

# Search for Charged Lepton Flavor Violation at the Mu2e Experiment

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*En mémoire de ma grand-mère, Fernande Bonneton (27/11/1931 - 12/04/2025)*

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---

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## ABSTRACT

The Muon to Electron conversion experiment (Mu2e) is a particle physics experiment under construction at the Fermi National Accelerator Laboratory (FNAL or Fermilab). Its goal is to search for signature of Charged Lepton Flavor Violation (CLFV) using the channel of neutrinoless muon conversion to electron in an aluminum target. It aims to improve the current limit by four orders of magnitude, reaching a single-event sensitivity of  $3 \times 10^{-17}$ . The experimental signal is an electron with a  $105 \text{ MeV c}^{-1}$  momentum being ejected from the stopping target. The main backgrounds are Standard Model muon decays in the stopping target, cosmic ray induced electrons, and radiative pion captures.

The Mu2e experiment contains two main detectors: a low-mass highly segmented tracker that measures the momentum of electrons, and an electromagnetic calorimeter that measures the energy of incoming charged particles. The calorimeter is composed of inorganic crystal scintillators that have been prepared and tested at Caltech and INFN before being assembled in the final structure at Fermilab. The Caltech group has also been involved in the energy calibration of the calorimeter through the design, commissioning, and operation of the source calibration system. It uses a neutron generator to activate a fluid containing fluorine atoms that radioactively decay into oxygen and generate  $6.13 \text{ MeV}$  gamma rays that are used as a reference energy for the calorimeter crystals.

The analysis of the results of the experiment has been developed to use the maximum likelihood estimation method. The choices of probability distribution functions used in the fit are described, and preliminary fitting results are displayed.

Finally, a phenomenological study has been performed to calculate the muon conversion rate of 236 isotopes. It includes the addition of muon X-ray experimental dataset to the existing electron scattering dataset, their combination using Barrett moment matching, the inclusion of permanent quadrupole deformation effect, and the estimation of neutron distribution for even-even nuclei.

## PUBLISHED CONTENT AND CONTRIBUTIONS

- [1] L. Borrel, D. G. Hitlin, and S. Middleton, “A New Determination of the (Z,A) Dependence of Coherent Muon-to-Electron Conversion”, [Nucl. Phys. A \*\*1062\*\*, 123161 \(2025\)](#),  
I am the main author of this published article that details the phenomenology study that I performed to improve the calculation of muon conversion rate.

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## NOMENCLATURE

**APD:** Avalanche Photodiode.

**BSM:** Beyond the Standard Model.

**CKM matrix:** Cabibbo-Kobayashi-Maskawa matrix.

**CLFV:** Charged Lepton Flavor Violation.

**COMET:** Coherent Muon to Electron Transition.

**DAQ:** Data Acquisition.

**DIRAC:** DIgitize and ReAdout Controller.

**DS:** Detector Solenoid.

**FEE:** Front-End Electronics.

**FWHM:** Full Width at Half Maximum.

**HRS:** Heat and Radiation Shield.

**INFN:** Istituto Nazionale di Fisica Nucleare, translated to National Institute of Nuclear Physics.

**LRU:** Light Response Uniformity.

**MEG:** Mu to E Gamma experiment.

**Mu2e:** Muon to Electron conversion experiment.

**Mu3e:** Anti-muons (Mu) to an electron and two positrons (3e) experiment.

**PDF:** Partial Distribution Function.

**PE:** Photoelectron.

**PMNS matrix:** Pontecorvo-Maki-Nakagawa-Sakata matrix.

**PMT:** Photomultiplier Tube.

**PS:** Production Solenoid.

**ROU:** Read-Out Unit.

**SM:** Standard Model.

**ST:** Stopping Target.

**STM:** Stopping Target Monitor.

**TS:** Transport Solenoid.

## INTRODUCTION

The Muon to Electron conversion experiment [1] (Mu2e) is a particle physics experiment under construction at the Fermi National Accelerator Laboratory (FNAL or Fermilab). Its goal is to search for signature of Charged Lepton Flavor Violation (CLFV) using the channel of neutrinoless muon conversion to electron in an aluminum target. It aims to improve the current limit by four orders of magnitude, reaching a single-event sensitivity of  $3 \times 10^{-17}$ . The experimental signal is an electron with a  $105 \text{ MeV c}^{-1}$  momentum being ejected from the stopping target. The main backgrounds are Standard Model muon decays in the stopping target, cosmic ray induced electrons, and radiative pion captures.

The Mu2e experiment contains two main detectors: a low-mass highly segmented tracker that measures the momentum of electrons, and an electromagnetic calorimeter that measures the energy of incoming charged particles. The calorimeter is composed of inorganic crystal scintillators that have been prepared and tested at Caltech and INFN before being assembled in the final structure at Fermilab. The Caltech group has also been involved in the energy calibration of the calorimeter through the design, commissioning, and operation of the source calibration system. It uses a neutron generator to activate a fluid containing fluorine atoms that radioactively decay into oxygen and generate  $6.13 \text{ MeV}$  gamma rays that are used as a reference energy for the calorimeter crystals.

The analysis of the results of the experiment has been developed to use the maximum likelihood estimation method. The choices of probability distribution functions used in the fit are described, and preliminary fitting results are displayed.

Finally, a phenomenological study has been performed to calculate the muon conversion rate of 236 isotopes. It includes the addition of muon X-ray experimental dataset to the existing electron scattering dataset, their combination using Barrett moment matching, the inclusion of permanent quadrupole deformation effect, and the estimation of neutron distribution for even-even nuclei.

## *Chapter 1*

### THEORETICAL OVERVIEW

#### 1.1 Charged Lepton Flavor Violation (CLFV)

Charged Lepton Flavor Violation (CLFV) is a BSM (Beyond the Standard Model) process in which a charged lepton (electron, muon, or tau) converts into another particle without respecting flavor conservation rules.

Particle flavor refers to the different species of particles of the same family. Figure 1.1 displays the elementary particles in our current understanding of the Standard Model of physics. The quarks are the elementary particles that are subjected to the four fundamental interactions (strong, weak, electromagnetic, and gravity), while the leptons are not subjected to the strong interaction. There are six different flavors of quarks (up, down, charm, strange, top, and bottom) and six different flavors of leptons (three charged leptons: electron, muon, tau ; three neutral leptons: electron neutrino, muon neutrino, tau neutrino).

Quarks and leptons can be divided into three generations, each generation having very similar properties (i.e. they behave the same way under the electromagnetic, weak, and strong interaction) but different masses. This mass difference makes particles from the second and third generations unstable, such that they decay rapidly into particles from the first generation. Consequently, all the matter in the universe is made of particles from the first generation: up and down quarks make protons and neutrons, and electrons orbit nuclei (formed by protons and neutrons) to form atoms. Particles from the second and third generations only appear at medium to high energy ( $\Lambda > 105 \text{ MeV}^1$ ). Thus, they can only be produced naturally (astrophysical events such as supernovae, gamma-ray bursts, and solar eruptions) or in artificial setups (particle accelerators).

In the Standard Model (SM), flavor is “approximately” conserved, and the only flavor violating force is the weak interaction carried by a massive W boson (see Feynman diagrams in Figure 1.2). The word “approximately” is used to emphasize that flavor violating processes are rare, due to the fact that the weak interaction is much weaker than the strong and electromagnetic interactions. Flavor-violating processes in the quark sector, also called quark mixing, are represented by the CKM matrix (Figure 1.3a).

In the neutral lepton sector (electron neutrino, muon neutrino, and tau neutrinos), the discovery of neutrino oscillation in 2001 at the Sudbury Neutrino Observatory (SNO) and described by the

---

<sup>1</sup>the mass of the muon



# Standard Model of Elementary Particles

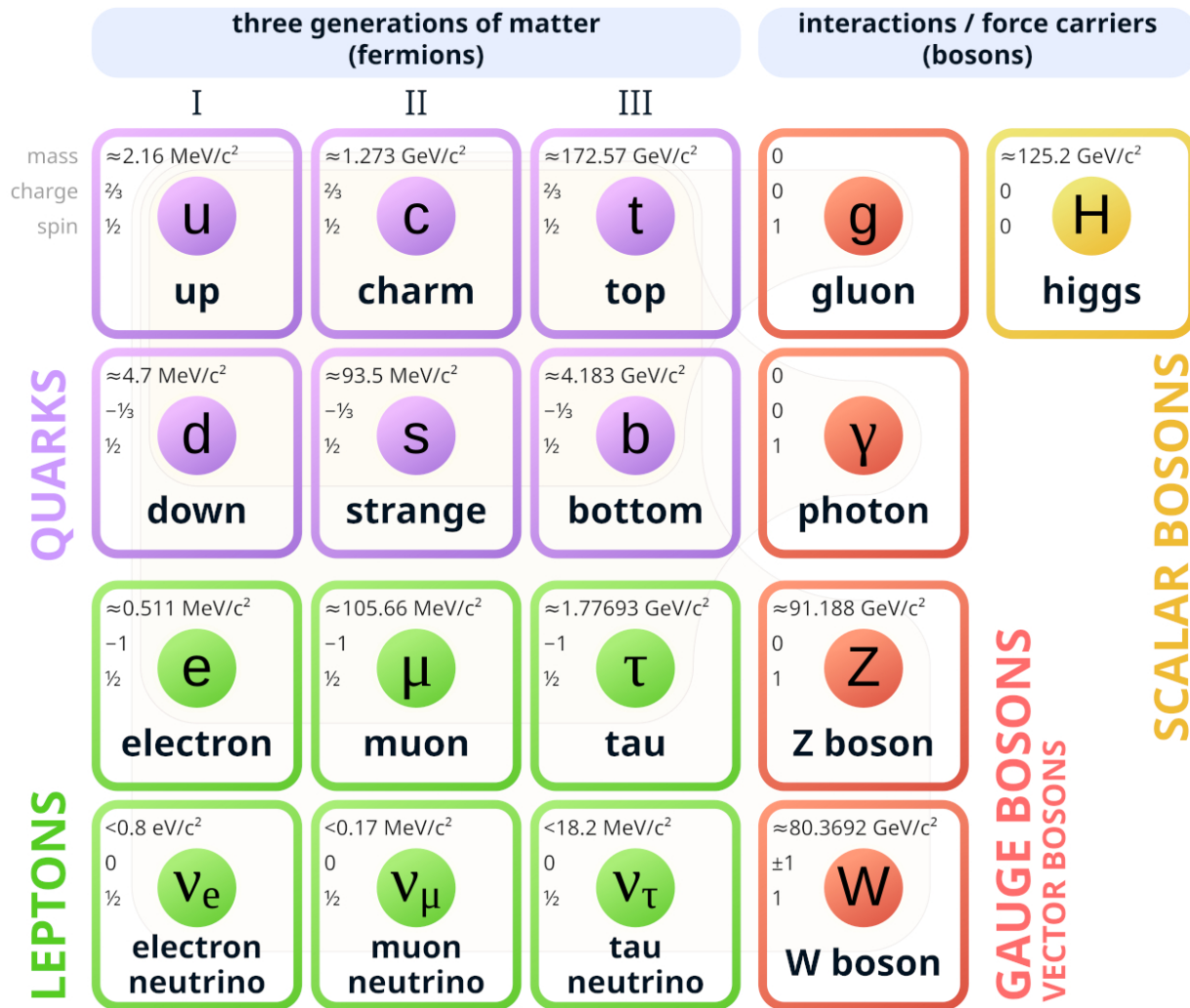
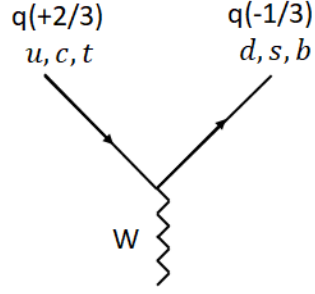


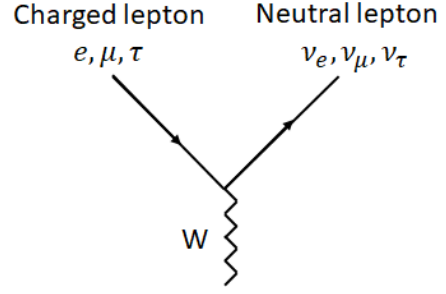
Figure 1.1: The Standard Model of Elementary Particles (adapted from [Wikipedia](#))

PMNS matrix (Figure 1.3b) shows that flavor violation is also possible in the neutral lepton sector.

Finally, flavor violation in the charged lepton sector has never been observed yet, but the discovery of quark mixing and neutrino oscillation led theorists to wonder whether it exists but hasn't been discovered due to a very low rate. The search for CLFV has been ongoing [3, 4] since the discovery of the muon in 1936 at Caltech by Carl Anderson and Seth Neddermeyer [5], and has seen renewed interest over past decades with the proposals for two new experiments: Mu2e at Fermilab [1] and COMET at J-PARC [6, 7].

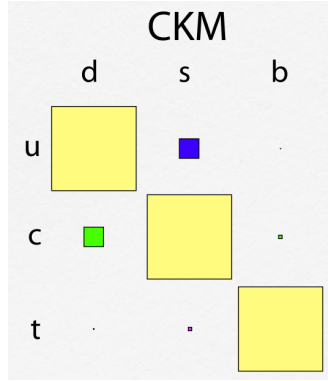


(a) Weak interaction in the quark sector

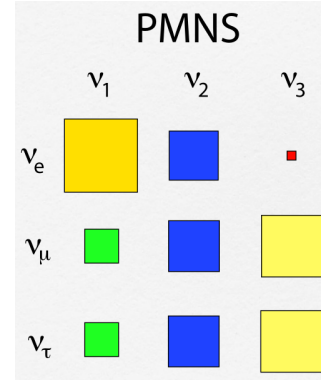


(b) Weak interaction in the lepton sector

Figure 1.2: Feynman diagrams of the weak interaction in the quark and lepton sectors



(a) Cabibbo-Kobayashi-Maskawa (CKM) matrix



(b) Pontecorvo-Maki-Nakagawa-Sakata (PMNS) matrix

Figure 1.3: CKM and PMNS matrices ; the area of each square is proportional to the magnitude of the matrix element. Taken from [2]

## 1.2 Standard Model prediction

According to the Standard Model, a muon decays into an electron, a muon neutrino, and an electron antineutrino (see Feynman diagram in Figure 1.4).

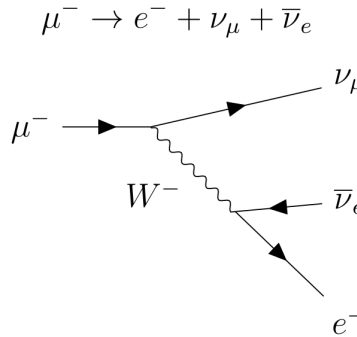


Figure 1.4: Feynman diagram of the Standard Model muon decay

The Standard Model predicts the existence of neutrinoless muon conversion to electron following

the Feynman diagram depicted in Figure 1.5.

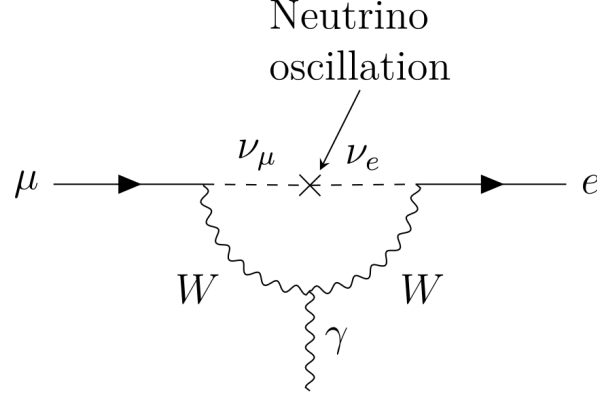


Figure 1.5: Feynman diagram of standard model muon to electron conversion

The Standard Model rate can be computed [4, 8] from this diagram to be:

$$B(\mu \rightarrow e\gamma) = \frac{3\alpha}{32\pi} \left| \sum_i U_{\mu i}^* U_{ei} \frac{m_i^2}{m_W^2} \right|^2 \sim 10^{-54} \quad (1.1)$$

where  $U_{ik}$  is the neutrino mixing matrix and  $m_i$  are the masses of the neutrino mass eigenstates.

This process requires neutrino oscillation from a muon neutrino to an electron neutrino, and thus the branching ratio is highly suppressed by a factor  $\sim \left( \frac{\Delta m_{\nu}^2}{m_W^2} \right)^2 \sim 10^{-54}$ . This rate is unreachable by any experiment in the near or distant future, thus CLFV search does not have any Standard Model background rate, and any observation would be a clear sign of Beyond the Standard Model physics.

### 1.3 Experimental signature of CLFV

#### 1.3.1 Muon

The muon has a mass of 105.7 MeV and a mean lifetime of 2.20  $\mu$ s [9]. As its mass is below the hadronization energy scale, it only has a few possible decay channels. This is also limited by kinematic constraints:  $\mu \rightarrow e$  is not possible as four-momentum cannot be conserved, thus it requires an additional particle or a nucleus in the vicinity. Because of the low mass of muons, the only available particles are up and down quarks (i.e. nearby nucleus), another electron-positron pair, or a photon. This leads to 3 main decay channels:

$\mu^+ \rightarrow e^+ \gamma$ : The choice of positive muons in lieu of negative ones is to prevent muons from interacting with nuclei

$\mu^+ \rightarrow e^+ e^- e^+$ : same for the choice of positive muons

$\mu^- \mathbf{N} \rightarrow e^- \mathbf{N}$ : The nucleus is there for conservation of 4-momentum

### 1.3.2 Tau

The Tau lepton has a mass of 1.78 GeV and a mean lifetime of 290 fs [9]. This high mass leads to hadronization decays, and thus many more decay channels exist. There are no dedicated experiments looking for neutrinoless tau conversion, however B factories (such as the Babar, Belle and Belle-II experiments) generate many taus.

Due to the very small lifetime of tau leptons, they cannot be observed directly, but we can study the daughter particles to reconstruct the parent tau particles, and look for missing energy that would correspond to neutrinos.

