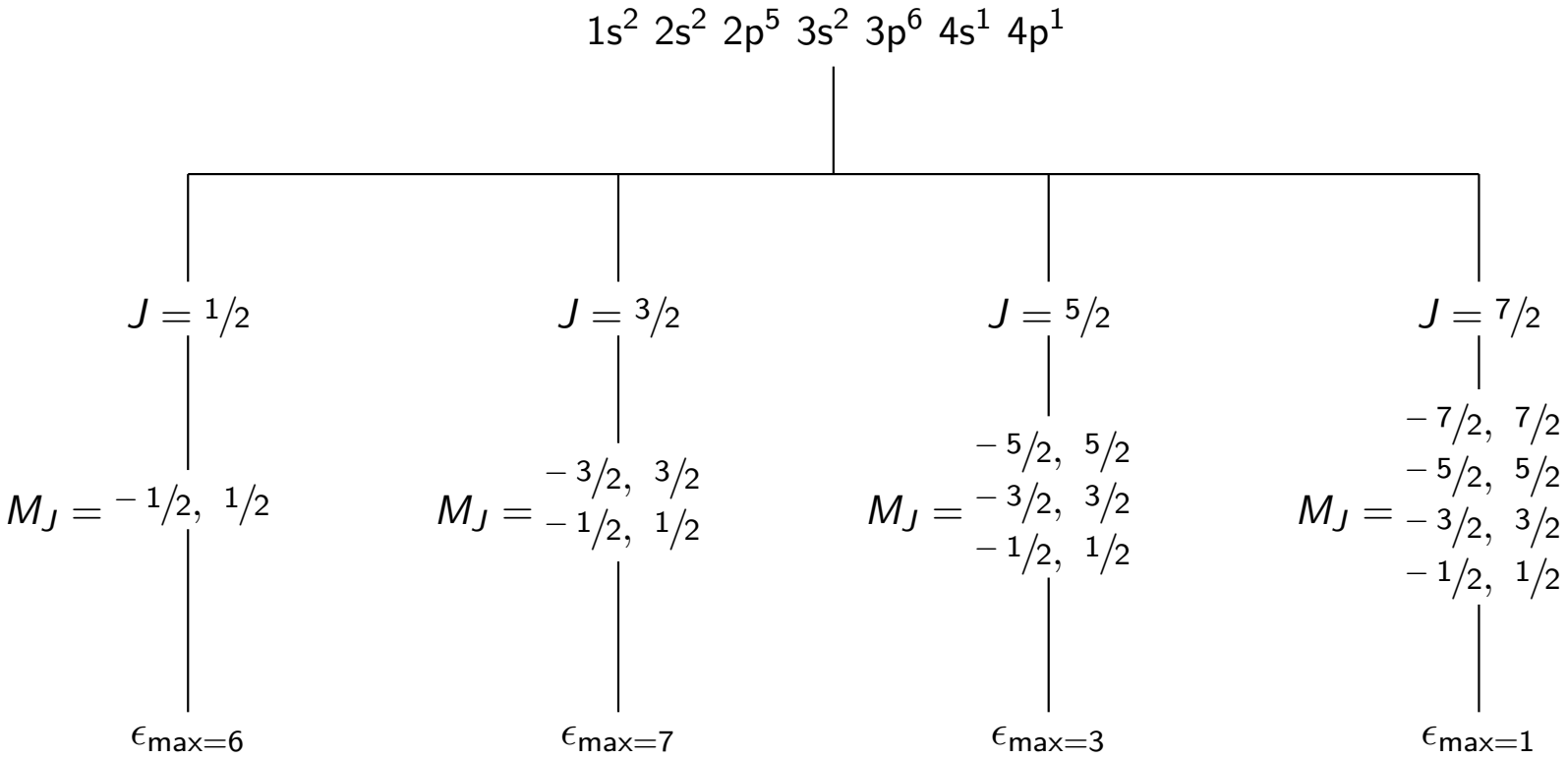
$J = {}^5/_2$					
2p		4s		4p	
M_l	M_s	M_l	M_s	M_l	M_s
1	$-{}^1/_2$	0	${}^1/_2$	1	${}^1/_2$
1	${}^1/_2$	0	$-{}^1/_2$	1	${}^1/_2$
1	${}^1/_2$	0	${}^1/_2$	1	$-{}^1/_2$

The level manifold

This set of possibilities and rearrangements form what we call the level manifold. In addition, a $2J+1$ level degeneracy is accounted for.



