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Muon Cascade Calculations

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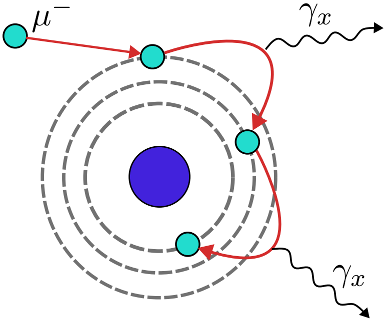
Introduction



- Elemental analysis is a modern usage of negative muons

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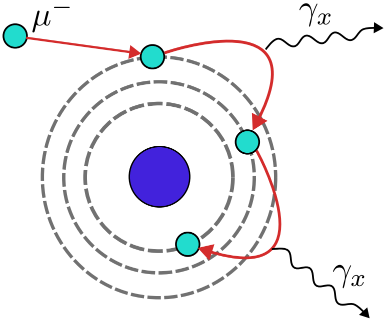

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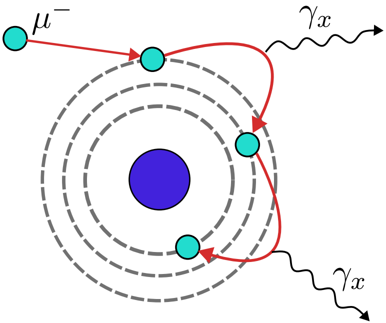

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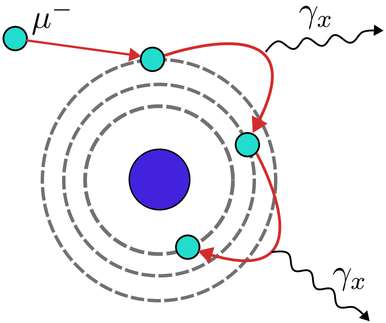

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- Negative muons are implanted into a material and are captured by the atoms of the composing elements
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- As the muon transitions down the energy levels of the atom, X-rays are released, which are measured by detectors

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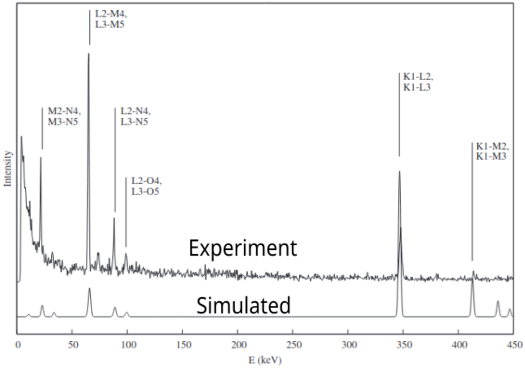

Fig. 1: X-ray spectrum by Sturniolo[1]

- These X-rays are unique to each element, and so elements in a given sample can be identified

[1]S. Sturniolo and A. Hillier, Mudirac: A Dirac Equation Solver for Elemental Analysis with Muonic X-Rays, X-Ray Spectrometry 50, 180 (2021).

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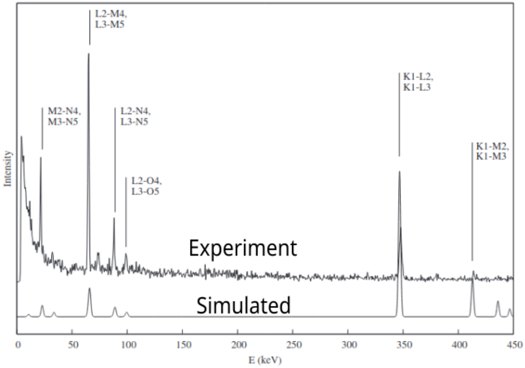

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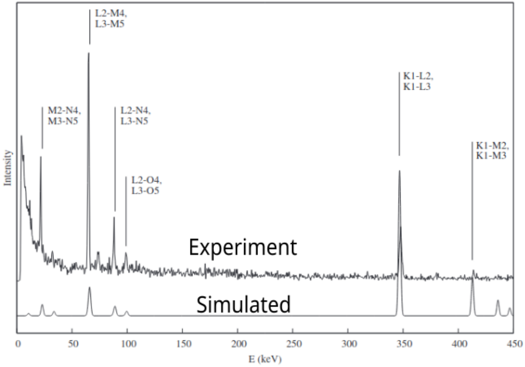

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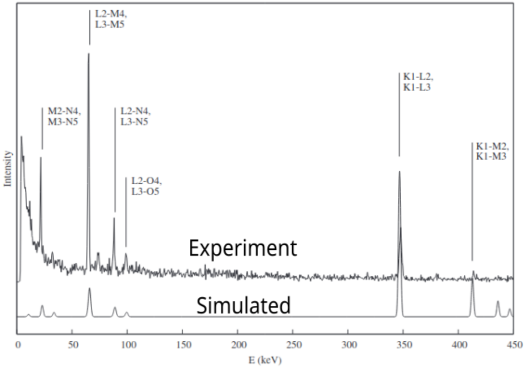