### 1.3.3 Present and future experimental bounds

CLFV has already been probed by several experiments in the past century (Figure 1.7) using multiple channels (Figure 1.6 taken from [10])

| Process                               | Experiment | Limit                                        | C.L. |
|---------------------------------------|------------|----------------------------------------------|------|
| $\mu^+ \rightarrow e^+ \gamma$        | MEG        | $4.2 \times 10^{-13}$ [101]                  | 90%  |
| $\mu^+ \rightarrow e^+ e^- e^+$       | SINDRUM    | $1.0 \times 10^{-12}$ [136]                  | 90%  |
| $\mu^- N \rightarrow e^- N$           | SINDRUM-II | $6.1(7.1) \times 10^{-13}$ Ti (Au) [137,138] | 90%  |
| $\mu^- N \rightarrow e^+ N'$          | SINDRUM-II | $5.7 \times 10^{-13}$ [139]                  | 90%  |
| $\tau^\pm \rightarrow e^\pm \gamma$   | BaBar      | $3.3 \times 10^{-8}$ [140]                   | 90%  |
| $\tau^\pm \rightarrow \mu^\pm \gamma$ | BaBar      | $4.4 \times 10^{-8}$ [140]                   | 90%  |
| $\tau \rightarrow eee$                | Belle      | $2.7 \times 10^{-8}$ [141]                   | 90%  |
| $\tau \rightarrow \mu\mu\mu$          | Belle      | $2.1 \times 10^{-8}$ [141]                   | 90%  |
| $\tau \rightarrow \mu ee$             | Belle      | $1.8 \times 10^{-8}$ [141]                   | 90%  |
| $\tau \rightarrow e\mu\mu$            | Belle      | $2.7 \times 10^{-8}$ [141]                   | 90%  |
| $\tau \rightarrow \pi^0 e$            | Belle      | $8.0 \times 10^{-8}$ [142]                   | 90%  |
| $\tau \rightarrow \pi^0 \mu$          | BaBar      | $1.1 \times 10^{-7}$ [143]                   | 90%  |
| $\tau \rightarrow \eta e$             | Belle      | $9.2 \times 10^{-8}$ [142]                   | 90%  |
| $\tau \rightarrow \eta \mu$           | Belle      | $6.5 \times 10^{-8}$ [142]                   | 90%  |
| $\tau \rightarrow \rho^0 e$           | Belle      | $1.8 \times 10^{-8}$ [144]                   | 90%  |
| $\tau \rightarrow \rho^0 \mu$         | Belle      | $1.2 \times 10^{-8}$ [144]                   | 90%  |

Figure 1.6: Current experimental upper limits on the branching ratios of CLFV processes for leptons (taken from [10])

For muon experiments, the figure of merit to measure is the rate of neutrinoless muon conversions called  $R_{\mu e}$ . More specifically for the  $\mu^- N \rightarrow e^- N$  channel, experiments use the muon capture rate

as a denominator to normalize the result and make it look like a branching fraction:

$$R_{\mu e} = \frac{\Gamma(\mu^- + {}^A_Z\text{N} \rightarrow e^- + {}^A_Z\text{N})}{\Gamma(\mu^- + {}^A_Z\text{N} \rightarrow e^- + {}^A_{Z-1}\text{N})} \quad (1.2)$$

The last measurement of  $\mu^- \text{N} \rightarrow e^- \text{N}$  was performed in 2006 by the SINDRUM-II experiment using a gold and a tungsten target. For gold, the current limit set is  $7.1 \times 10^{-13}$  [11]. The aim of the upcoming Mu2e experiment is to improve this sensitivity by four orders of magnitude using an aluminum target, to reach a single-event sensitivity of  $3 \times 10^{-17}$  [1].

Multiple BSM models predict a CLFV rate that would be within the reach of the new generation of CLFV experiments (Mu2e [1], COMET [6], MEG-II [12], Mu3e [13]) that will obtain results by the end of the decade (Figure 1.7).

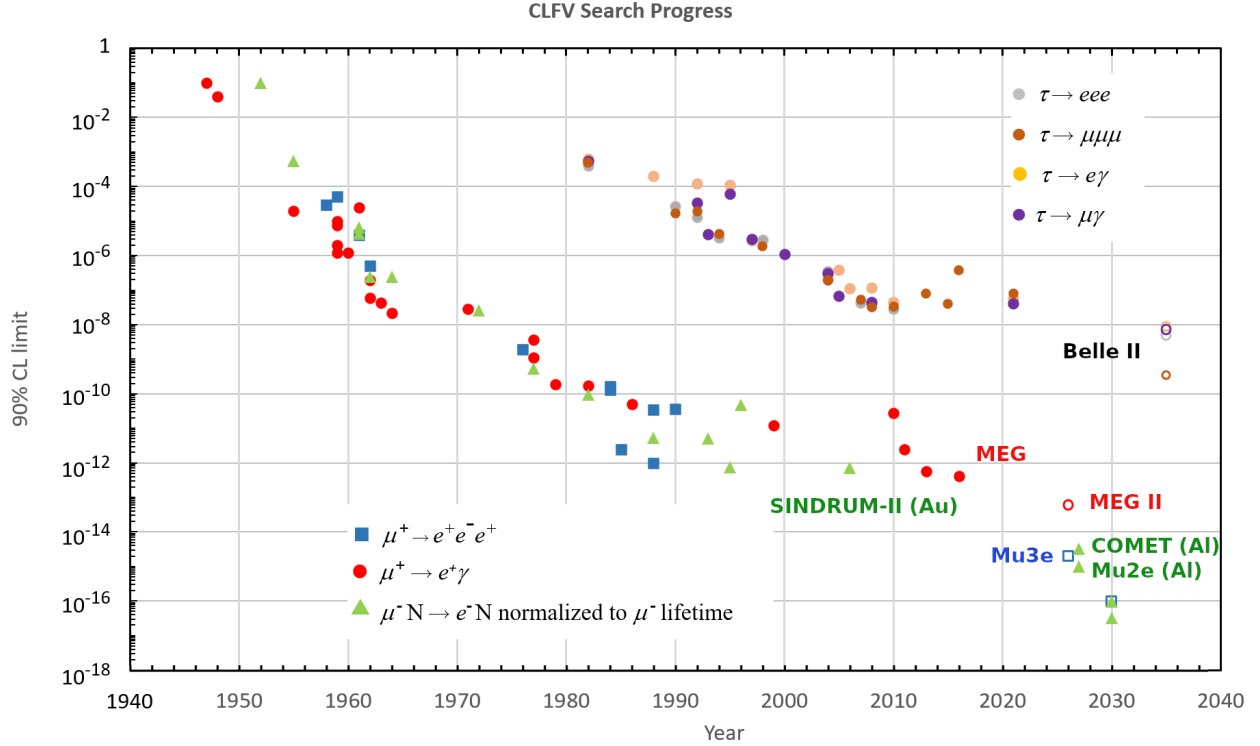


Figure 1.7: History of CLFV experiments [14]. The different colored shapes represent different CLFV channels

#### 1.4 BSM models predicting CLFV

This section is based on the article from Raidal *et al.* [15] that describes the different BSM models that can produce Charged Lepton Flavor Violation.

We know that the current Standard Model (SM) does not provide a complete description of our current knowledge of particle physics.

One of the main signatures of new physics beyond the Standard Model (BSM) is the discovery of neutrino oscillation that proves that neutrinos have a non-zero mass.

The following will quickly present some BSM models that predict CLFV at the level that can be observed by the new generation of CLFV experiments.

#### 1.4.1 Leptoquark

Leptoquarks are theoretical particles that would mediate interactions between leptons and quarks. In this model, the CLFV process is at tree level as seen in the Feynman diagram in Figure 1.8.

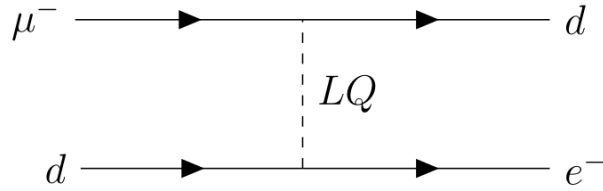


Figure 1.8: Feynman diagram of a leptoquark mediating neutrinoless muon decay

#### 1.4.2 Heavy neutrinos

The mass of the neutrino is several orders of magnitude smaller than the mass of all the other particles in the Standard Model. One of the theories that would be able to explain this difference is the seesaw mechanism, which predicts the existence of an undiscovered heavy neutrino. This heavy neutrino would be able to contribute to neutrinoless muon decay with the same diagram as the Standard Model contribution, but the rate would not be suppressed as much.

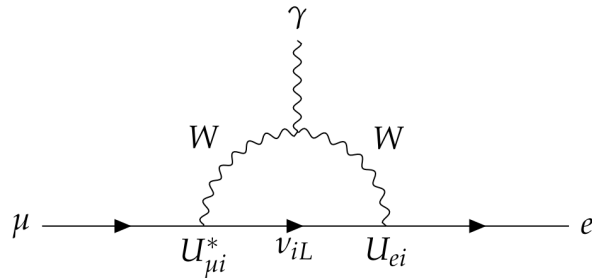


Figure 1.9: Feynman diagram of a muon to electron conversion mediated by a heavy neutrino

#### 1.4.3 Multi-Higgs doublet

In the standard model, one Higgs doublet is required to generate gauge boson and lepton masses through the Higgs mechanism. However, in order to generate neutrino masses, the Higgs sector

needs to be extended to have at least two Higgs doublets. Flavor violation can be found inside the new Yukawa coupling, creating tree-level contribution as well as loop diagram.

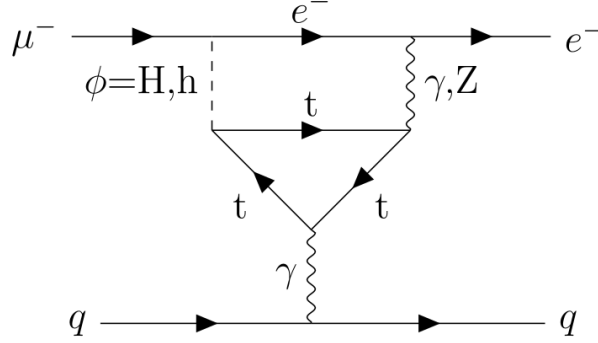


Figure 1.10: Feynman diagram of muon conversion mediated by a second Higgs doublet

#### 1.4.4 Supersymmetry

Supersymmetric (SUSY) models have been popularized to solve multiple problems faced by the Standard Model. We can include CLFV in the new interaction in the supersymmetric sector. The Standard Model lepton will produce a slepton and a neutralino, the slepton will convert to a slepton with a different flavor, and then recombine with the neutralino to form a different flavor lepton.

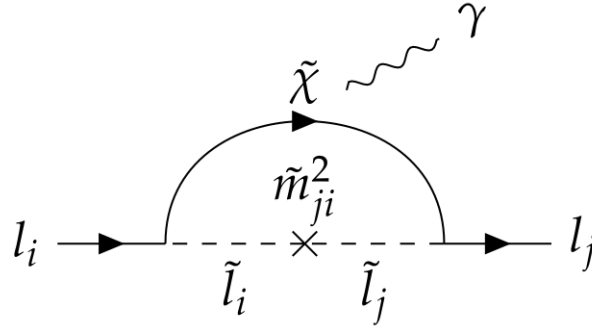


Figure 1.11: Feynman diagram of muon conversion mediated by sleptons  $\tilde{l}$  and neutralinos  $\tilde{\chi}$

#### 1.5 Effective Field Theory and mass reach

We can look into Charged Lepton Flavor Violation using the Effective Field Theory (EFT) formalism [16]. This approach looks at all the possible operators from the Lagrangian, and constrains them based on available experimental measurements of specific channels. There can be a lot of possible operators, thus restrictions are applied to look only at operators that have an impact at tree level on the channel that we are interested in.

For CLFV in muon decay, we can write the effective Lagrangian [16]:

$$\mathcal{L}_{CLFV} = \frac{1}{(1 + \kappa_D)\Lambda^2} m_\mu \bar{\mu}_R \sigma_{\alpha\beta} e_L F^{\alpha\beta} + \frac{\kappa_D}{(1 + \kappa_D)\Lambda^2} \bar{\mu}_L \gamma_\alpha e_L (\bar{u}_L \gamma^\alpha u_L + \bar{d}_L \gamma^\alpha d_L)$$

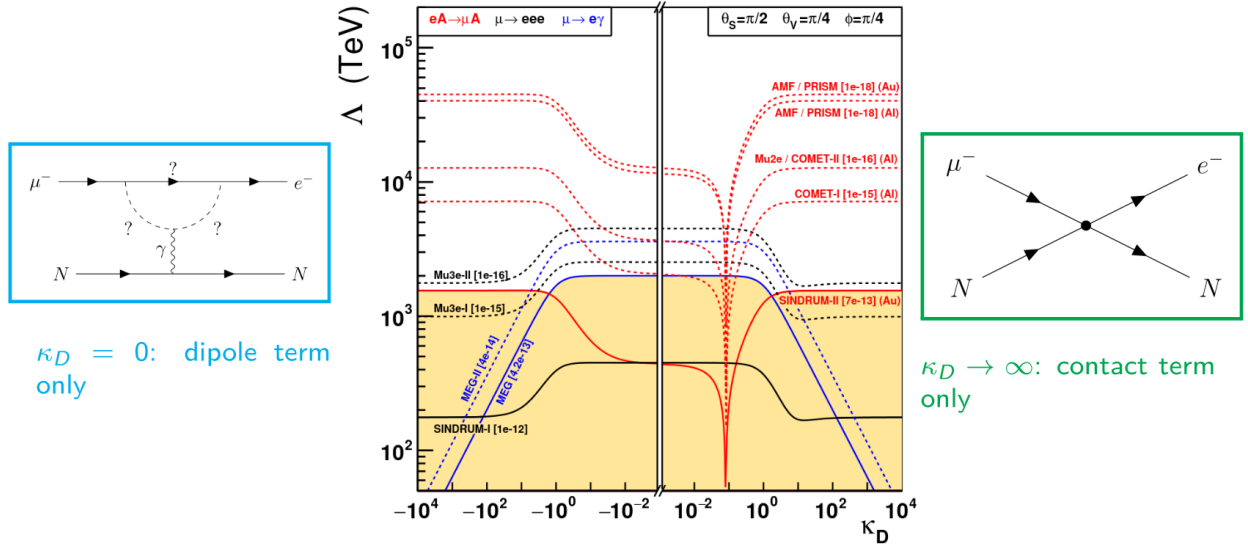


Figure 1.12

The first term is the dipole term, which is the only contributor to the  $\mu \rightarrow e\gamma$  channel, and can also contribute to the other two channels through the diagram on the left of Figure 1.12. The second term, the contact term, does not affect the  $\mu \rightarrow e\gamma$  channel, but is the main contributor to the  $\mu N \rightarrow eN$  channel. The plot in the center of Figure 1.12 represents the effective mass reach of the combination of the different operators, and the current and projected experimental limits.

## 1.6 Signal shape and background

This section will provide details on the five main backgrounds and the signal of the Mu2e experiment.

### 1.6.1 Conversion electrons

The conversion electron signal comes from BSM neutrinoless muon decay into an electron. The four-momentum conservation forces the outgoing electron to be monoenergetic with an energy of 104.973 MeV.

An EFT approach has been used in reference [17] to provide a more detailed shape of this theoretical signal that includes nuclear and radiative effects.



### 1.6.2 Michel spectrum and Decay-In-Orbit (DIO)

A free muon decays after a mean lifetime of  $2.2\mu\text{s}$  into an electron, a muon neutrino and an electron anti-neutrino. Using the conservation of four-momentum, the neutrinos take a fraction of the energy and momentum of the initial muon. The energy spectrum of the outgoing electron is described by the Michel parameters (see [18, 19]):

$$\frac{d^2\Gamma}{dx d\cos\theta} \propto x^2 \left[ (3 - 3x) + \frac{2}{3}\rho(4x - 3) + P_\mu \xi \cos\theta \left( (1 - x) + \frac{2}{3}\delta(4x - 3) \right) \right] \quad (1.3)$$

where  $x = \frac{E_e}{E_{\text{max}}}$  is the energy of the outgoing electron divided by its maximum possible energy  $E_{\text{max}} = m_\mu/2 = 52.8\text{ MeV}$  ;  $\rho, \xi$ , and  $\delta$  are the Michel parameters ; and  $P_\mu$  is the polarization of the muon beam.

We integrate over the angle  $\cos\theta$  and substitute the value of the Michel parameter  $\rho = 3/4$  to get the energy spectrum of the outgoing electron:

$$\frac{d\Gamma}{dx} \propto 2x^2 \left( (3 - 3x) + \frac{2}{3}\rho(4x - 3) \right) = x^2(3 - 2x) \quad (1.4)$$

The energy spectrum of the Michel electron was last measured by the TWIST experiment [19] in 2011 and is plotted in Figure 1.13 in red.

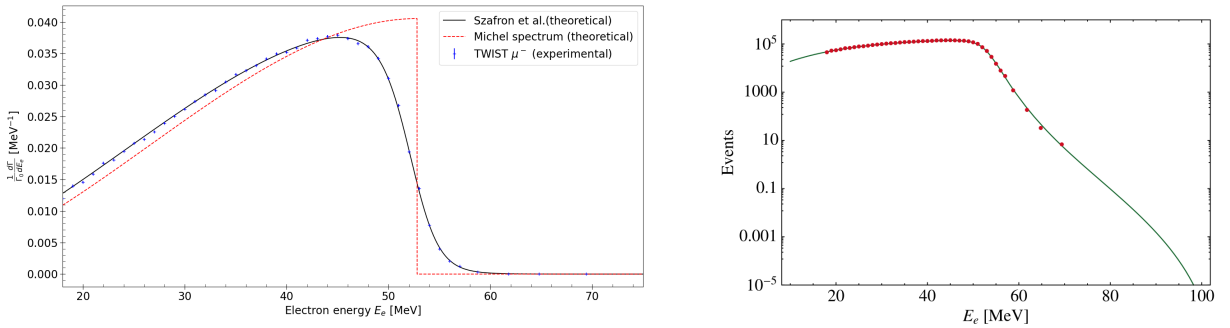


Figure 1.13: Left: energy spectrum of Michel electrons (red), DIO predicted by theory [20] (black), and DIO measured experimentally [19] (blue). Right: same on a logarithmic scale with the DIO theory in black and the DIO experimental in red

Because their maximum energy is way below the expected signal energy, Michel electrons are not a background of the experiment, but their rate is very high and they can overwhelm our detectors. Consequently, the Mu2e experiment detectors are designed with an annular shape to prevent Michel electrons from interacting with them. Indeed, the trajectory of charged particles in a uniform magnetic field is an helix with a radius proportional to the momentum of the particle. A

50 MeV electron will have a small radius and travel through the hole of the annular-shaped detectors (see an illustration in Figure 1.14)

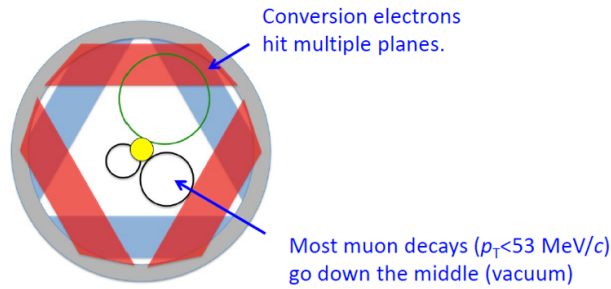


Figure 1.14: Illustration of a Michel electron going through the hole of the Mu2e tracker, while a conversion electron interacts with the detector

As we are looking at muon decaying into an electron while orbiting a nucleus, the muon is not “free” but bound to the nucleus, thus the energy spectrum of the outgoing electron is distorted. These electrons, called Decay-In-Orbit or DIO, can have an energy up to  $E_{end} = 104.973$  MeV, which is the energy of the electron produced by a neutrinoless muon conversion. However, the energy spectrum decreases sharply above 50 MeV (see Figure 1.13 for a linear scale (left) and logarithmic scale (right)).