$6+7+3+1=17$ levels

$6\times 2+7\times 4+3\times 6+1\times 8=66$ states

Level calculations with *mcdfgme*

A calculation was performed for each existent level.
In each of them, a level was treated as a linear combination of state wavefunctions (associated with the eigenvalues) with mixing coefficients:

$$|\Psi\rangle = a_1 |\psi_1\rangle + a_2 |\psi_2\rangle + \dots$$

Self-consistent field

- Coulomb interactions
- Breit considerations
- Vacuum Polarization

Perturbation theory

Self-energy

Evaluating the calculation

What to look out for:

- Orthogonality conservation
- Energy divergences
- Effective nuclear charge

Evaluating the calculation

What to look out for:

- Orthogonality conservation
- Energy divergences
- Effective nuclear charge

Due to the method's numerical nature, orthogonality problems may surge.
We look at overlap values for similar orbitals (same l_j) and set a maximum threshold:

$$|\langle n\ l_j | m\ l_j \rangle| \leq 10^{-6}$$

Evaluating the calculation

What to look out for:

- Orthogonality conservation
- Energy divergences
- Effective nuclear charge

A component of the energy is computed through two different methods. For good convergence, the difference in their values should not be above 1 eV.

$$|E_1 - E_2| \leq 1 \text{ eV}$$

Evaluating the calculation

What to look out for:

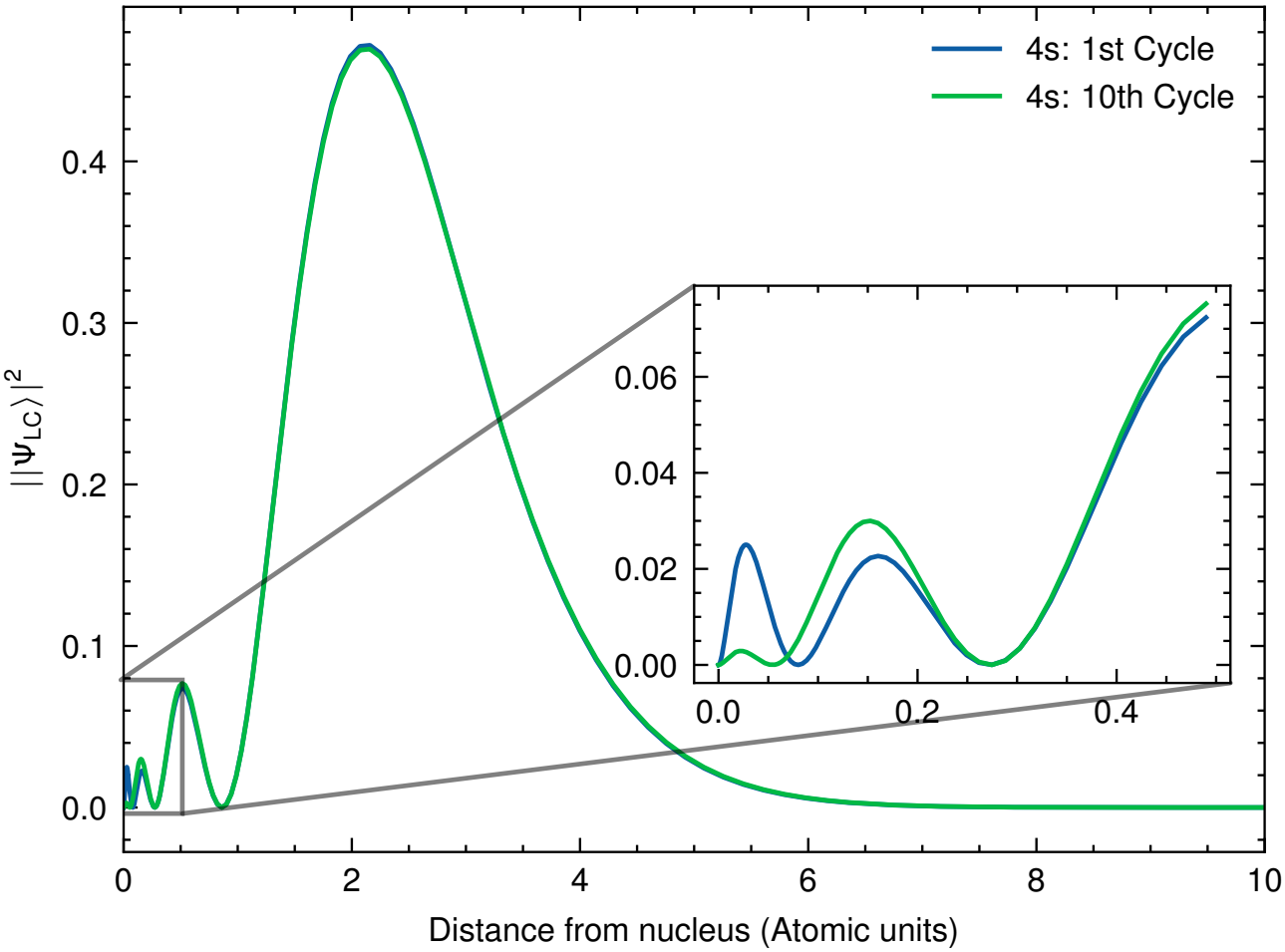
- Orthogonality conservation
- Energy divergences
- Effective nuclear charge