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- Calculating the positions of peaks is simple, but calculating relative intensities is a difficult problem, as it relies on the initial muon population
- Mudirac[1], a modern code for negative muon spectroscopy, gets the peak positions correct, but not the intensities
- **We want a robust and predictive method for calculating muonic X-ray intensities**

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  - **Uses non-relativistic, hydrogen-like radial wavefunctions for both electrons and muon**

Non-relativistic, hydrogen-like approximation

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- For a hydrogen-like atom, separate the total wavefunction into radial and angular parts

$$\psi_{n,l}(r,\theta,\phi) = R_{n,l}(r)Y_{l,m}(\theta,\phi)$$

- Bound muonic radial solutions are analytic, taking the familiar form of

$$R_{nl}(r) = \sqrt{\frac{Z(n-l-1)!}{n^2a[(n+l)!]^3}}e^{-\rho/2}\rho^{l+1}L_{n+l}^{2l+1}(\rho)$$

- Similarly, we have analytic solutions for continuum electrons

$$R_{e2}(r_2) \quad = \quad \sqrt{\frac{m_e}{\hbar}}2^{l+1}k^{l+\frac{1}{2}}e^{ikr_2}r_2^l e_1^{\frac{\pi y}{2}}F_1(l+1-iy;2l+2;-2ikr_2)\frac{|\Gamma(l+1-iy)|}{(2l+1)!}$$

- y is a dimensionless parameter which is inversely proportional to the kinetic energy of the emitted electron; larger y means a larger rate

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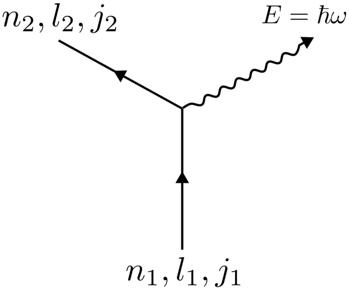
  - **Calculates radiative transitions up to and including octupole**

Radiative Transitions



Radiative Transition

- We only consider the electric transition multipole operator, as magnetic multipoles proceed significantly slower

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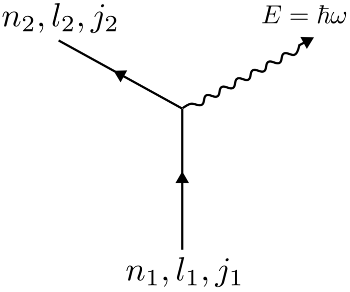

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$$\mathcal{M}^{E}_{LM}(\mathbf{r}) = e\left(\frac{|\mathbf{r}|Z}{a_\mu}\right)^{L} Y^{*}_{LM}(\hat{\mathbf{r}})$$

where L is the multipolarity of the transition

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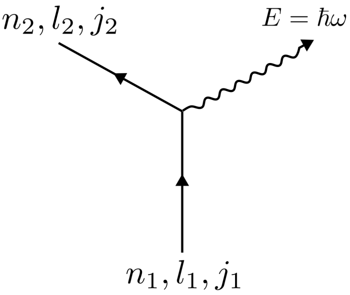

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- Total radiative rate can be computed by computing the matrix element:

$$\Gamma_R^{LM} = \frac{8\pi(L+1)}{L[(2L+1)!!]^2}\frac{1}{\hbar}\left(\frac{a_\mu\omega}{Zc}\right)^{2L+1} |\langle f|\mathcal{M}^E_{LM}|i\rangle|^2$$

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  - **Calculates Auger transitions up to and including octupole**

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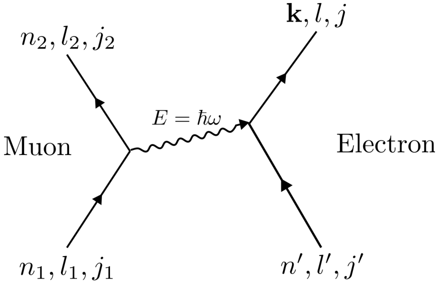
Auger Transitions



Auger Transition

- In the non-relativistic scheme, product wavefunctions can be used to find the Auger rate

$$\begin{aligned}\Gamma_A^L &= \left| \int_0^\infty dr_1 \int_0^\infty dr_2 R^*_{\mu 2}(r_1) R^*_{e2}(r_2) \right. \\ &\times \left. \frac{r_<^L}{r_>^{L+1}} R^*_{\mu 1}(r_1) R^*_{e1}(r_2) r_1^2 r_2^2 \right|^2 \\ &\times |\text{Angular Part}|^2 \times |\text{Electron population}|\end{aligned}$$