### 1.6.3 Cosmic rays

For an experiment located on the surface of the Earth, it will have to deal with a constant cosmic ray muon flux of  $O(10^4)$  muon per square meter per minute. These muons are created by very high energy cosmic ray protons interacting in the upper atmosphere, and thus can create electrons with an energy around 105 MeV through Standard Model decay, as illustrated in Figure 1.15.

In addition, a high-energy cosmic muon can also be misidentified as an electron by the detector because it will have the same helix radius (see Equation 4.3). For the Mu2e experiment, this background would produce about one signal-like event per day, when the requirement for the entire experiment would be less than 0.1 events.

There are two ways of removing this background: the first one is to place the experiment deep underground, as it can reduce the cosmic muon rate by a couple of orders of magnitude, but it is almost impossible to place an entire particle accelerator hundreds of meters underground. The chosen solution is to combine a passive shielding and an active detector that can veto a time window when it detects an incoming cosmic ray (see more details in Section 2.7). In addition, we can use calorimeter information to distinguish between a muon having the same helix radius as a conversion electron, as their shower profile in the crystals is different.

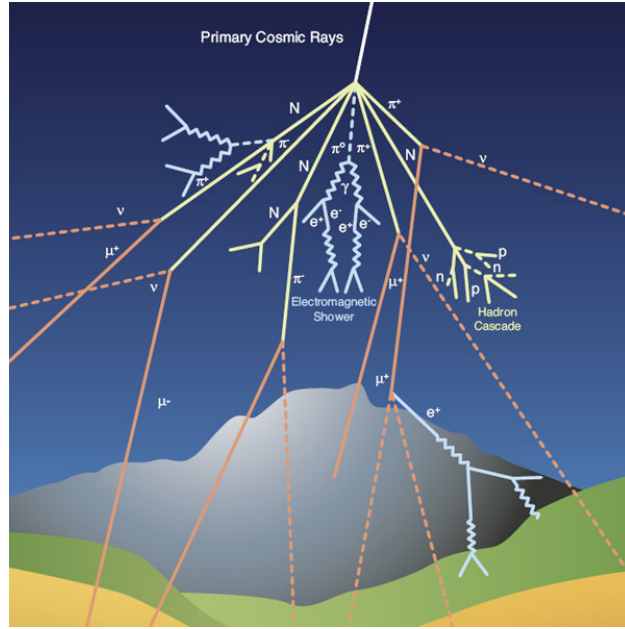


Figure 1.15: Cosmic ray shower in the atmosphere producing cosmic muons (source: [CERN](#))

#### 1.6.4 Radiative Pion Capture (RPC)

Radiative Pion Capture (RPC) is a process in which a negative pion  $\pi^-$  replaces an electron in the orbit of a nucleus, and then emits a high-energy photon. Figure 1.16 displays the Feynman diagram of radiative pion capture.

Radiative pion capture

$$\pi^- + {}^A_Z N \rightarrow {}^A_{Z-1} N + \gamma$$

Figure 1.16: Radiative Pion Capture diagram

The energy of the photon has been measured experimentally on a magnesium target ( $Z = 12$ , one less than aluminum) [21] and its energy spectrum is plotted in Figure 1.17.

The high-energy photon can then produce an asymmetric electron-positron pair, generating an electron with an energy comparable to a conversion electron. If the photon produced is virtual (real), the process is called internal (external) RPC. The two processes are very similar, but they are quantum mechanically different and thus their rates are slightly different.

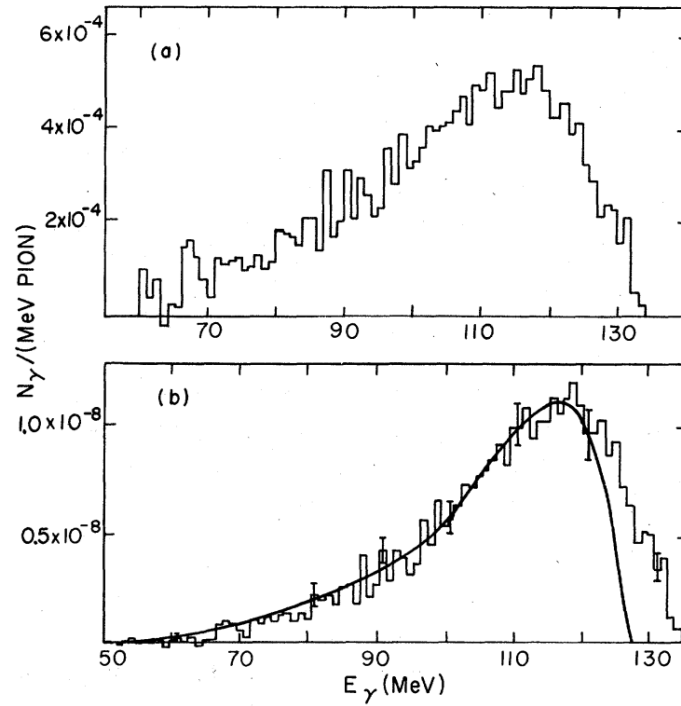


FIG. 7. Energy spectrum of photons from radiative pion capture in magnesium. (a) Spectrum with efficiency divided out (see note, Fig. 4). (b) Measured spectrum with in-flight background subtracted; solid line: pole-model predictions.

Figure 1.17: Energy spectrum of photons produced through radiative pion capture in an Mg target (source: [21])

The technique used by the Mu2e experiment to remove this background is to exploit the difference between the pion lifetime ( $\tau_\pi = 26$  ns) and the lifetime of muons orbiting an aluminum nucleus ( $\tau_\mu^{\text{Al}} = 864$  ns). By using a pulsed muon beam with a delayed time window, we can wait out the pions to decay in the target (see Figure 1.18)

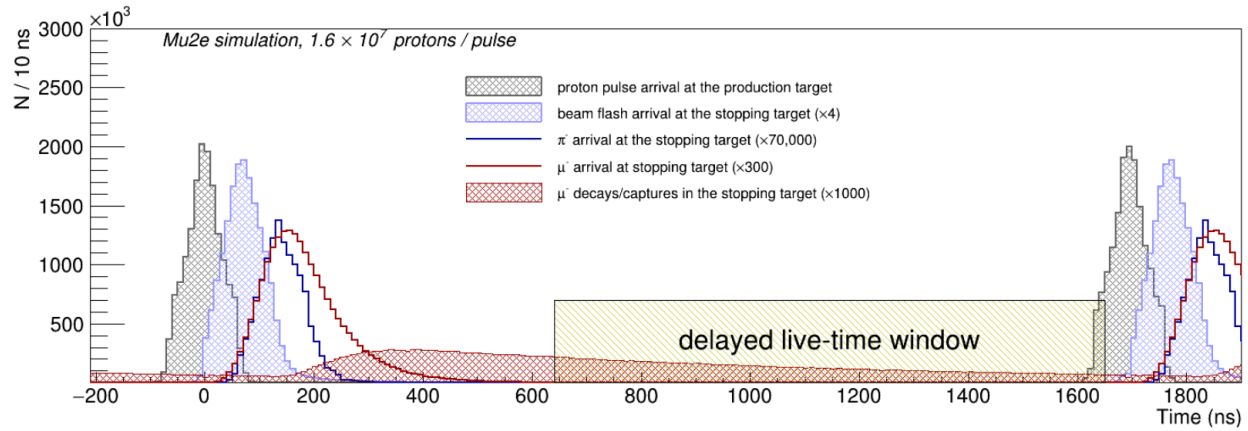


Figure 1.18: Time structure of the Mu2e experiment, using a delayed time window to remove radiative pion capture background

## *Chapter 2*

### THE MU2E EXPERIMENT

The Mu2e experiment [1] is located on the Muon campus at the Fermi National Accelerator Laboratory (Fermilab). It is designed to search for neutrinoless muon decay into an electron on an aluminum target with a single event sensitivity of  $3 \times 10^{-17}$  [1] ( $3 \times 10^{-16}$  in run 1 [22]).

The main goal of an experiment that aims to detect neutrinoless muon decay in the vicinity of a nucleus is to measure the momentum of outgoing electrons with high precision. The main difference between the Standard Model decay (shown in 1.4) and the conversion process is the emission or not of neutrinos. This has a strong impact on the kinematics of the interaction:

- If no neutrinos are emitted, conservation of four-momentum requires an additional particle (photon) or a nucleus in the vicinity. We then have a two-body decay, and four-momentum conservation constrains the outgoing electron to be monoenergetic (up to radiative corrections).
- If neutrinos are emitted, we have a three-body decay, and the outgoing neutrinos can also carry some of the four-momentum, relaxing the constraints on the outgoing electron four-momentum. The outgoing electron energy spectrum is described by the Michel spectrum, modified to account for the presence of the nucleus.

A derivation of the Michel spectrum and the values of the Michel parameters can be found in reference [4], and a plot showing the different spectra is displayed in Figure 2.1).

## 2.1 Experimental concept

This section gives an overview of the main steps that are needed to make an experiment capable of measuring muon conversion rate.

### 2.1.1 Muon beam

First, we need a muon beam. Because muons have a mean lifetime of  $2.2 \mu\text{s}$ , the experiment needs to be located on a particle accelerator. Currently, one of the most efficient way to produce muons is to strike high-energy protons onto a target to produce charged pions  $\pi^\pm$ , which then decay rapidly ( $\tau_{\pi^\pm} = 26 \text{ ns}$ ) into muons.

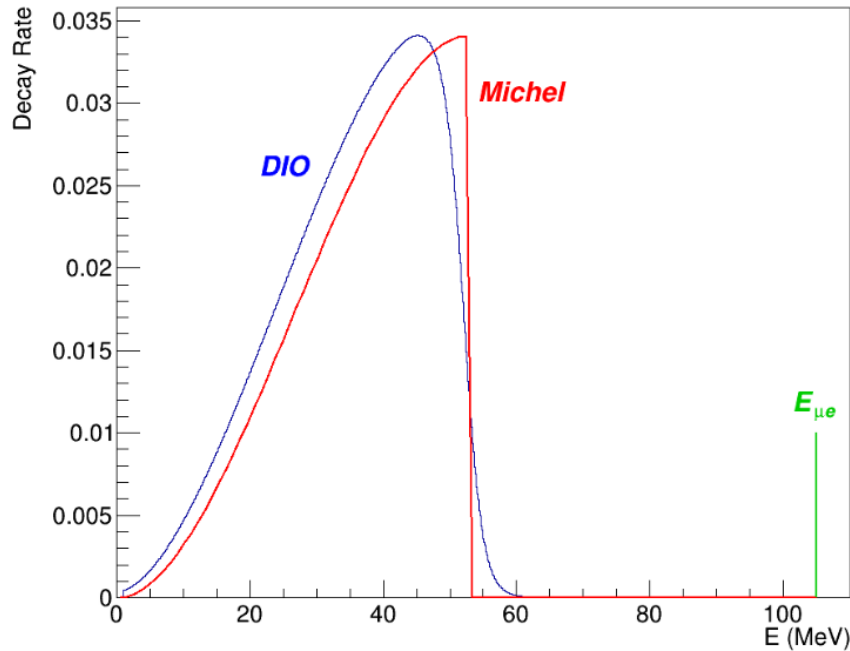


Figure 2.1: Theoretical decay rate as a function of the energy of the outgoing electron for conversion electron, Decay-In-Orbit (DIO), and free muon decay (Michel spectrum)

### 2.1.2 Muon stop

We want to measure muon decays close to a nucleus such that the nucleus can participate in the four-momentum conservation equation. Because negative muons and electrons interact with other particles in the same way, muons can replace electrons orbiting a nucleus and create a muonic atom. To increase the probability of muons stopping in the stopping target, the muon momentum needs to be low (so that it does not break through the stopping target unimpeded).

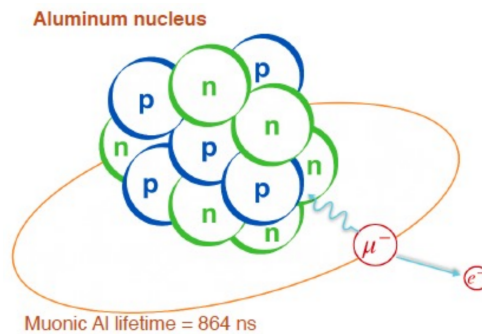


Figure 2.2: Depiction of a muon replacing an electron orbiting an aluminum nucleus and ejecting an electron after conversion

### 2.1.3 Electron measurement

Once the muon is orbiting the target nucleus, it rapidly cascades into the 1s orbit while emitting characteristic X-rays. Then, it will decay into an electron after a short amount of time depending on the nucleus (between  $O(\text{ns})$  for high-Z elements to  $O(\mu\text{s})$  for low-Z elements). As described at the beginning of this chapter, the measurement of the momentum of the outgoing electron is the key to differentiate between Standard Model muon decay and Beyond the Standard Model muon conversion. Hence, detectors are placed downstream of the stopping target to measure electron momentum and energy.

We can use the COMET and the Mu2e experiment as examples to see how they use those principles.

### 2.1.4 Example with the COMET experiment

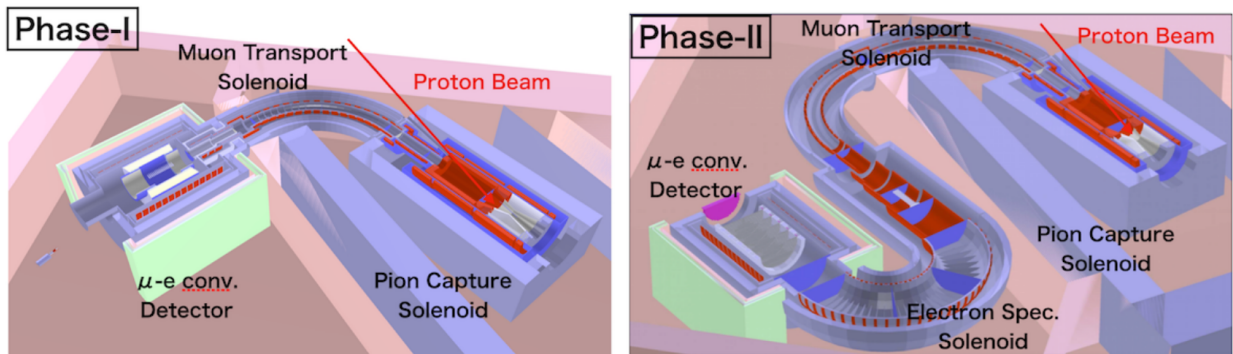


Figure 2.3: The two phases of the COMET experiment [23]

1. The COMET experiment [6, 7] is located at the J-PARC accelerator facility in Japan. Its 8 GeV proton beam is directed on a tungsten target<sup>1</sup> to produce pions.
2. Low-momentum, backward-going pions are transported in a curved solenoid where they decay into muons, which stop in an aluminum stopping target.
3. In Phase-I, the stopping target is surrounded by the CyDET (Cylindrical Detector), a cylindrical drift chamber that measures the momentum of the outgoing electrons. In Phase-II, the electrons ejected from the stopping target travel through a system similar to a mass spectrometer: a curved solenoid separates the electrons depending on their momentum (low momentum electrons get absorbed into blockers at the bottom of the solenoid), and their precise momentum and energy is measured by the StrECAL (Straw and Electromagnetic Calorimeter) with a precision better than 200 keV/c

<sup>1</sup>COMET will use a graphite target for its Phase-I, but will change it to a tungsten target for Phase-II



## 2.2 Overview the Mu2e experiment

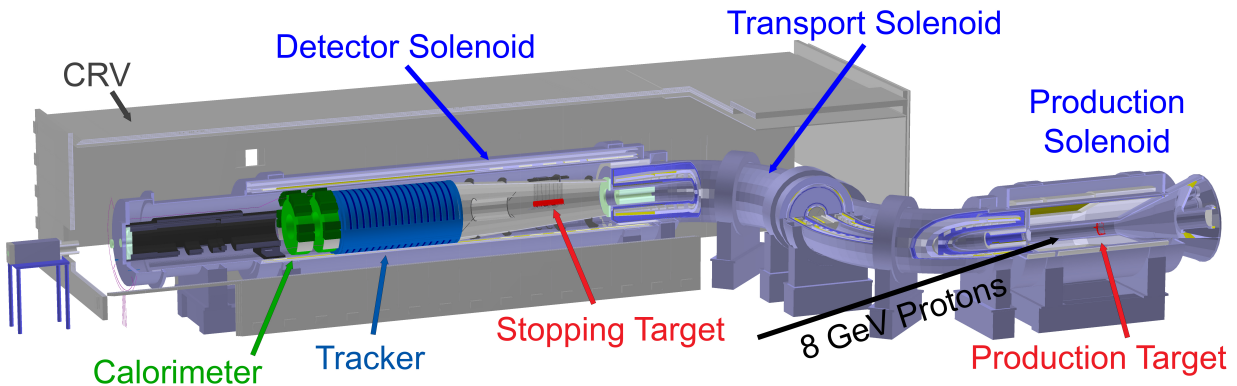


Figure 2.4: CAD drawing of the Mu2e experiment

The Mu2e experiment is located at the Fermi National Accelerator Laboratory to use its 8 GeV proton beam. The proton beam enters the Production Solenoid (PS) to strike the production target made of inconel to produce pions.

The low-momentum, backward-going pions decay into muons and are directed toward the Transport Solenoid (TS), an “S”-shaped solenoid with a collimator in the middle that selects the charge of the particles going through. The negatively-charged muons arrive in the Detector Solenoid (DS) and stop in an aluminum stopping target.

After the muons decay into electrons, the outgoing electrons go through a tracker and a calorimeter that measure their momentum and energy respectively.

The entire detector solenoid is surrounded by a Cosmic Ray Veto (CRV), which goal is to detect incoming cosmic ray, one of the main background of the experiment.

The next sections in this chapter will detail the different components that make the Mu2e experiment.

## 2.3 Muon beamline

Mu2e is located on the muon campus at the Fermi National Accelerator Laboratory (Fermilab), on the M4 beamline, downstream of the g-2 experiment (see Figure 2.5).