The presence of inner electrons leads to a shielding of the positive nuclear charge. As so, outer electrons will be subject to an attenuated positive charge. This effect has been previously studied, and the obtained values should be benchmarked.

Methods for solving the convergence problems

- Changing the number of self-consistent cycles.
- Altering cycle parameters, such as accuracy.
- Choosing the initial trial wavefunctions for select orbitals (e.g. Hydrogenoids or obtained through the Thomas Fermi potential).
- Changing the method for solving the Dirac equation.
- Enforcing the node number for the wavefunctions

Changes in wavefunctions after the variational process



Total number of calculated levels

For the 19 performed calculations,

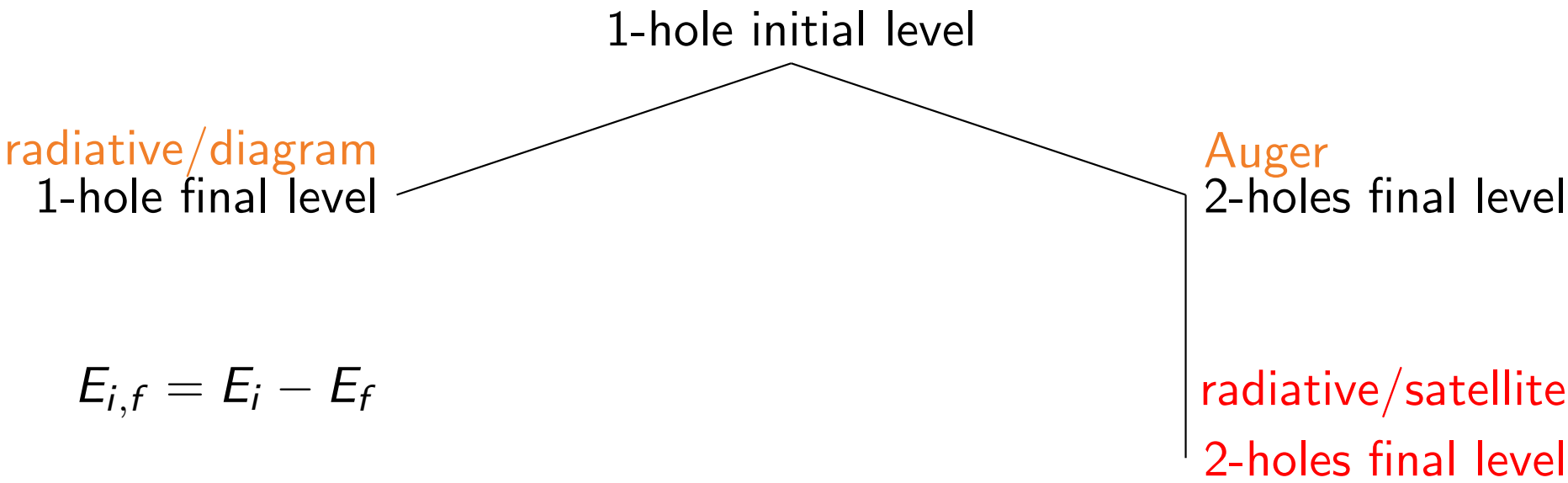
- 1601 1-hole levels
  - 166 manually converged
- 20550 2-holes levels
  - 1678 manually converged

Leaving a total of:

- 22151 levels calculated
- 1844 levels manually converged

Atomic transitions

When a system is not found in its least energetic state various processes will occur until the most stable one is reached.
In this way, for every level, calculations were performed for decays to all possible lower energy states.