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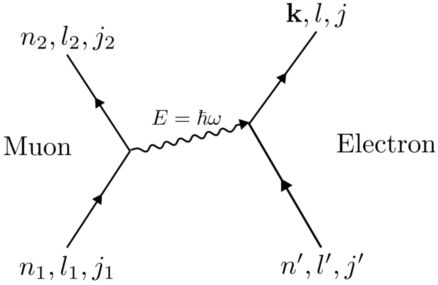

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- Penetration occurs where the muon and electronic orbits overlap, and this is approximated by fitting to a simpler function

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  - Calculates Auger transitions up to and including octupole
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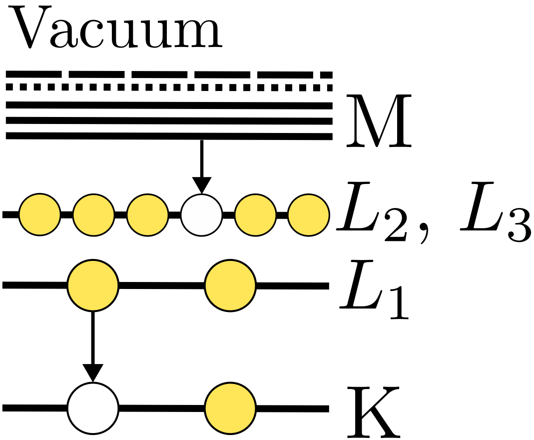
Electron Refilling



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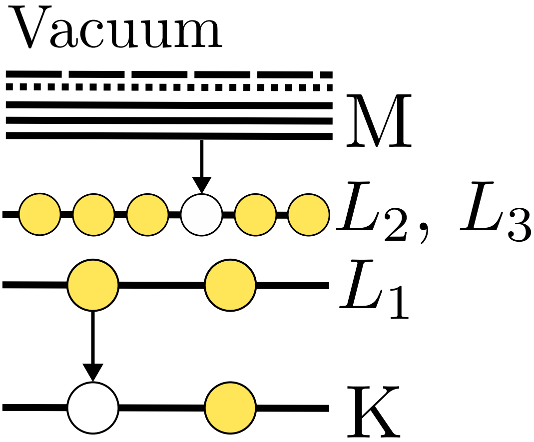

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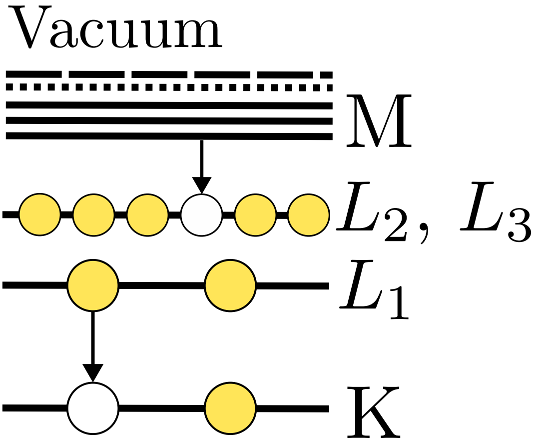

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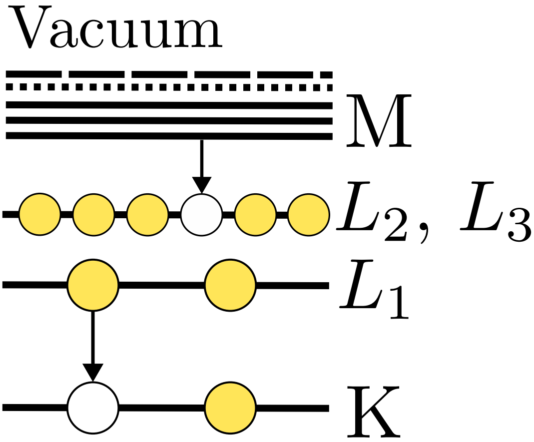

- As the Auger transitions occur, empty electron subshells are left behind
- K electron refilling is formally treated[1] through perturbation theory
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- L and M electrons are either never refilled, or refilled instantly

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  - **Two different built in l-distributions, with custom distribution allowed as input**

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l-distributions

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- Free parameters need to be chosen in some way; use a least squares regression using available experimental data:

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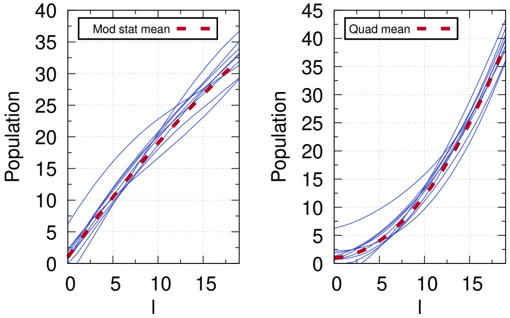
- Gaussian Processes can allow us to take samples using the fitted distribution as the mean