The steps that the protons take from generation to delivery to the Mu2e experiment are detailed below [25]:

1. Protons are generated and accelerated in the linear accelerator (LINAC) to 400 MeV.

2. They are injected into the 8 GeV rapid-cycling-synchrotron booster operating at 15 Hz ; one proton booster batch contains  $4 \times 10^{12}$  protons and is made of eighty-one 19 ns (53 MHz) bunches (thus each booster batch is  $81 \times 19 \approx 1.5 \mu\text{s}$  long).
3. Up to two booster batches are then transferred to the recycler ring through the MI-8 beamline and re-bunched into four (or eight for 2 booster batches) 2.5 MHz bunches, each containing  $1 \times 10^{12}$  protons.
4. The beam is transported to the delivery ring, one bunch at a time
5. Finally, an electrostatic septum is used to resonantly extract the beam into the M4 beamline to be delivered to the Mu2e experiment production target.

The resulting proton beam hitting the production target in the production solenoid has the time structure described in Figure 2.6. Each proton pulse is separated by 1695 ns, has a duration of 250 ns, a geometrical rms radius of 1 mm, and contains  $3.9 \times 10^7$  protons. Using 2 booster batches per main injector cycle, the experiment can receive  $6 \times 10^{12}$  protons per second ( $1.2 \times 10^{20}$  protons

per year), corresponding to a beam power of 7.3 kW. The resulting muon beam reaching the stopping target has an intensity of  $O(10^{10})$  muons per second [22], making it the most intense pulsed muon beam in the world.

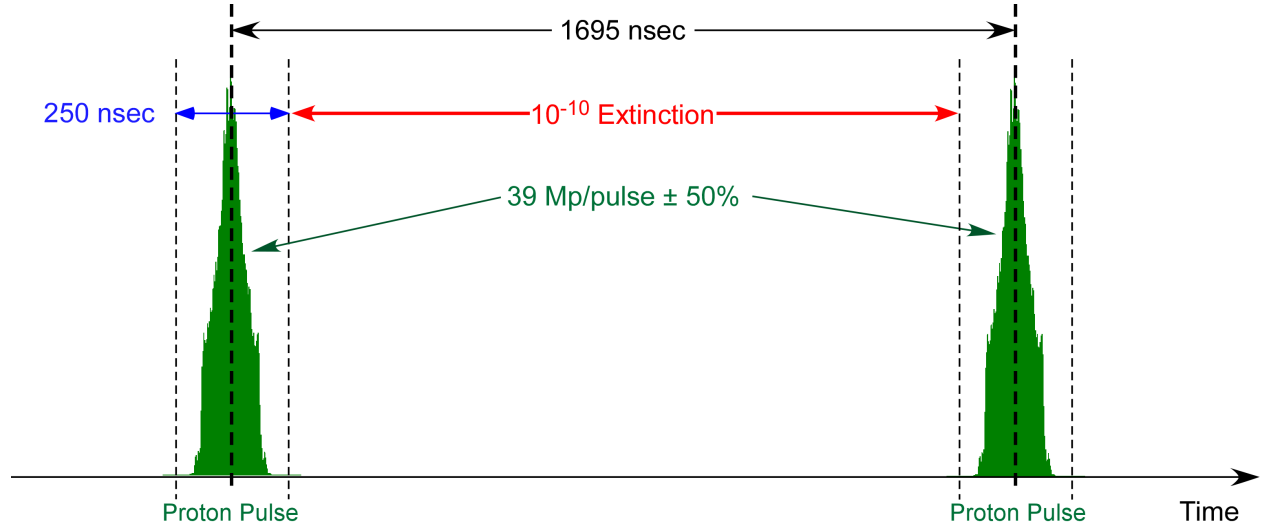


Figure 2.6: Time structure of the Mu2e beam [25]

In order to limit secondary beam particles reaching the detectors and creating additional background signal, we need to suppress residual beam in between proton pulses by a factor  $10^{-10}$ . The recycler re-bunching process provides a beam extinction of  $10^{-4}$ , and an additional set of 2 AC dipoles located inside the M4 beamline improves the extinction by an additional factor of  $10^{-7}$  (both contributions on the time structure of the beam are depicted in Figure 2.7). These 2 high high-frequency dipole magnets deflect the out-of-time beam towards an absorbing collimator.

To monitor the performance of the extinction system, the extinction monitor system consists of two collimators, a permanent magnet, a tracker, and a range stack, all located downstream of the proton beam (Figure 2.8), slightly off-axis above the beam dump in order to limit radiation from the beam.

The first collimator selects secondary particles produced by the interaction of the proton beam with the production target. The permanent magnet bends the trajectory of the charged particles toward another collimator, filtering out neutral particles. The tracker, made of two sets of 4 pixel detector planes separated by a spectrometer magnet, reconstructs the trajectory of charged particles before and after being bent by the magnet, providing a measurement of their momentum. Finally, the range stack is composed of four scintillating planes separated by steel absorber plates, and its goal is to identify muons.

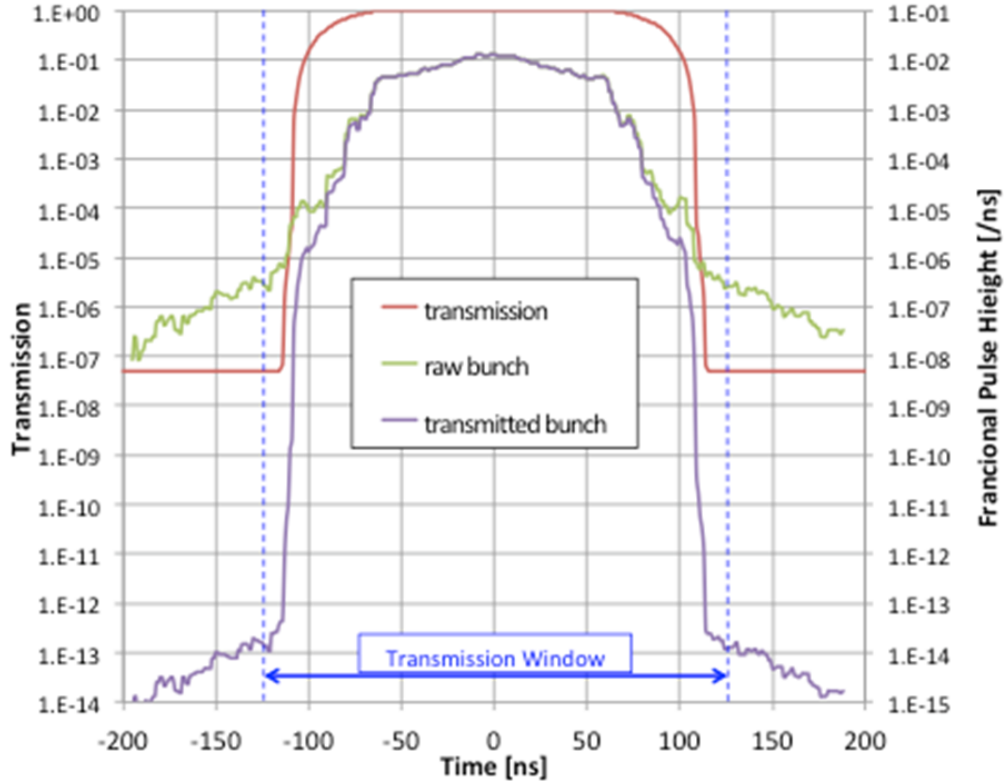


Figure 2.7: Performance of the extinction systems : the red curve (using the left scale) represents the transmission of the AC dipole ; the green curve (using the right scale) is the proton time shape in the recycler ring ; the blue curve is the convolution of the previous two curves and corresponds to the total extinction [25].

## 2.4 Solenoids

The Mu2e experiment consists of 3 large superconducting solenoids that are magnetically coupled and serve different purposes:

**The Production Solenoid (PS)** contains the production target that is hit by the proton beam to produce pions ;

**The Transport Solenoid (TS)** is shaped like an “S”, it transports low-momentum muons to the stopping target in the detector solenoid, and removes neutral and positively charged particles;

**The Detector Solenoid (DS)** houses the stopping target, the tracker and the electromagnetic calorimeter.

Each solenoid is made of several cylindrical layers assembled one inside another (example for the DS in Figure 2.10).

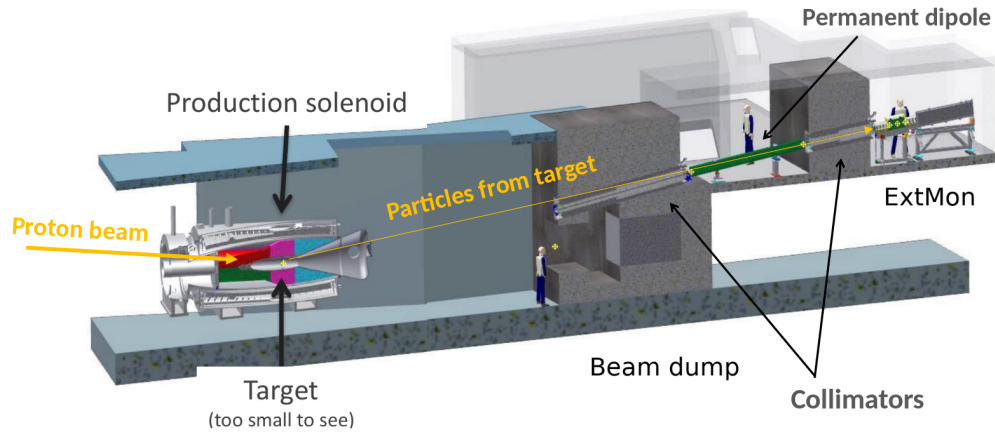


Figure 2.8: Extinction monitor system

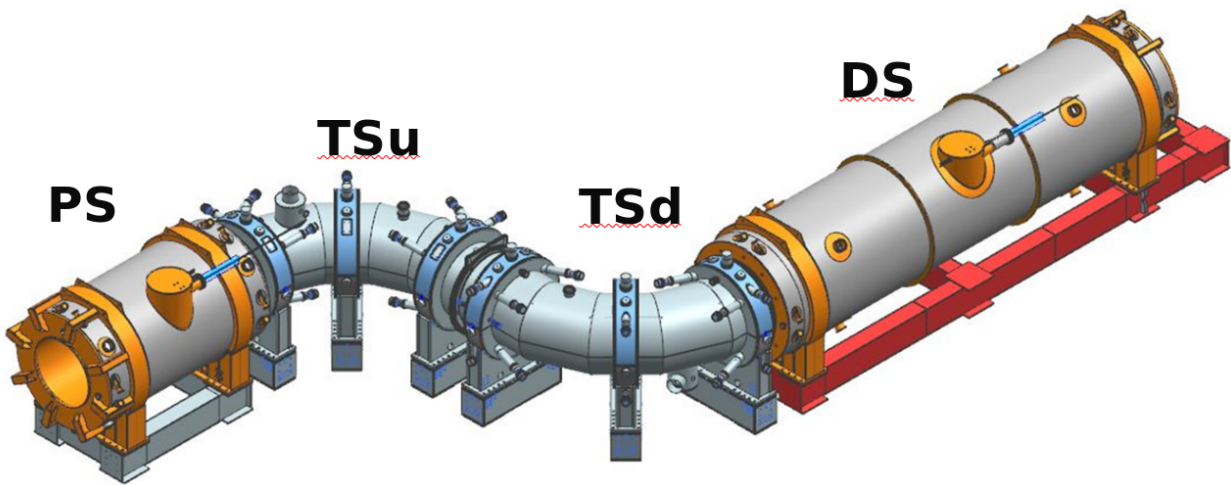


Figure 2.9: The 3 superconducting solenoids of Mu2e ; from left to right: the Production Solenoid (PS), the Transport Solenoid upstream (TSu) and downstream (TSd), and the Detector Solenoid (DS)

- the innermost layer is the inner bore, which forms the interface with the vacuum at room temperature.
- Surrounding the inner bore is the inner thermal shield that is cooled to liquid nitrogen temperature ( $T_{LN_2} = 80 \text{ K}$ ) ; the thermal shield is thermally insulated on both sides by Multi-Layer Insulation (MLI).
- The MLI is used to block radiation heating between the different layers.
- The cold mass hosts the superconducting cables that need to be cooled at liquid helium temperature ( $T_{LHe} = 4.7 \text{ K}$ ). It is suspended inside the vacuum vessel to minimize heat transfer with the other layers.

- Another thermal shield surrounded by MLI is separating the cold mass from the outer vacuum vessel
- The Vacuum vessel is the outermost layer, it provides mechanical support for the solenoid.

## DS Layers

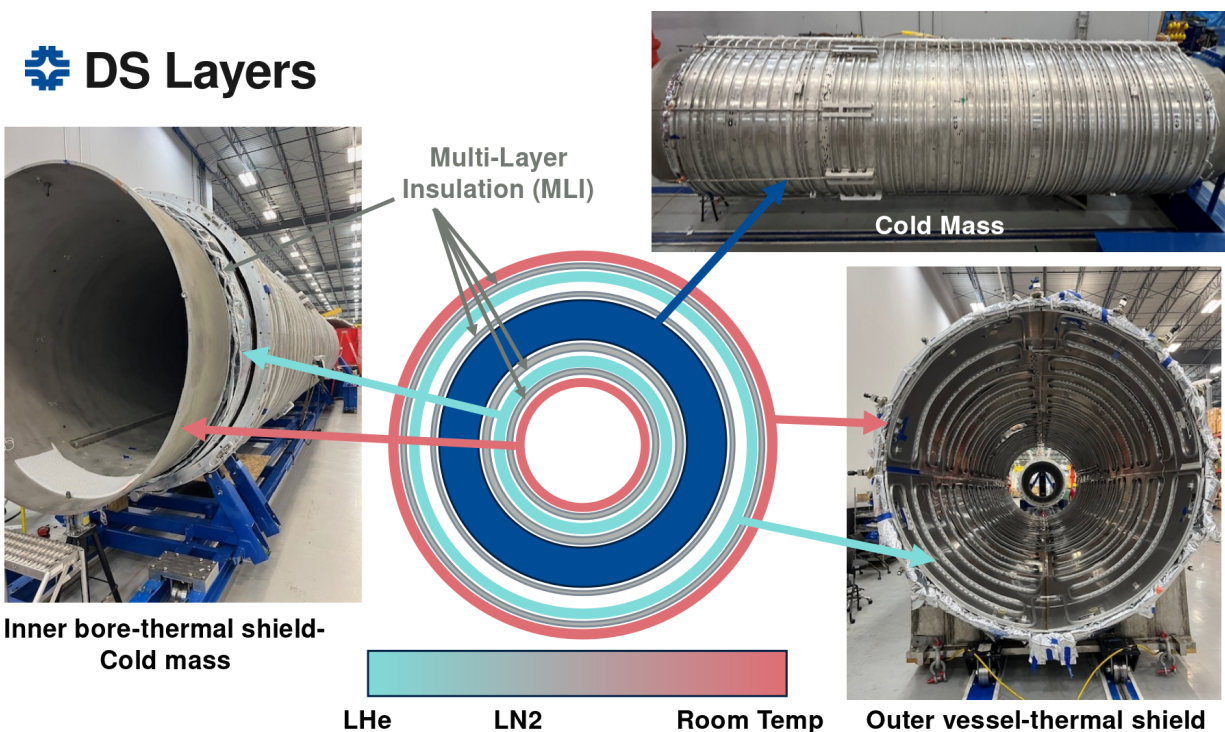


Figure 2.10: Schematics of the different layers that compose the Detector Solenoid (credit: K. Badgley [26])

The magnetic field is generated by coils wound from  $\varnothing 40 \mu\text{m}$  Al-stabilized NbTi superconducting cable. The cables are electrically insulated from one another using a combination of layers of G-10 epoxy, polyimide (Kapton<sup>®</sup>), and pre-preg E-glass. To achieve a 5 T magnetic field in the production solenoid, an operating current of 10 kA is necessary [27]. The Mu2e solenoids are all connected to a single cryogenic system that provides cooling at both liquid nitrogen temperature and liquid helium temperature.

The vacuum system is divided into two distinct volumes separated by a window located in the middle of the transport solenoid. The first vacuum volume contains the production solenoid and the upstream section of the transport solenoid. The pressure needs to be lower than  $1 \times 10^{-5}$  Torr in order to maximize the lifetime of the production target. The second vacuum volume contains the downstream section of the transport solenoid and the detector solenoid. A pressure of  $1 \times 10^{-4}$  Torr for the detector solenoid is required to minimize secondary interactions of the electron before it is measured.



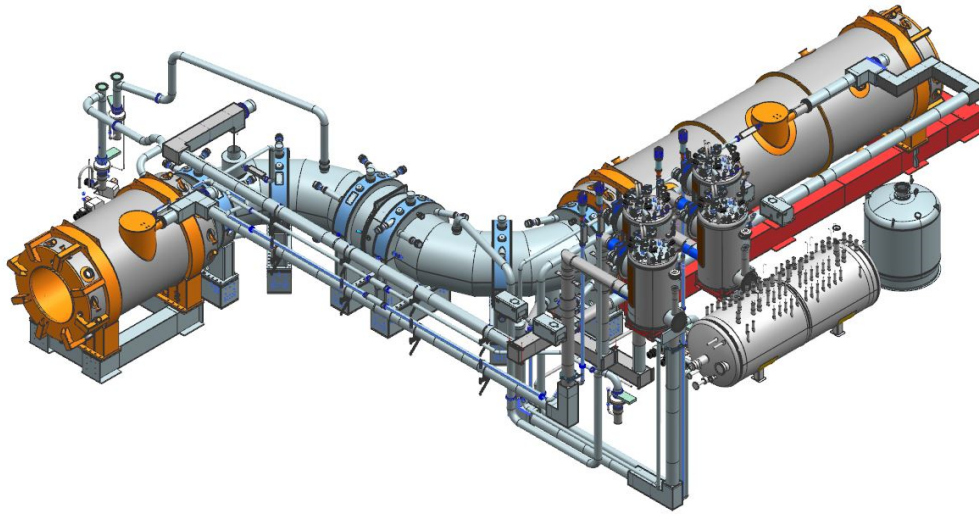


Figure 2.11: The Mu2e superconducting solenoids with their cooling system

To achieve this vacuum level, a standard multistage sequence is used: roughing pumps reduce the pressure from atmospheric pressure to a threshold at which diffusion pumps can be started.

#### 2.4.1 Production Solenoid (PS) and production target

The Mu2e Production Solenoid (PS) is a 4 m long superconducting solenoid with a 1.5 m inner bore diameter, generating a homogeneous axial magnetic field up to 5 T. The magnetic field is graded from 4.5 T to 2.5 T at the interface with the Transport Solenoid.

The 8 GeV pulsed proton beam supplied by the Fermilab accelerator complex enters the PS and strikes the production target to produce pions (and many other particles). The charged pions decay rapidly ( $\tau = 26$  ns) into muons with a branching ratio above 99.9 % [9].

The gradient magnetic field creates a magnetic mirror effect: low-momentum charged particles are reflected back toward the lower magnetic field. This allows Mu2e to be located off-axis with regards to the proton beam, thus considerably reducing beam flash effects. The forward-going particles end in the beam stop situated downstream of the proton beam, while low-momentum particles (backward-going particles and particles with a high transverse momentum) are directed toward the transport solenoid.