Radiative transitions

Given the set of all 1-hole levels, with n elements, the total number of these transitions (without accounting for level degeneracy), N, is simply given by the amount of combinations of two elements between the set:

$$N = \frac{n!}{2 \cdot (n-2)!}$$

For these transitions, full orbital relaxation was allowed.
The *mcdfgme* calculation yields the rates for each Electric and/or Magnetic component/pole for both Coulomb (length) and Lorentz (velocity) gauges.

Auger transitions

The total number of Auger transitions can not be calculated *a priori*. Since the 1-hole and 2-holes level sets are "independent", the level structure needs to be calculated in order to fully resolve the number of transitions. For computing these transitions, the free-electron wavefunction has to be computed for the initial state potential, and orthogonality is enforced between the free-wave and bound orbitals.

All calculated transitions

In total, for this work,

- 70885 diagram radiative
- 452988 Auger
- 6684258 satellite radiative

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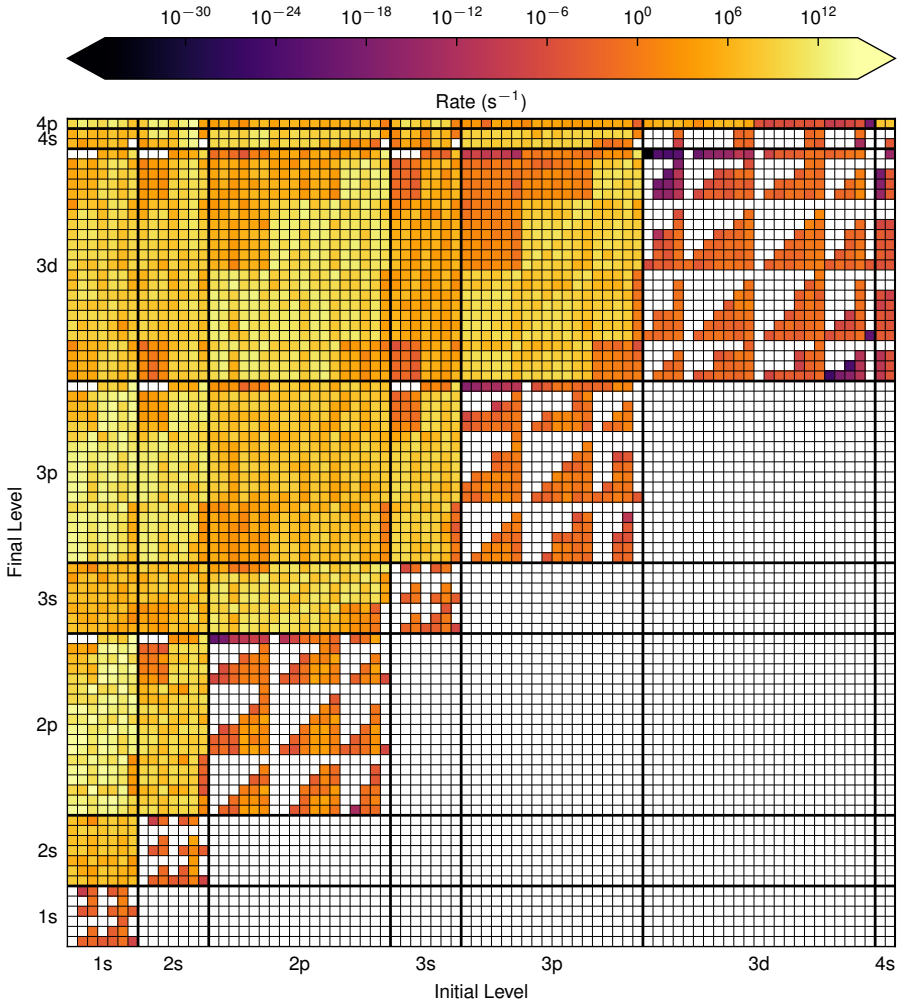
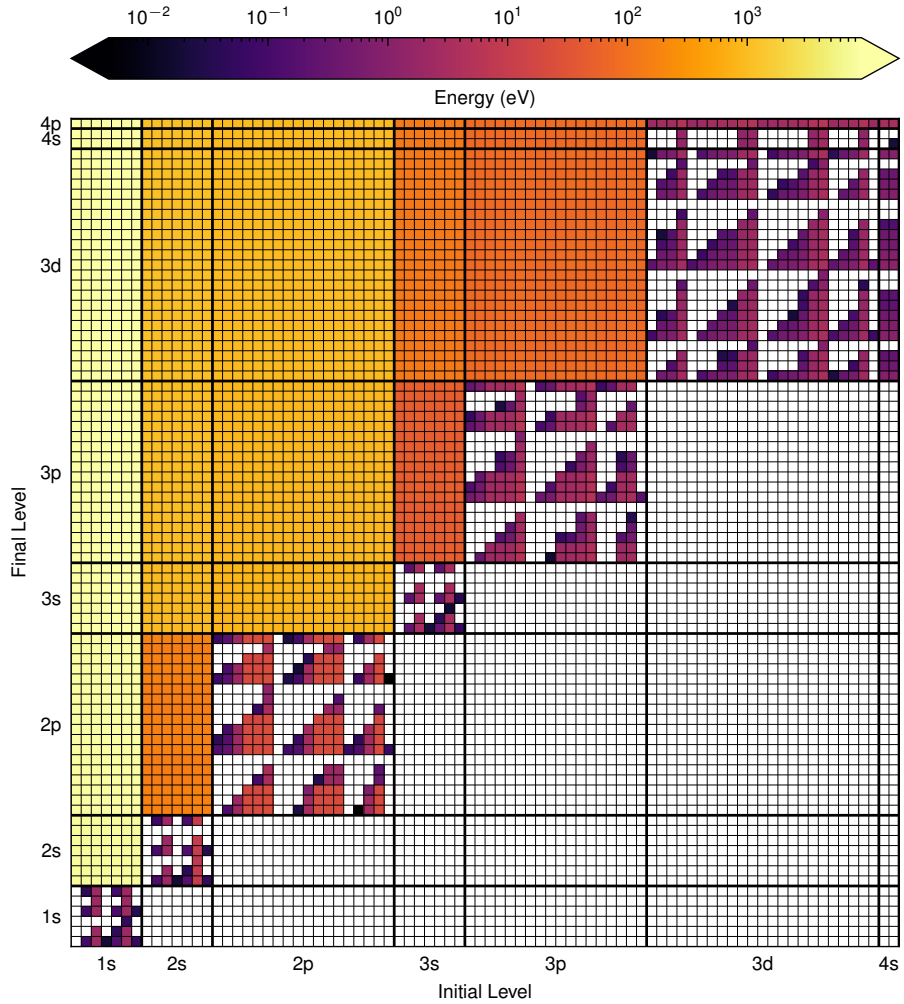
transitions were calculated, totaling to 7208131 computations performed.

