

Muon Cascade Calculations

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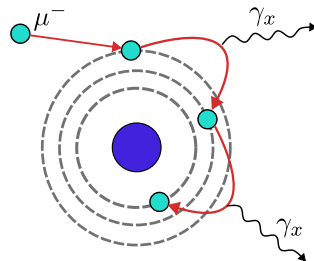
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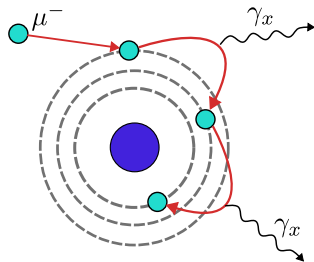
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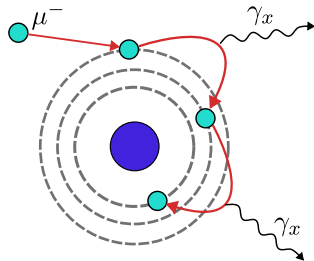
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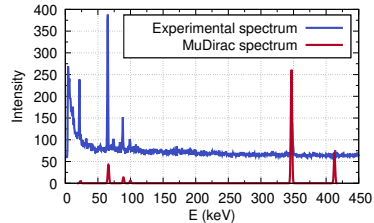
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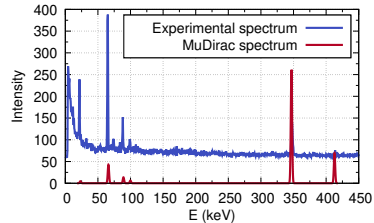
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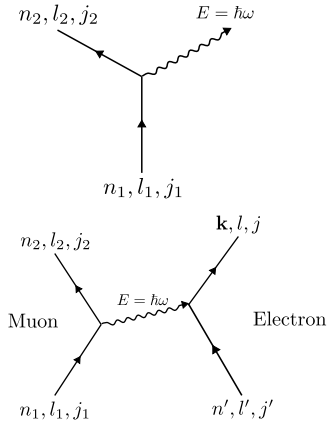


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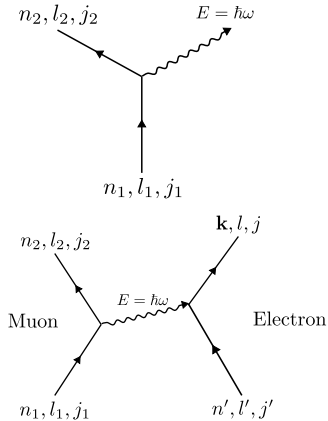


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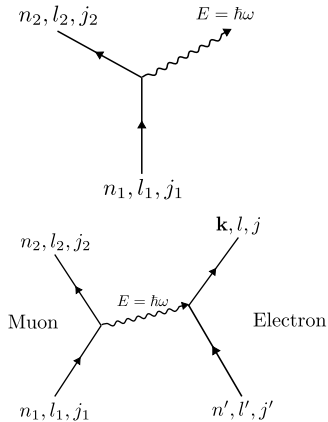
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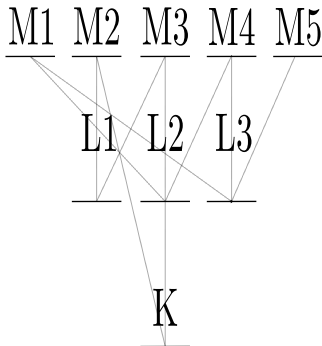
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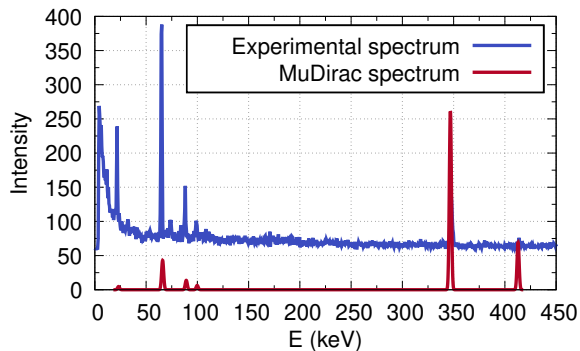
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- The final measurable intensities are therefore a function of **all possible previous transitions**

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- **This is useful for validation of new relativistic results**

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- Energies are calculated accurately through the use of Dirac spinors, finite nuclear models, and QED corrections
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- Radiative dipoles are calculated, but Auger transitions, electron refilling, and angular momentum distributions are not considered

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- The full relativistic, radiative transition rate between an **initial** and **final** muon state is found to be

$$\Gamma_R = \frac{4E_{if}}{3c} |\langle \psi_f | (\boldsymbol{\alpha} \cdot \hat{\mathbf{e}}_\lambda) e^{-i\mathbf{k}_\lambda \cdot \mathbf{r}} | \psi_i \rangle|^2 \quad (2)$$

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- The exponential can be expanded out in Taylor series, and each term in the expansion corresponds to a term in the multipole expansion

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- Electric quadrupole rates were derived and tested in `MuDirac`
- Comparison to the Akylas-Vogel code is valid for systems in the non-relativistic limit i.e low Z atoms
- Individual quadrupole rates were compared for a given set of transitions:

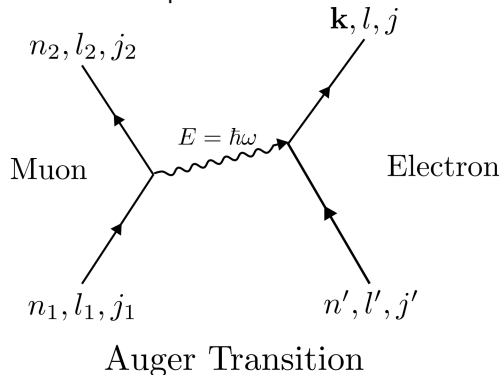
(n,l) pairs	Akylas-Vogel	Fine pairs	MuDirac
(3,2)→(1,0)	5.48×10^9	K1-M4	3.70×10^9
		K1-M5	1.61×10^9
		Sum	5.31×10^9
(3,2)→(2,0)	4.72×10^8	L1-M4	3.18×10^8
		L1-M5	1.39×10^8
		Sum	4.57×10^8

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- Validation against Akylas-Vogel is yet to be performed

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- TCDFT has been used for electron-positive muon systems, including a parameterisation of the correlation functional
- Being able to solve this problem for the negative muon would give a more accurate description of the system

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- A natural route to the full interacting muon-electron problem would come through this implementation
- Ultimately, the ability to solve for muonic states in a bulk system may allow for more accurate capture probabilities, potentially leading to better intensities

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- MuDirac does not get intensities correct due to missing physics
- Relativistic radiative and Auger transitions are the first steps taken to getting correct intensities, with the radiative rates being successfully validated against the Akylas-Vogel code

References

- 1 S. Sturniolo and A. Hillier, Mudirac: A Dirac equation solver for elemental analysis with muonic X-rays, X-Ray Spectrometry 50, 180 (2021)
- 2 V. R. Akylas and P. Vogel, Muonic Atom Cascade Program, Computer Physics Communications 15, 291 (1978)
- 3 M. Goli and S. Shahbazian, Two-component density functional theory for muonic molecules: Inclusion of the electron-positive muon correlation functional, The Journal of Chemical Physics 156, 044104 (2022).
- 4 S. J. Clark, M. D. Segall, C. J. Pickard, P. J. Hasnip, M. I. J. Probert, K. Refson, and M. C. Payne, First principles methods using CASTEP, Zeitschrift Für Kristallographie - Crystalline Materials 220, 567 (2005).

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