The 8 GeV proton beam striking the production target generates a lot of heat and radiation. This leads to the necessity for the Heat and Radiation Shield (HRS), a 29 000 kg bronze cylinder that surrounds the production target to protect the solenoid.

The production target is designed to maximize pion production from proton interactions. It is

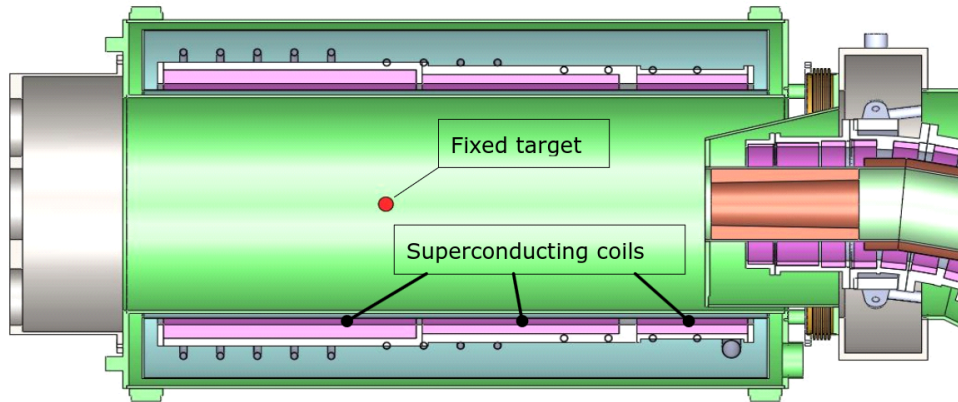


Figure 2.12: Top view of the cross-section of the Production Solenoid ; a section of the Transport Solenoid can be seen on the right

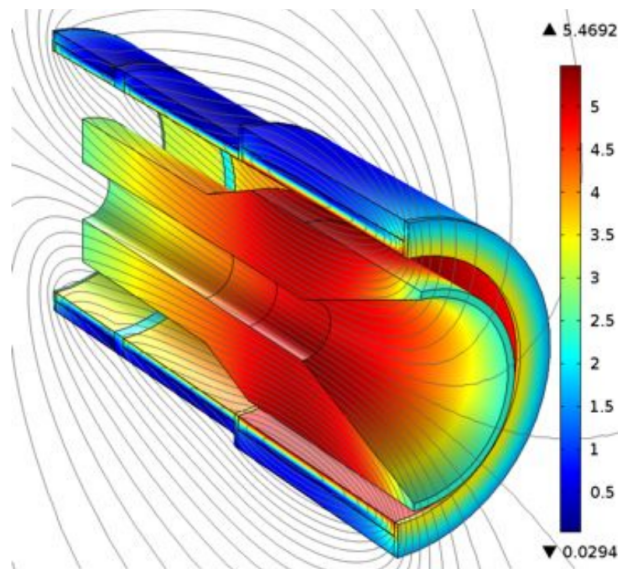


Figure 2.13: Map of the magnetic field generated by the Production Solenoid (taken from [1])

located in the path of the proton beam, thus it is subject to very intense radiation and extreme heat.

The choice of inconel-718 [28] and a very specific design (see Figure 2.14) had been optimized to survive this environment for at least one year. Indeed, no material can sustain this environment on a long term, so the target needs to be replaced once a year, during the summer shutdown of the accelerator. A robotic arm has been designed to replace the production target through a small port in the PS.

#### 2.4.2 Transport Solenoid (TS)

The Mu2e Transport Solenoid (TS) is a 13 m long assembly of superconducting solenoids in the shape of an “S”. The solenoids have a 0.5 m inner bore diameter, and generate a gradient magnetic



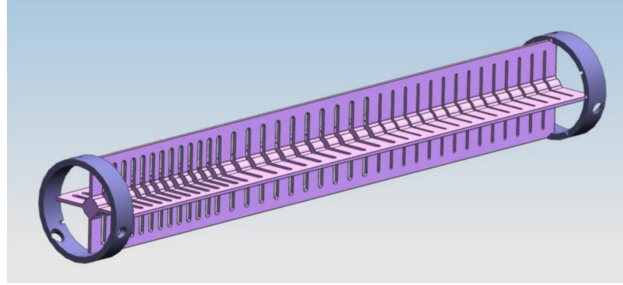


Figure 2.14: drawing of the production target (Hayman2 design)

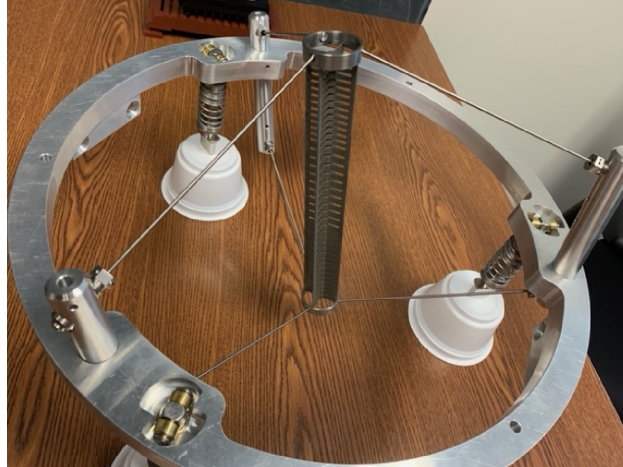


Figure 2.15: photo of the production target (Hayman2 design)

field from 2 T (at the interface with the Detector Solenoid) to 2.5 T (at the interface with the Production Solenoid).

The TS “S” shape removes all neutral particles as they go straight through because their trajectories are not bent by the magnetic field. Negative and positive particles have a different trajectory while moving along the TS, and the center of their helix is translated vertically at the center of the “S”. This is where a rotating collimator is placed to enable the experiment to choose the charge of the particles that go through. The second bend allows the charged particles to move back to the center of the solenoid before they enter the Detector Solenoid.

Finally, an anti-proton window is located in the middle of the TS as a way to reduce the background from anti-proton produced by the stopping target

### 2.4.3 Detector Solenoid (DS)

The Detector Solenoid (DS) is the largest of the Mu2e solenoid, with its length of 11 m and its 2 m inner bore diameter. Its main purpose is to house the Stopping Target (ST) surrounded by the Inner and Outer Proton Absorbers (IPA and OPA), the two main detectors: the tracker and the electromagnetic calorimeter ; and finally downstream of the detectors the Muon Beam Stop (MBS).

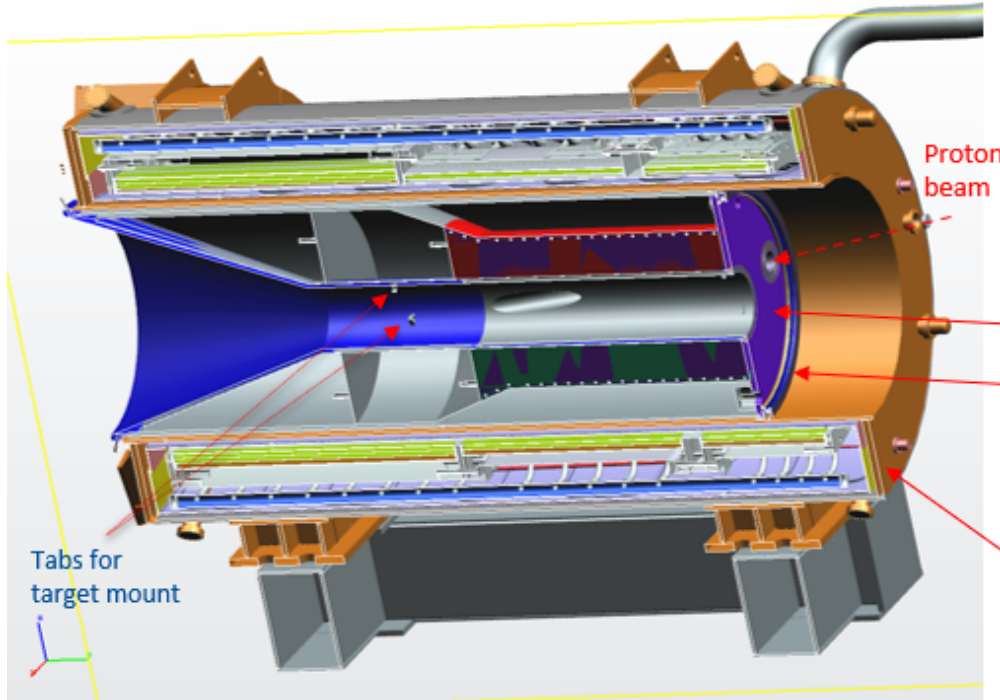


Figure 2.16: Drawing of the Heat and Radiation Shield inside the Production Solenoid

All of these components are not directly attached to the DS, but are set on a rail system, such that they can be extracted from the solenoid for maintenance and calibration.

The magnetic field has a gradient in the stopping target region, reducing from 2 T at the interface with the transport solenoid to 1 T, and is then constant at 1 T in the detector region.

## 2.5 Tracker

The goal of the tracker detector [29] is to measure the momentum of charged particles going through the detector. Using the homogeneous 1 T magnetic field in the downstream section of the detector solenoid, the charged particles exhibit helical trajectories with a radius proportional to their momentum. To minimize scattering and other energy losses (which worsen the momentum resolution), the detector needs to use as little material as possible and is placed in a  $10^{-4}$  Torr vacuum in the detector solenoid.

The Mu2e experiment uses a low-mass highly segmented straw tracker in the shape of an annuli, its momentum resolution is required to be better than 180 keV [29]. This specific annular shape is useful to remove the beam flash and Michel electrons (with momentum  $< 50$  MeV) backgrounds, as they go through the hole in the detector without interacting with it. The inner radius of the tracker (and the calorimeter) is calculated to maximize the detection efficiency of  $O(105$  MeV) electrons while rejecting lower momentum charged particles.



(a) The Production Solenoid being lowered in its final location (in August 2025)



(b) The Heat and Radiation Shield being inserted inside the Production Solenoid (in October 2025)

Figure 2.17: Pictures of the Production Solenoid

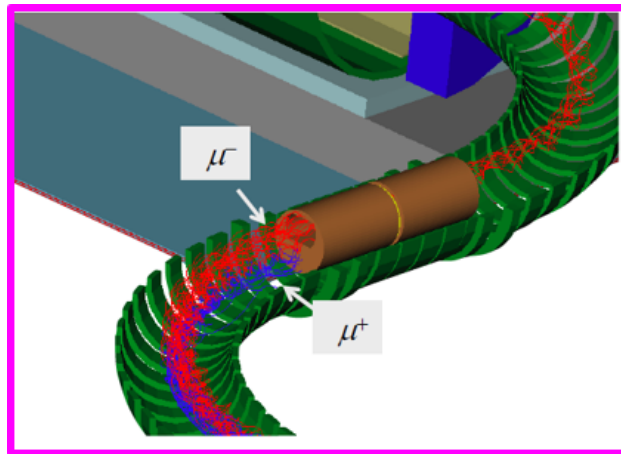


Figure 2.18: Collimator TS

When a charged particle goes through a straw, it ionizes the gas inside the straw, creating a positive ion and an ionization electron. The straw has metallized walls (cathode) and a center wire (anode) with a difference of potential, such that ionization electrons drift from the wall to the wire, where it generates a Townsend avalanche<sup>2</sup> that creates a current spike in the wire. The transient current is

<sup>2</sup>A Townsend avalanche happens in a gaseous medium with an electric field. An initial ionized electron is

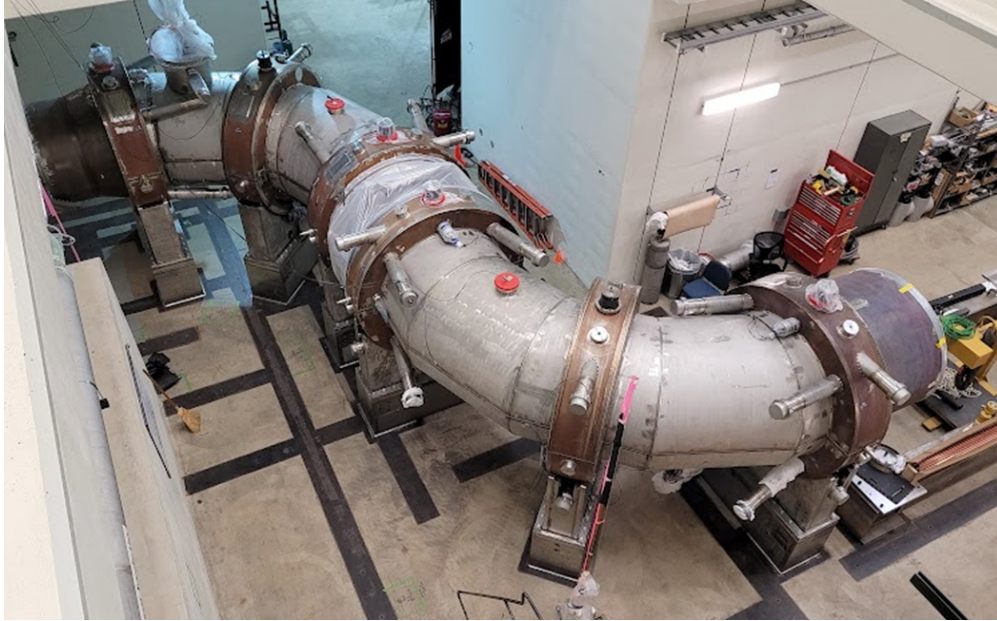


Figure 2.19: TS built

detected at both ends of the straw by a preamplifier connected to a TDC (Time-to-Digital Converter), and the time difference between the detection at each end of the straw gives the position of the event along the length of the straw. The TDC have a required time resolution of 35 ps to achieve a 1 cm position resolution on the position of the ionization event.

The straws have a length varying between 330 mm and 1200 mm and a diameter of 5 mm. They are made of two layers of 6  $\mu\text{m}$  Mylar<sup>®</sup> spiral wound using a 3  $\mu\text{m}$  layer of adhesive. The straw walls are metallized on both the inner and outer surface with a 500 Å aluminum layer (for electrostatic shielding) and an additional 200 Å gold layer on the inner surface that acts as the cathode. The center wire is a 25  $\mu\text{m}$  gold-plated tungsten wire. The straws are filled with a gas mixture of 80 % Ar and 20 % CO<sub>2</sub> at a pressure of 1 atm.

The tracker is composed of 20 736 straws organized in panels, planes and stations:

**A panel** is made of two layers of straws (96 straws in total) covering a 120° arc

**A plane** is assembled from two layers of 3 panels that cover the entire 360° ring ; there is a 30° rotation between the two layers.

**A station** consists of two planes, where the second plane is rotated 180°.

accelerated by the electric field and knocks electrons from the gas molecules, which themselves get accelerated by the electric field and knock more electrons from the gas medium, creating an avalanche that reach the anode and generates a current spike in the wire.



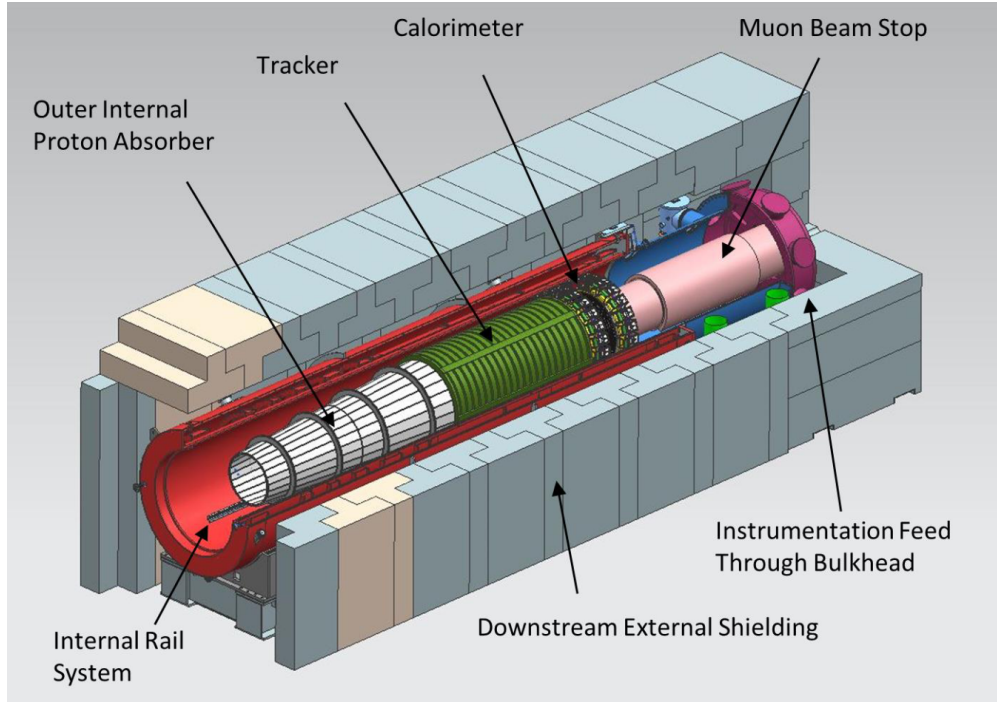


Figure 2.20: Drawing of the Detector Solenoid showing all the components present inside

**The tracker frame** is made of 18 stations that span 3195 mm (3051 mm active length)

The calibration of the tracker for 105 MeV electrons is based on a cosmic ray runs and measurements of known background signal (DIO, RPC) during special runs.

## 2.6 Calorimeter

In particle physics, an electromagnetic calorimeter is a detector tasked to measure the energy deposited by particles via electromagnetic interaction. The Mu2e electromagnetic calorimeter [30] is located downstream of the tracker<sup>3</sup>, and is composed of two annular disks containing 1348 pure cesium iodide (CsI) scintillating crystals. The two disks are separated by 700 mm (which corresponds to half of the wavelength of a 105 MeV electron) to almost guarantee that conversion electrons will intersect at least one of the disks (see Figure 2.26).

It has three main purposes:

- Provides particle identification capabilities to reject muons and pions by using the fact that the shape of the particle shower generated by muons, pions, and electrons are all different.
- generates a fast online trigger filter to keep or not the event based on total energy deposited in the calorimeter.

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<sup>3</sup>because it is a destructive measurement



Figure 2.21: The Detector Solenoid cold mass being inserted inside the vacuum vessel at the vendor factory (in October 2025)

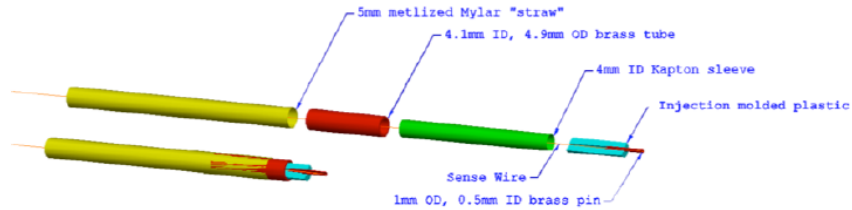


Figure 2.22: tracker straw

- helps the reconstruction algorithm by giving a starting point (or seed) to complement tracker information.