Rate and Energy matrices

To evaluate and benchmark a calculation, a visualization tool was used, where the calculated energy and rate values were displayed in a grid-like view.

Rate and Energy matrices





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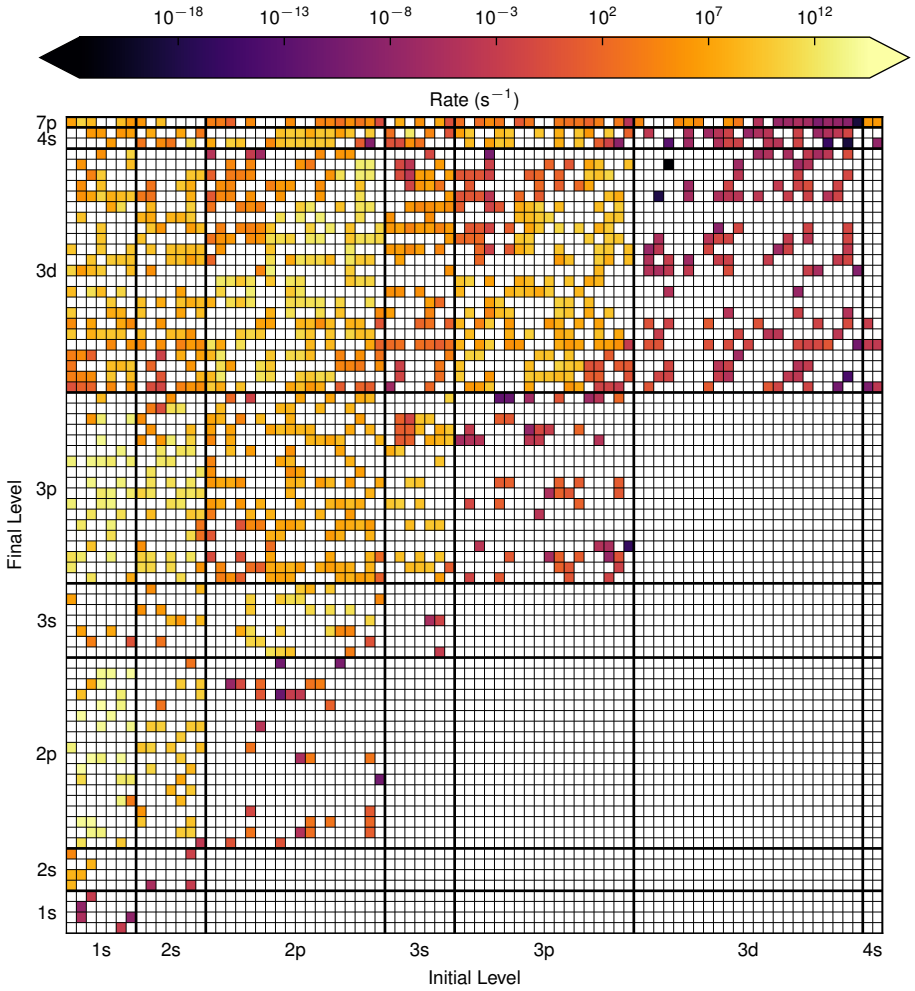