Gaussian Process Sampling



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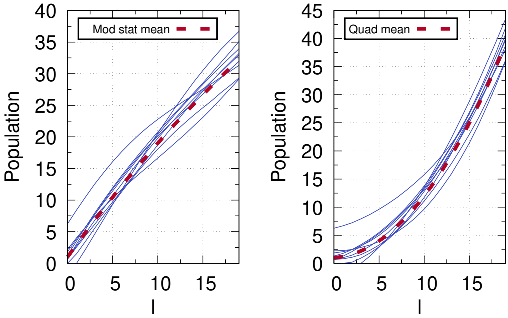

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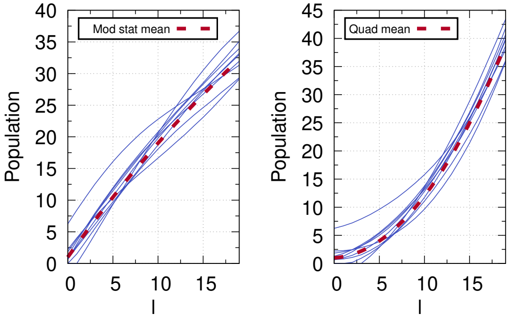

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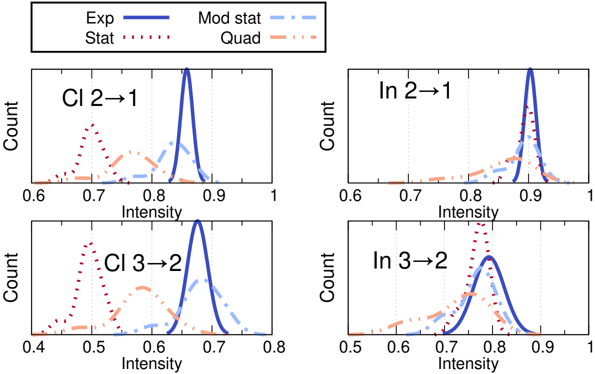
$$P_\lambda(l) = \mu_\lambda(l) + \mathcal{GP}$$

- Each sample population will correspond to a single intensity

Results



- Each distribution gives massively different intensity distribution compared to experiment for low Z (chlorine)
- For large Z (indium), the distributions are in much better agreement with both each other and experiment
- K, L, and M electrons are less strongly perturbed for larger Z atoms

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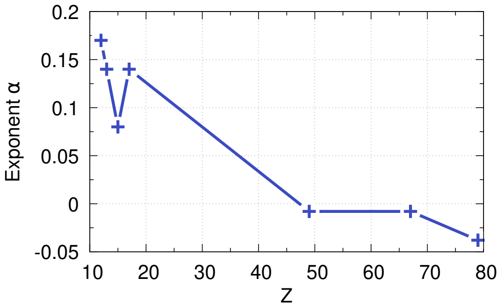

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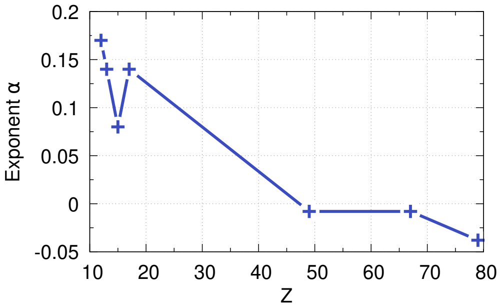

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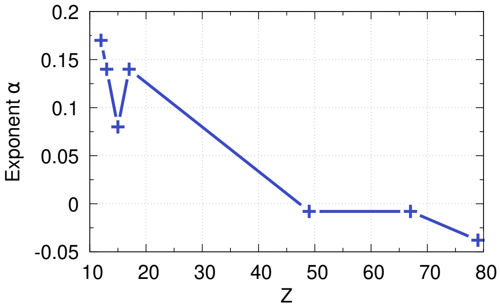

- Optimised exponents were calculated for several elements using available experimental data
- Rough trend of decreasing α with Z corresponding to a flatter distribution
- With more data, predictive trends could be feasible

What's next?

- **Implement Auger rates in Mudirac, and add the cascade functionality**
- Treat electrons and muon fully quantum mechanically and relativistically
- Investigate l-distributions, particularly the integral derived from the classical slow down of the muon:

$$\Delta N(l) = \frac{h^2 l \Delta l \pi}{m} \int_0^\infty \frac{R(E)}{E} dE \int_{E-E_{bar}(l)}^\infty \frac{dP_t(\epsilon)}{d\epsilon} d\epsilon$$

- More systematic description of electron refilling, potentially ab initio

Acknowledgements

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- Dr. Albert Bartók-Pártay
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