To achieve these goals, the Mu2e calorimeter is required to have a large geometric acceptance, a time resolution better than 0.5 ns, an energy resolution better than 10 %, and a position resolution of 1 cm for 105 MeV electrons, while being able to operate in a 1 T axial magnetic field, under vacuum ( $10^{-4}$  Torr), in a heavy radiation environment (total ionization dose in the order of 100 krad, neutron flux of  $10^{12}$  n/cm<sup>2</sup> 1 MeV equivalent neutron).

A more detailed description of the calorimeter is given in Chapter 3.

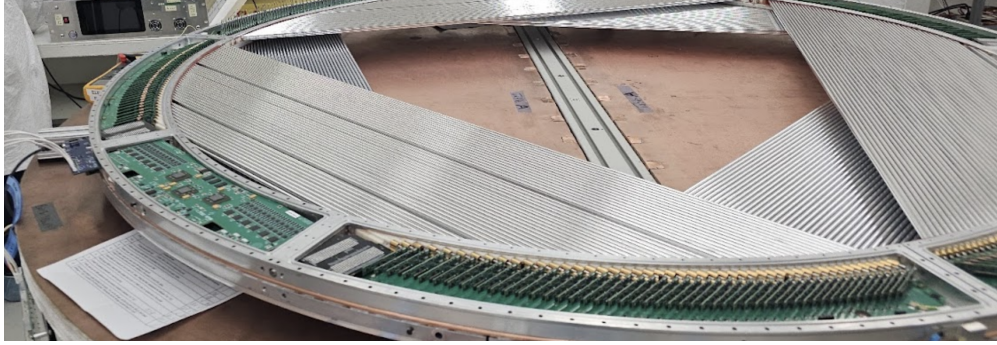


Figure 2.23: One station of the tracker

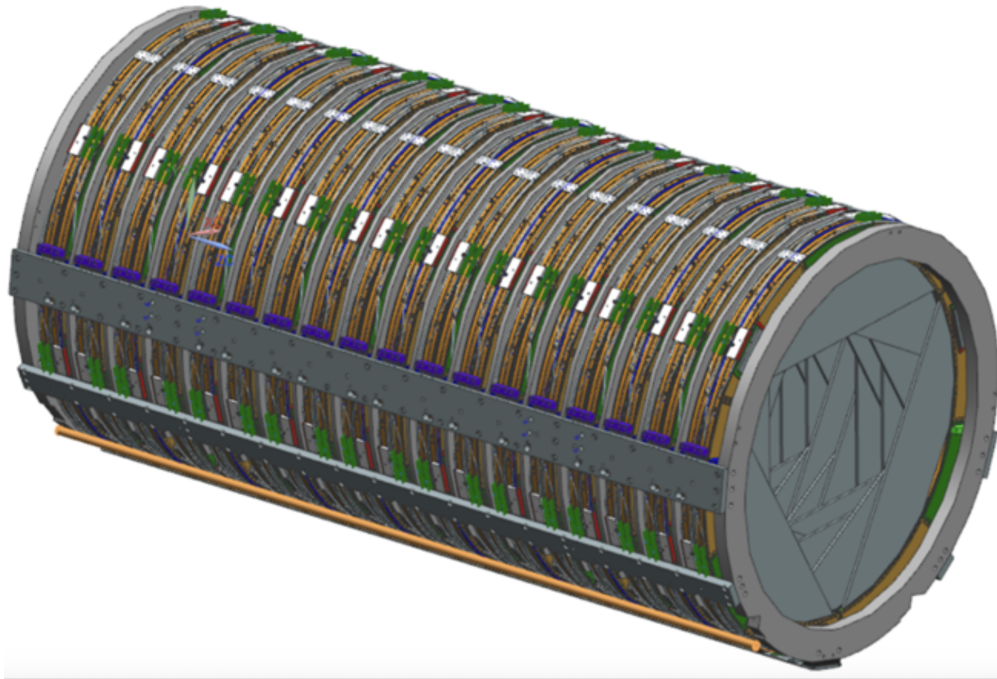


Figure 2.24: CAD drawing of the tracker

## 2.7 Cosmic Ray Veto (CRV)

The largest background in the Mu2e experiment is produced by cosmic rays, generating about one signal-like event a day. To achieve the required sensitivity of less than 0.1 signal-like cosmic ray event over the entire Mu2e run, this background rate needs to be suppressed by a factor 10 000, meaning that the cosmic ray veto system has to have an efficiency greater than 99.99 %.

To achieve this, the detector solenoid and the upstream transport solenoid are covered on all sides by the Cosmic Ray Veto (CRV) [31], whose goal is to detect incoming cosmic rays. It is made of multiple modules of different size that cover a total area of 335 m<sup>2</sup> and is made of a total of 5344 counters. Each plastic scintillator strip has a 20 mm × 50 mm cross-section and a length that varies (between 3 m and 6.6 m) depending on its location. Once a cosmic ray is detected, the CRV stores



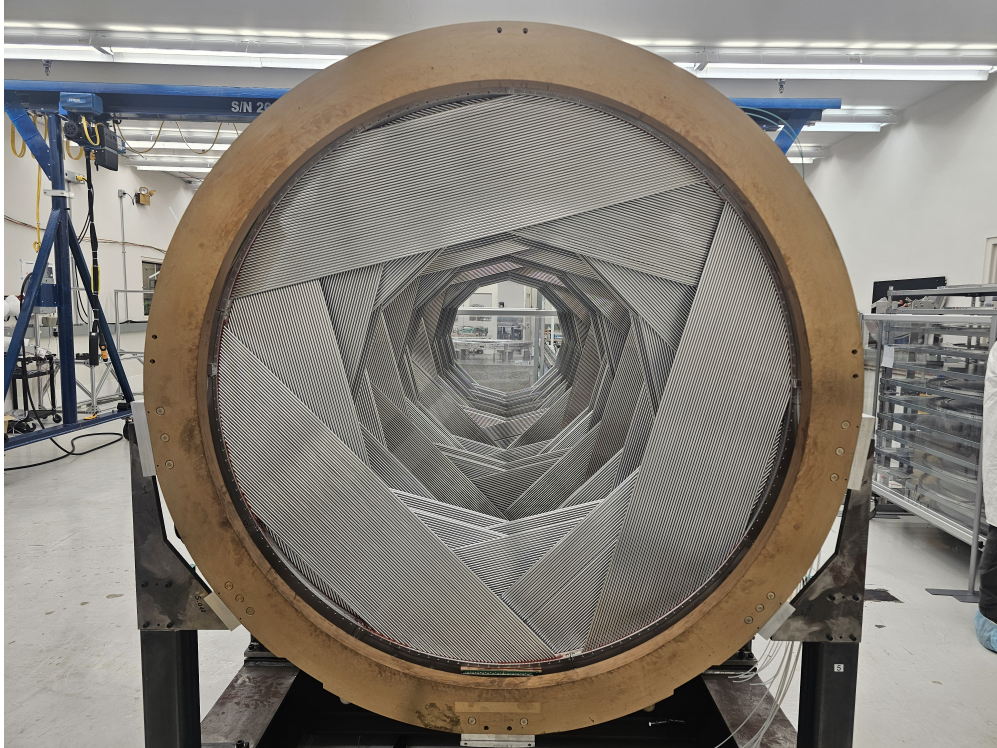


Figure 2.25: Hole in the center of the tracker

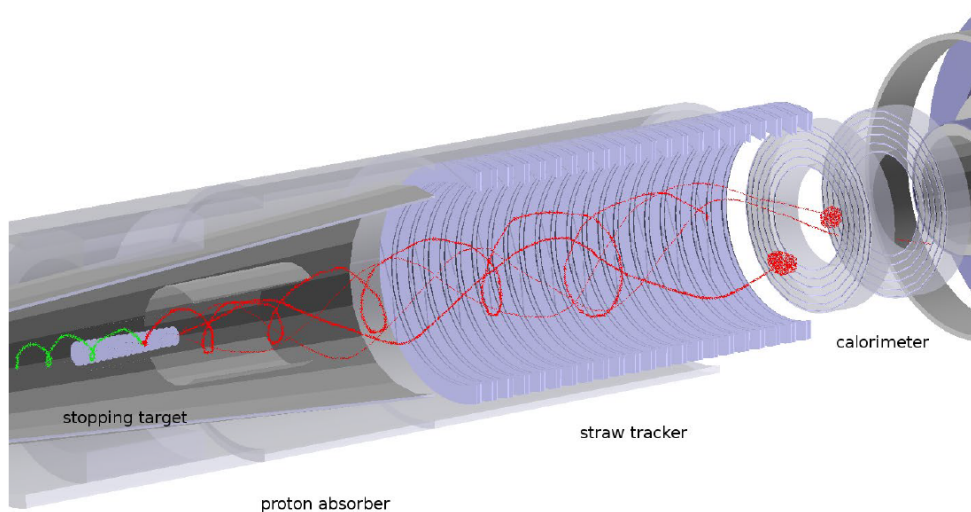


Figure 2.26: Conversion electron events intersecting both calorimeter disks

its timing and energy so that it can be vetoed later in the analysis process: events taken within a time window around the CRV hit can be ignored.

The cosmic ray system is divided into two different parts, a passive shielding and an active veto system (see Figure 2.30).



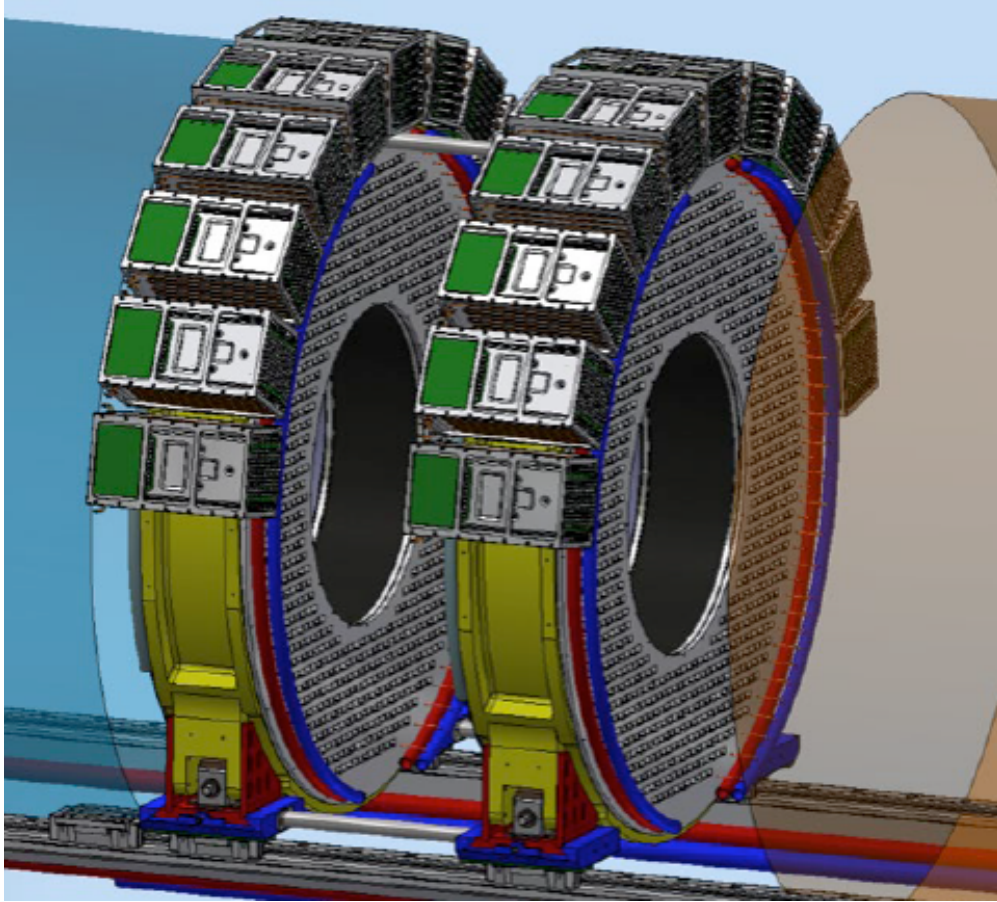


Figure 2.27: CAD drawing of the two calorimeter disks

The passive shielding is made of large concrete blocks that reduce the amount of cosmic rays reaching the detectors.

The active cosmic ray veto (CRV) system consists of four layers of extruded plastic scintillator strips with a layer of aluminum absorber in between each scintillator layer.

The plastic used for the scintillator is a polystyrene base doped with 1 wt.% 2,5-diphenyloxazole (PPO) and 0.03 wt.% 1,4-bis(5-phenyloxazol-2-yl) benzene (POPOP) [32]. The plastic scintillators are co-extruded with a 0.25 mm thick reflective titanium dioxide ( $\text{TiO}_2$ ) cladding. They are embedded with 1.4 mm diameter wavelength-shifting fibers from Kuraray<sup>4</sup> that absorbs blue light ( $\sim 425$  nm) emitted by the scintillator and re-emits blue-green light in the 500 nm – 600 nm wavelength range that is more appropriate for the SiPMs used. Each scintillator counter is read-out on both sides by Silicon Photomultipliers (SiPMs) to use the time difference between the two sides to locate the position of the hit along the scintillator.

<sup>4</sup>Kuraray website

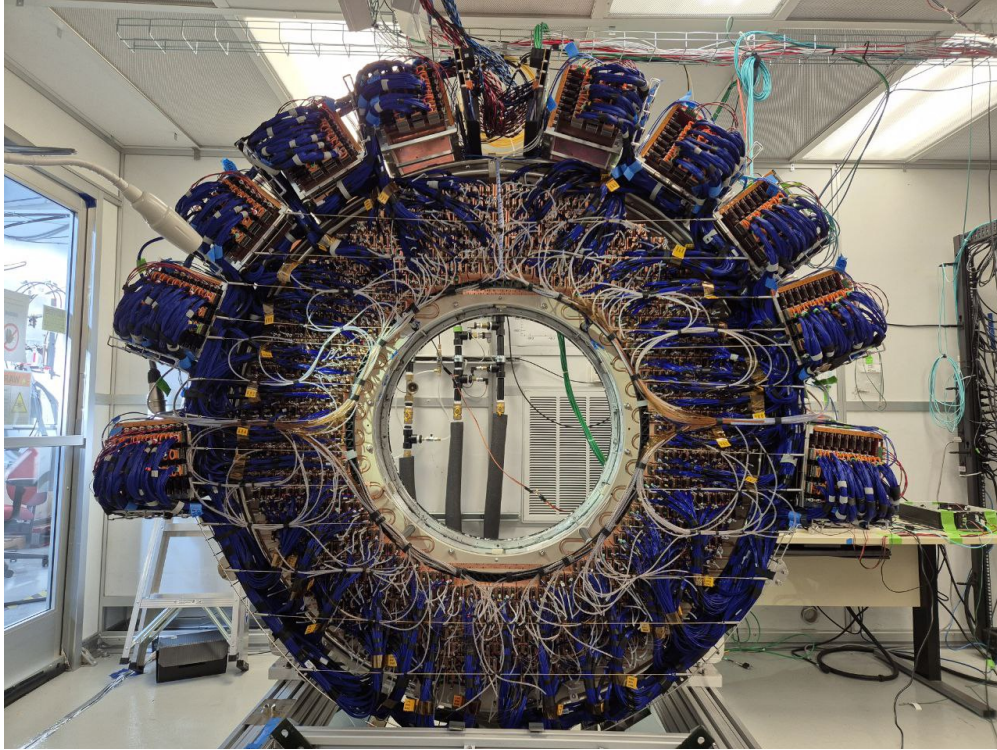


Figure 2.28: Calorimeter built and cabled

## 2.8 Stopping Target (ST) and Stopping Target Monitor (STM)

### 2.8.1 Stopping Target (ST)

The stopping target is composed of 37 thin annular aluminum foils, with a thickness of  $105\ \mu\text{m}$ , an inner radius of 21 mm and an outer radius of 75 mm. The target has a total length of 800 mm and is made of high purity aluminum ( $> 99.9\%$ ). The choice of aluminum is motivated by its low atomic number ( $Z = 27$ ) leading to a long muonic atom lifetime, as well as good mechanical and chemical properties. In order to remove Radiative Pion Capture (RPC) background that comes shortly after the beam flash, the experiment exploits the difference between the pion lifetime ( $\tau = 26\ \text{ns}$ ) and the lifetime of muonic aluminum atom ( $\tau = 864\ \text{ns}$ ). This way, we can use a delayed time window  $[700 - 1695\ \text{ns}]$  to remove most of the RPC background while keeping the majority of the muon decay events (more details available in Section 1.6.4). More details about the choice of stopping target material can be found in Chapter 5.

The geometry of the stopping target has been optimized to simultaneously maximize the number of muon captures and minimize outgoing electron energy loss through the target.

Surrounding the stopping target are two conical absorbers: the Inner Proton Absorber (IPA) and the Outer Proton Absorber (OPA). The IPA is located just downstream of the stopping target at a higher radius (between 335 and 353 mm), and the OPA surrounds both the stopping target and the

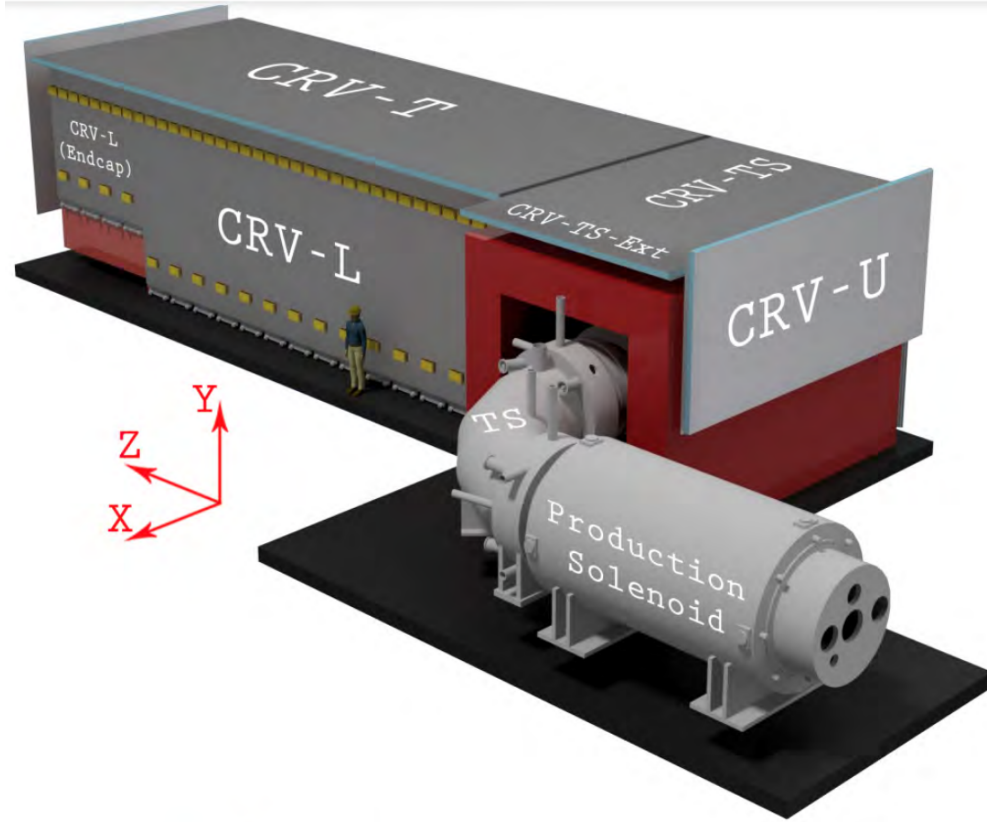


Figure 2.29: CAD drawing of the Cosmic Ray Veto surrounding the detector solenoid

IPA with a radius between 250 and 450 mm. Their goal is to reduce the number of protons reaching the tracker (they are very ionizing and can destroy the straws), while being mostly transparent for electrons. This requirement motivated the use of low-Z materials, and both the IPA and OPA are made of high-density polyethylene.