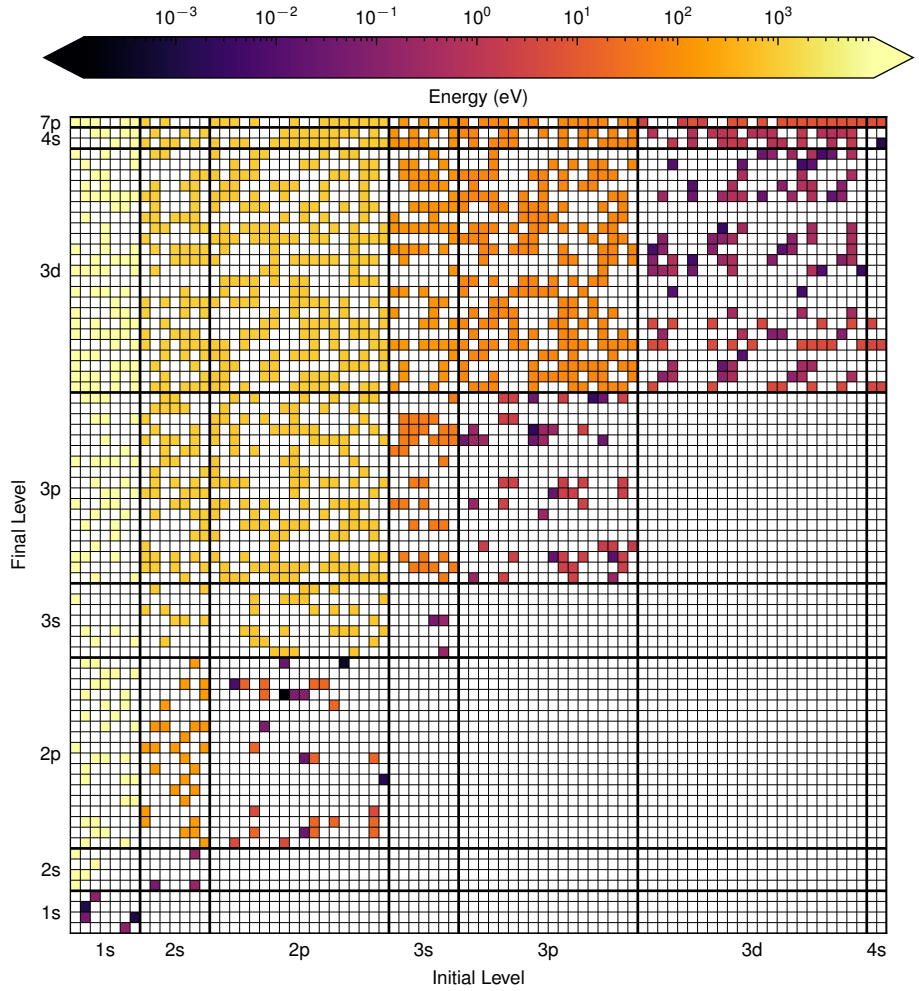

Overview

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Overview

Conclusion

Thank you
for your attention!