### 2.8.2 Stopping Target Monitor (STM)

The Stopping Target Monitor (STM) is an additional detector designed to count the number of muons that stop in the stopping target with a required accuracy of 10 %. The number of stopped muon is a critical value to measure as it is used to compute the rate of muon conversion:

$$R_{\mu e} = \frac{\Gamma(\mu^- + {}^A_Z\text{N} \rightarrow e^- + {}^A_Z\text{N})}{\Gamma(\mu^- + {}^A_Z\text{N} \rightarrow \nu_\mu + {}^A_{Z-1}\text{N})} \quad (2.1)$$

In Equation 2.1, the numerator is the rate of neutrinoless muon conversion and the denominator is the rate of muon capture.

This measurement is based on detecting gamma rays emitted during the muon capture process.



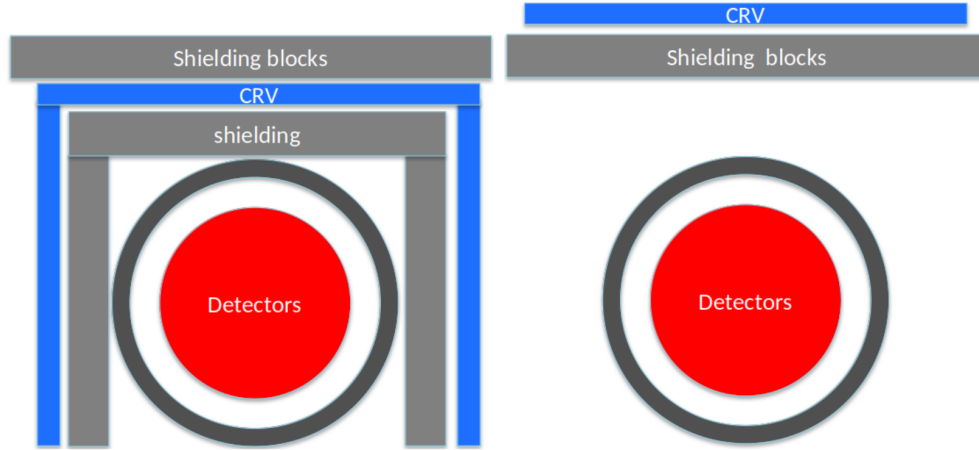


Figure 2.30: Configuration of the Cosmic Ray Veto with full coverage (on the left) and reduced configuration during run-I (on the right)

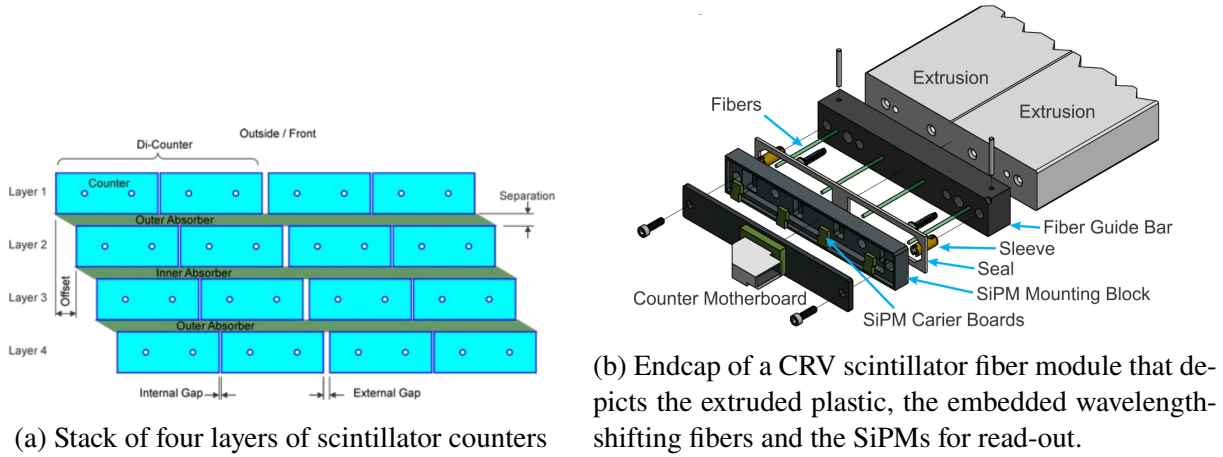


Figure 2.31: CRV modules

Figure 2.34 details the different steps in the muon capture process, with an emphasis on the energy of the emitted photons [33]. The three emission lines that are used in order of strengths are at 347 keV, 1809 keV, and 844 keV.

The STM system is composed of a collimator located just outside the CRV, downstream of the muon beam stop (on the far left on Figure 2.4, detailed in Figure 2.35), and a combination of two complementary detectors placed about 25 m downstream on the axis of the detector solenoid. The collimator limits the amount of charged particles reaching the detectors in order to limit their radiation damage (especially for the HPGe detector).

The first detector is a High-Purity Germanium (HPGe) detector with a very good energy resolution ( $O(1 \text{ keV})$ ) but a long recovery time ( $O(50 \mu\text{s})$ ) that implies a slow rate of data taking. To complement the HPGe semi-conductor detector, a  $\text{LaBr}_3$  inorganic scintillator detector provides



Figure 2.32: Picture of the stopping target

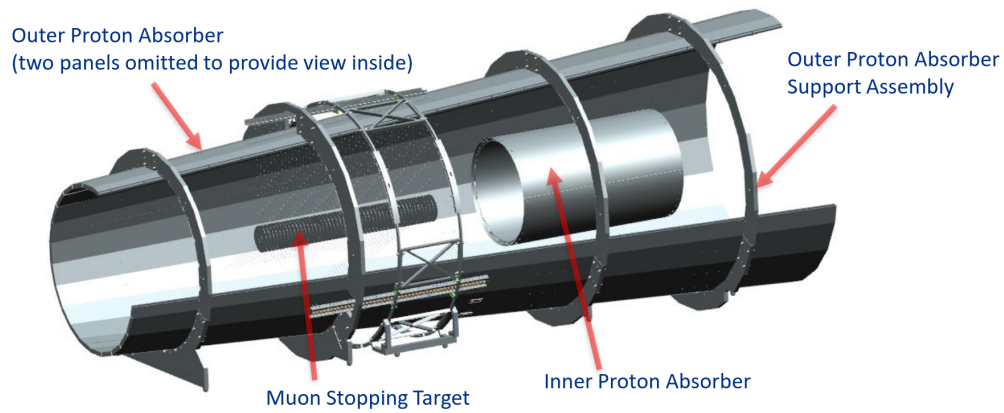


Figure 2.33: View of the stopping target, Inner Proton Absorber (IPA), and Outer Proton Absorber (OPA)

a fast recovery time ( $O(50 \text{ ns})$ ) at the cost of a worsened energy resolution ( $O(10 \text{ keV})$ ). The combination of the two detectors provides a continuous monitoring of the muon stopping rate during operation with the  $\text{LaBr}_3$  detector, and a more precise measurement of the rate offline with the HPGe detector.

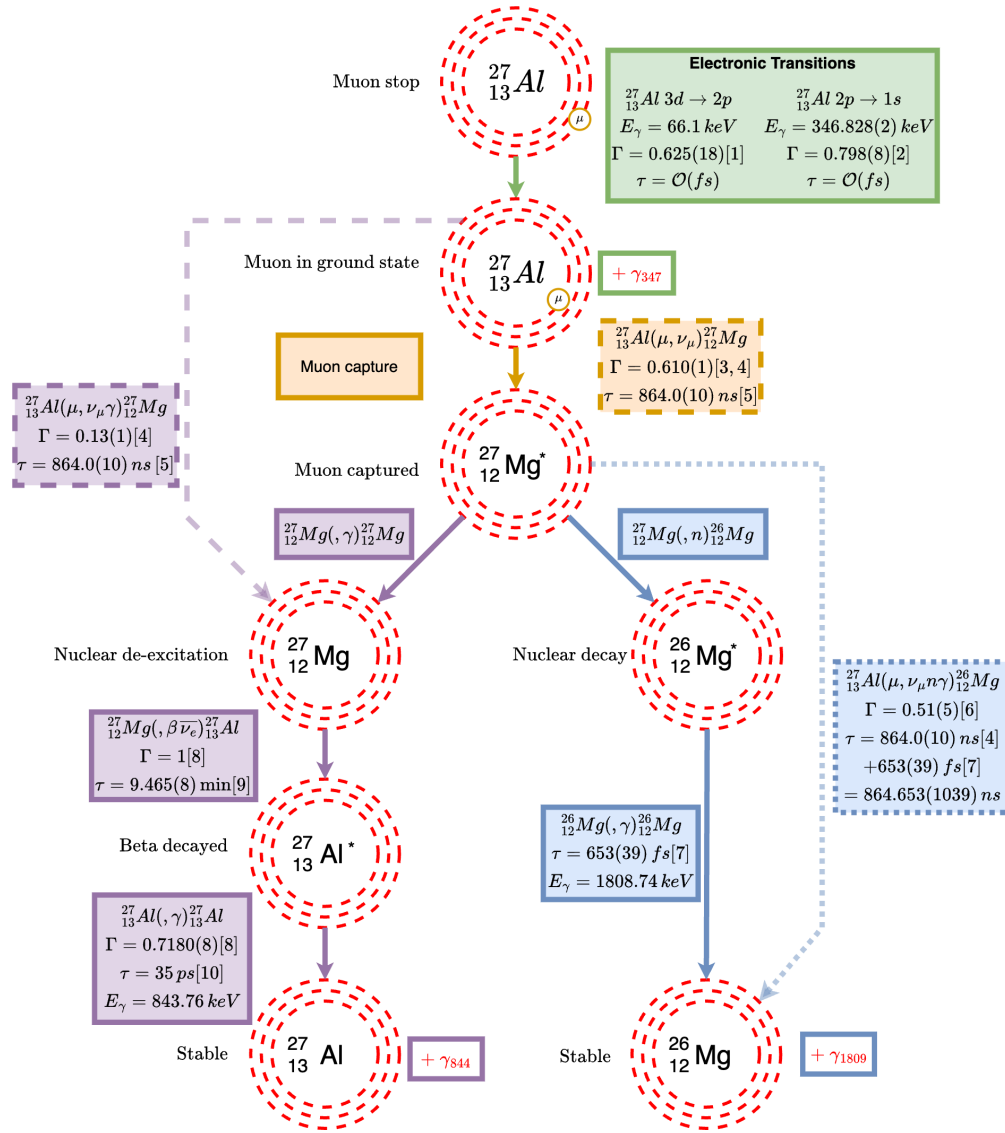


Figure 2.34: Muon capture decay chain (credit: Pawel Plesniak [33])

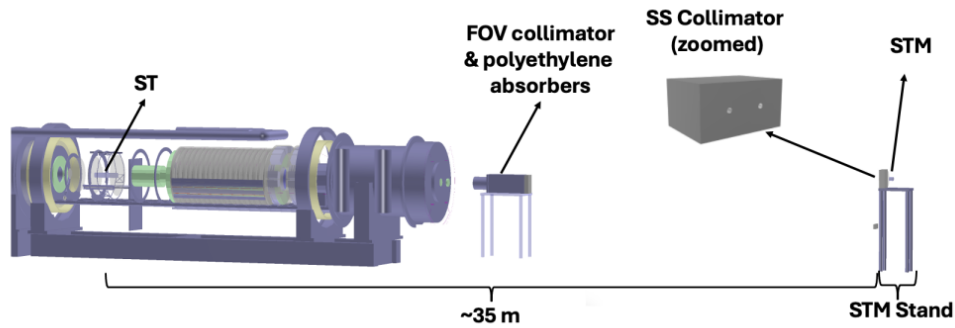


Figure 2.35: STM system (credit: Claudia Alvarez Garcia thesis)

## Chapter 3

### THE ELECTROMAGNETIC CALORIMETER

The Calorimeter [30] has been designed, tested, and built by groups from INFN (Istituto Nazionale di Fisica Nucleare, the Italian national laboratory for physics) and Caltech. While INFN has been leading the mechanical design and assembly, the Caltech group has been in charge of the energy calibration system and the crystal quality control.

#### 3.1 Calorimeter components

##### 3.1.1 Mechanical structure

The mechanical structure of the Mu2e calorimeter [34, 35] is made of a 146 mm thick aluminum outer ring with an inner [resp. outer] diameter of 1314 mm [resp. 1460 mm]. Its purpose is to support all the crystals as well as the data acquisition (DAQ) electronics placed in 10 crates around the calorimeter disk. The inner ring (with an inner [resp. outer] diameter of 672 mm [resp. 716 mm]) and the front plate can be traversed by particles before reaching the crystals, hence to minimize the energy loss of particles, they are made of carbon fibers with embedded aluminum honeycomb structures. The front plate is fitted with 10 thin-walled aluminum tubes used for the energy calibration system described in Section 3.1.4. The back plate is a 20 mm polyether ether ketone (PEEK) plate that supports the readout units and their cooling system. It hosts a network of 38 copper lines that circulates a cooling liquid at  $-15^{\circ}\text{C}$  to cool down the silicon photomultipliers (SiPMs).

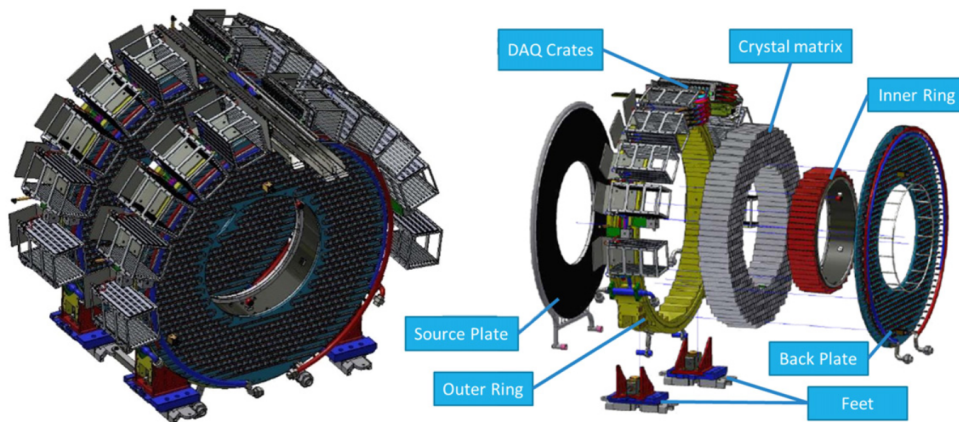


Figure 3.1: CAD drawing of the calorimeter disk [34]



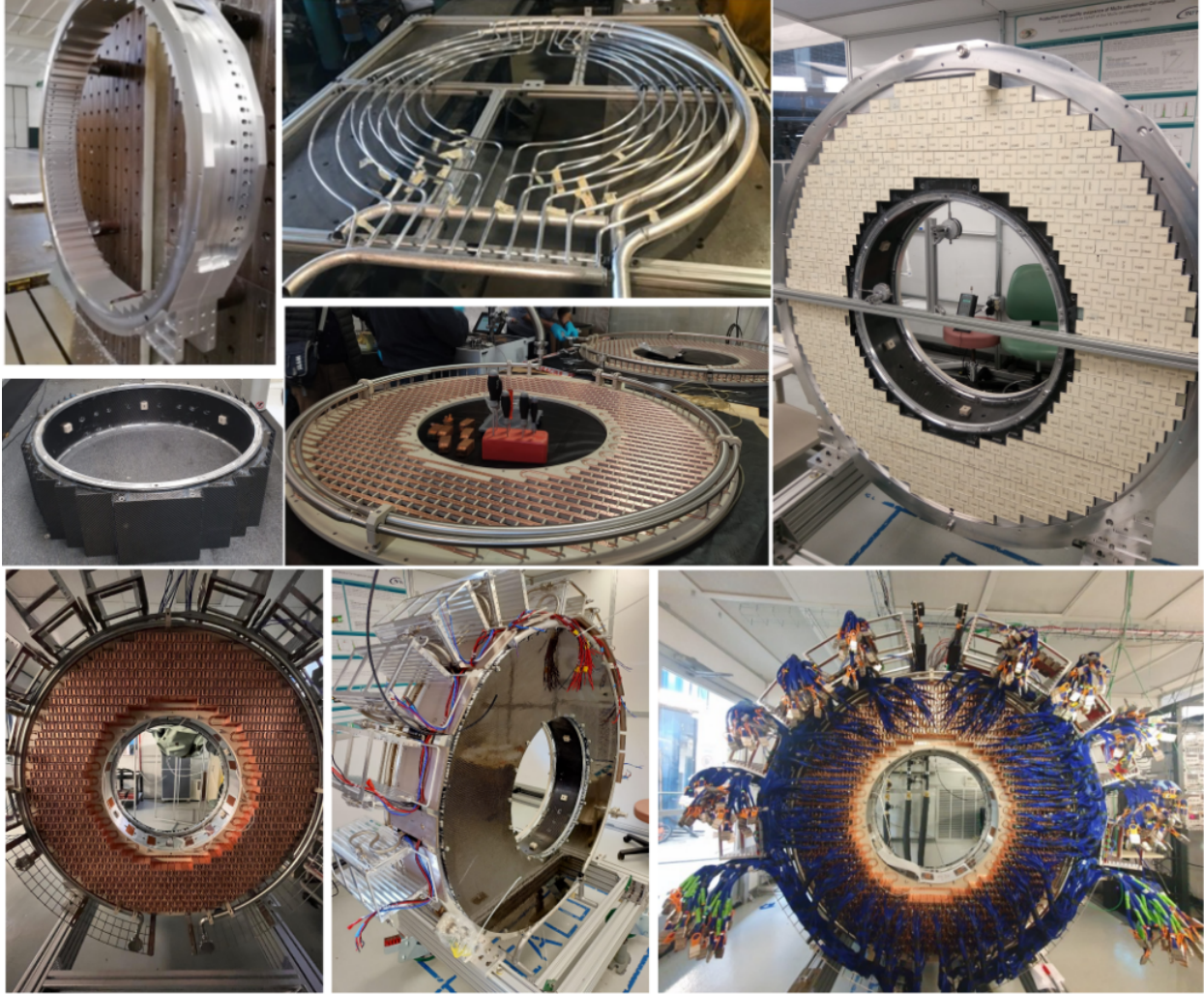


Figure 3.2: Pictures of the different parts of the calorimeter under construction outer ring (top-left); energy calibration tubes in the front place (top-center); crystal stacked in the disk (top right); inner ring (middle-left); back plate (center); read-out units installed in the back of the disk (bottom-left); front plate and electronic crates installed (front center); cable connected to the read-out units (bottom-right) [35].

### 3.1.2 Crystals

The crystals used in the Mu2e electromagnetic calorimeter are undoped cesium iodide (CsI), wrapped in a 150  $\mu\text{m}$  thick layer of reflective Tyvek<sup>®</sup> and its back endcap<sup>1</sup> is covered by 2 independent arrays of silicon photomultipliers (SiPMs). To reduce the optical cross-talk between crystals, an additional 50  $\mu\text{m}$  thick black Tedlar<sup>®</sup> foil is placed in between each crystal. Their dimensions are 34 mm  $\times$  34 mm  $\times$  200 mm (see Figure 3.3 [36]), where the length of 200 mm has been chosen to be about 10 times the radiation length in order to contain the entire particle shower.

<sup>1</sup>the front endcap is covered by a plastic endcap

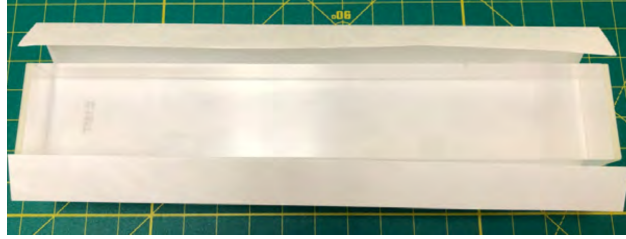


Figure 3.3: One CsI crystal for the Mu2e calorimeter

CsI main scintillation wavelength is 310 nm with a fast decay time of 20 ns that is capable of handling the high rates expected in Mu2e.

In addition to the CsI crystals, there are 4 LYSO (lutetium-yttrium oxyorthosilicate) crystals installed in four corners of the calorimeter (see 3.4)). These four crystals are analyzed separately, as they have a completely different goal than the calorimeter. Their purpose is to provide an alternative way to measure the number of muon stops, complementary to the stopping target monitor system. They can detect with high precision the 1809 keV photons produced during the muon capture process (see Section 2.8.2) with a much faster rate than the STM.

### 3.1.3 Front End Electronics (FEE) and readout electronics

Each array of SiPMs is made of two rows of 3 Hamamatsu UV-extended 6 mm  $\times$  6 mm with 50  $\mu$ m pixel size<sup>2</sup>. They have a high photon detection efficiency at the CsI emission wavelength peak (310 nm), are radiation hard, and have a very fast recovery time (below 100 ns). In order to operate in vacuum and keep outgassing rates low, the coupling between the crystal and the SiPMs isn't using any optical grease, thus reducing light yield. One crystal is readout by two of these SiPMs to provide redundancy, and the 2 SiPMs along with their necessary electronics (preamplifier and regulator) are encased inside a copper Faraday cage (to minimize electromagnetic interferences) are called a Read-Out Unit (ROU) [38].

The rest of the readout electronics [35, 39] are located in the 10 crates surrounding the calorimeter disk, each crate being able to hold 8 electronic boards, each board being responsible for 20 crystals (or 40 SiPMs). These electronic boards are made of two parts (see Figure 3.6): one “mezzanine” board that is responsible for distributing low and high voltage to the SiPMs and monitoring their temperature, and one readout and digitization board (DIGitization and ReAdout Controller, or DIRAC) which hold an Analog-to-Digital Converter (ADC) and other electronic components necessary to readout, amplify, and digitize the signal and send it via optical fibers to the servers.

<sup>2</sup>custom made by Hamamatsu based on model S13360-6050PE

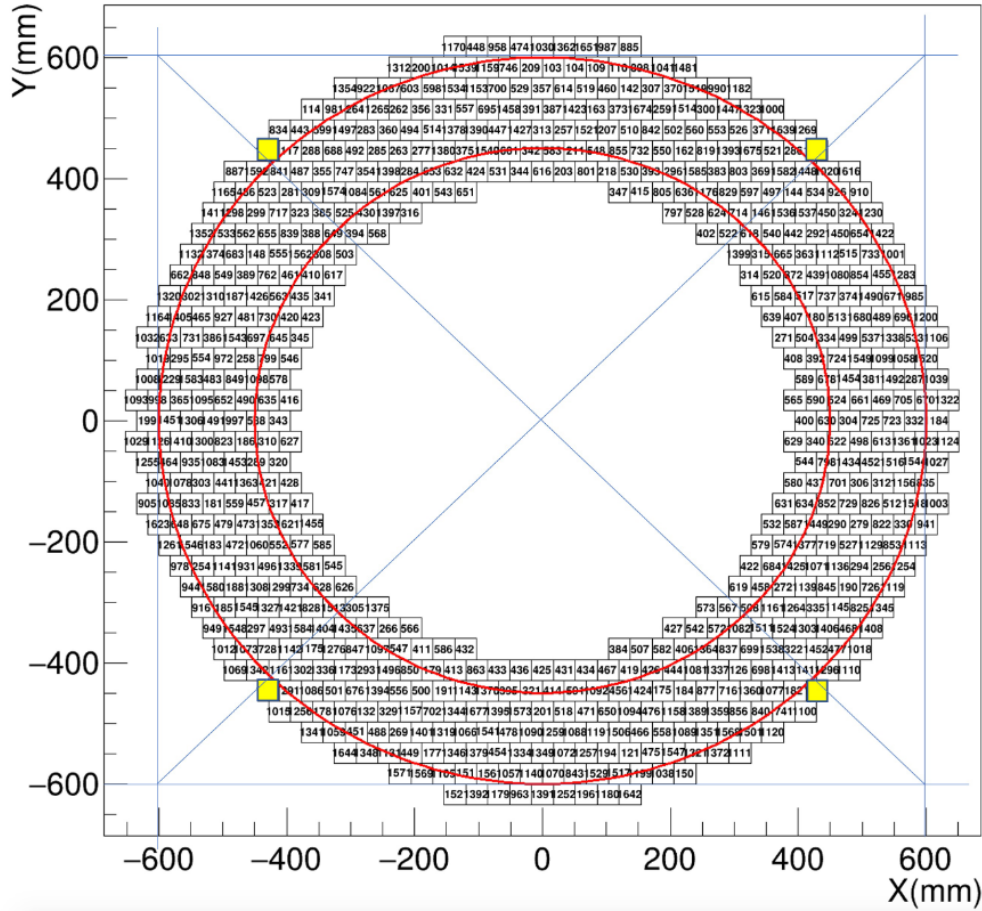


Figure 3.4: Position of the four LYSO crystals in the Mu2e calorimeter (credit: Simona Giovannella [37])

### 3.1.4 Calibration systems

The electromagnetic calorimeter has two main calibration systems that need to run regularly to maintain data consistency during physics runs. Additional calibration runs using cosmic rays or backgrounds can be used in special runs, but these will not be developed in the following sections.

### 3.1.5 Laser calibration

The goal of the laser calibration system [40] is to monitor the stability of the gain of the SiPMs and their time resolution. It uses a Standa STA-01SH-2<sup>3</sup> pulsed Nd:YAG laser to deliver green light (532 nm wavelength) to all of the crystals simultaneously. Figure 3.7 showcases the different components of the laser system.

<sup>3</sup>[website link](#)



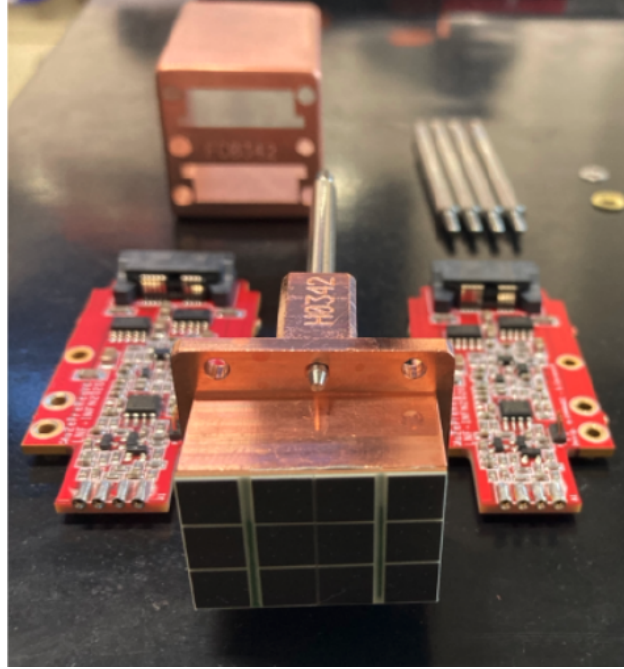


Figure 3.5: Calorimeter Front End Electronics

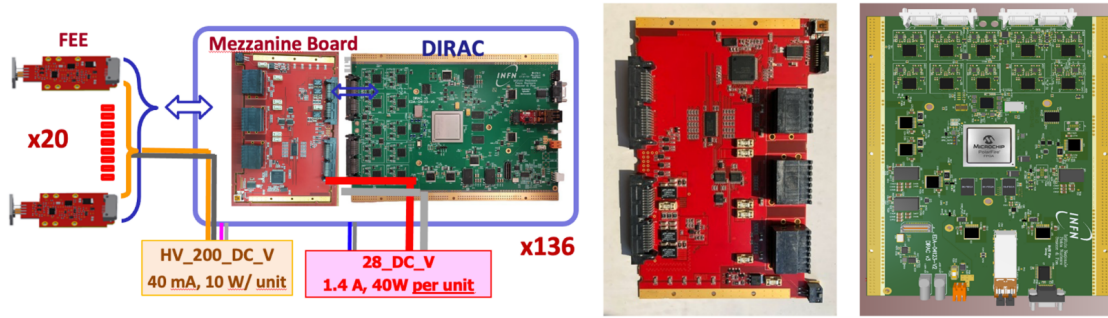


Figure 3.6: Electronic components of the calorimeter. Source: [35]

### 3.1.6 Energy calibration

In order to achieve an energy resolution better than 10 % at 105 MeV, the calorimeter needs to have an energy calibration system that can be run regularly to monitor the energy calibration of each ROU. The Mu2e calorimeter team decided to use a system previously used in the calorimeter of the BaBar experiment [41], where a 6.13 MeV photon is produced via a nuclear decay chain started by a neutron generator.

The decay chain equation (Equation 3.1) involves irradiating fluorine atoms with neutrons to create a 6.13 MeV photon with a half-time of 7 s.

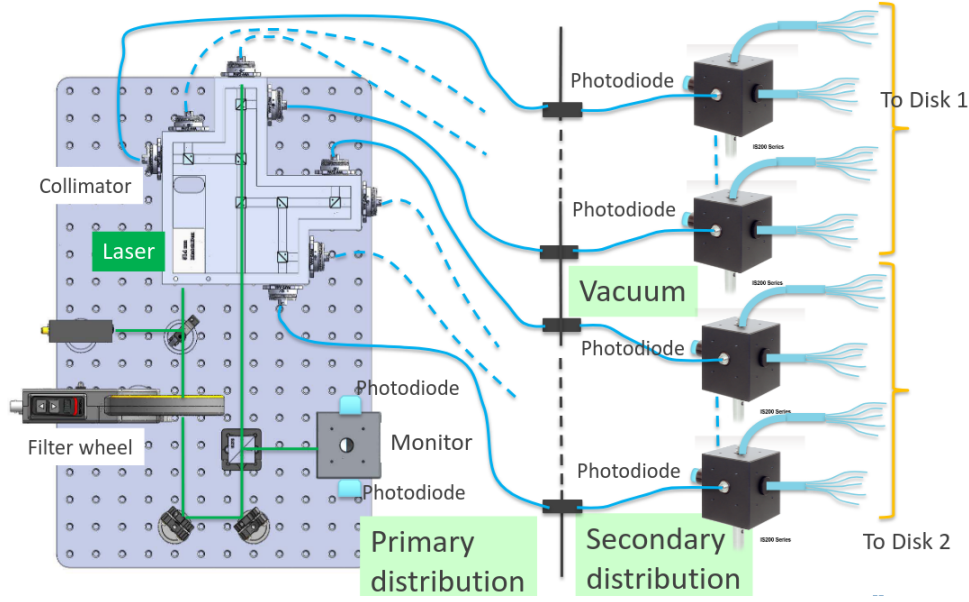
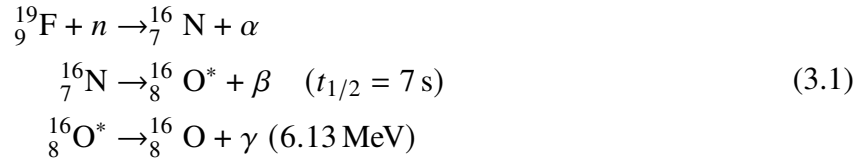


Figure 3.7: Laser calibration system for the calorimeter (credit: C. Ferrari [40])



Because of the short lifetime, this process needs to be done in situ. In addition, to be able to calibrate one entire calorimeter disk at once, we circulate a fluid containing fluorine atoms (Fluorinert™ FC-770) in aluminum tubes covering the front plate of the calorimeter. A circulation pump pushes the fluid between a reservoir placed in front of the Deuterium-Tritium (DT) generator and the calorimeter, as illustrated in Figure 3.8.

It takes about 20 minutes to generate at least 100 000 photons per crystal and obtain a calibration precision better than 1 %. A simulation of the resulting crystal response can be seen in Figure 3.9, in which the red curve is a fit of the simulated data in black. The fit is made by adding three different components and a background: the three components correspond to the 6.13 MeV photon absorption peak (yellow curve), the single escape peak (pink curve), and the double escape peak<sup>4</sup>(cyan curve), all three being fitted to three Crystal Ball distribution separated by  $m_e = 511 \text{ keV}$ , and a background approximated by a logistic function (blue curve) [43].

More details about the neutron generator and its commissioning are located in Section 3.4.

<sup>4</sup>when the photon deposits its energy in the crystal via an electromagnetic shower, if its energy is above 1.022 MeV, it can create an electron and positron through pair production; the positron will annihilate with a surrounding electron and produce two 511 keV photons; the single escape peak corresponds to the case when one of the two photon escapes the crystal without depositing its energy, and the double escape peak when both photons escape.

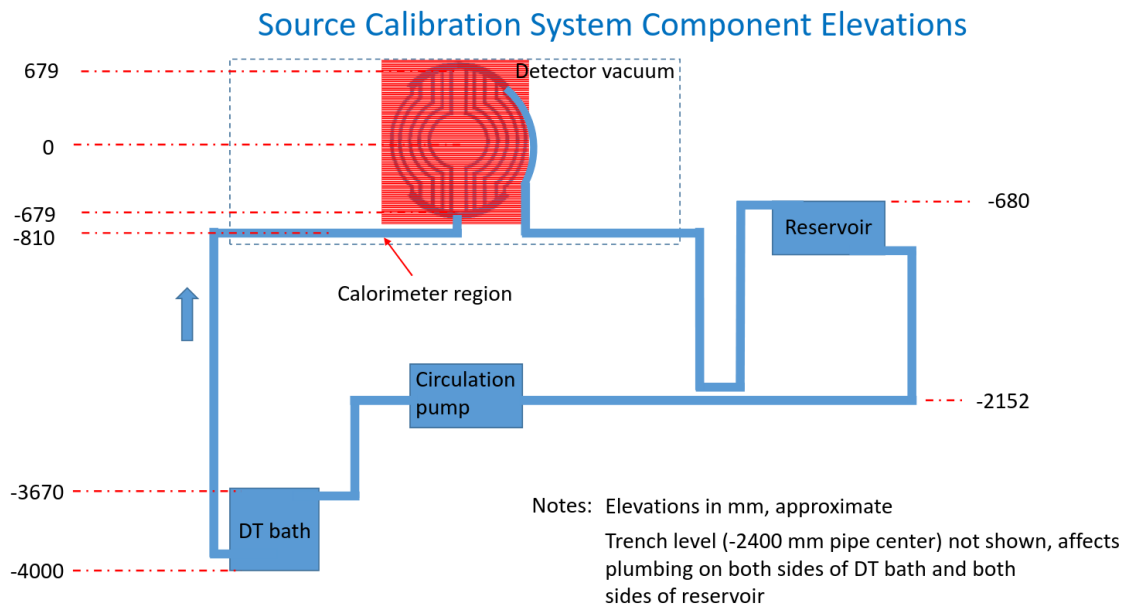


Figure 3.8: Calorimeter energy calibration system. Credit: Frank Porter [42]

### 3.2 Inorganic crystal scintillators

A material is said to have scintillation properties when it is able to absorb the energy of incoming high-energy particles (or photons) and re-emit this energy in the form of light at a specific wavelength. The absorption mechanism for scintillators is based on particle shower, and more particularly for electromagnetic calorimeter, it is restrained to particles that interact with the scintillation material through the electromagnetic force. An electromagnetic particle shower is the sequence of pair production (a high-energy photon converting into an electron-positron pair) and Bremsstrahlung (a decelerating high-energy charged particle produces photons to conserve four-momentum), creating a cascade of lower energy particles that deposit all of their energy in the medium.

There are three main mechanisms used by an incoming high-energy particle to deposit energy in the scintillation material, which are illustrated in Figure 3.10:

**Pair production:** limited to high energy ( $> 1$  MeV) required to produce an electron-positron pair, its probability increases with the atomic number of the scintillation material.

**Compton scattering:** a photon transfers a fraction of its energy to a valence shell electron that is ejected from its atomic orbit. It is the most probable process at medium energy (50 to 1000 keV) and is independent of atomic number.

**photoelectric effect:** the photon energy is entirely absorbed by a K-shell electron, the latter is ejected and leaves a vacancy that is filled, emitting a characteristic X-ray photon in the



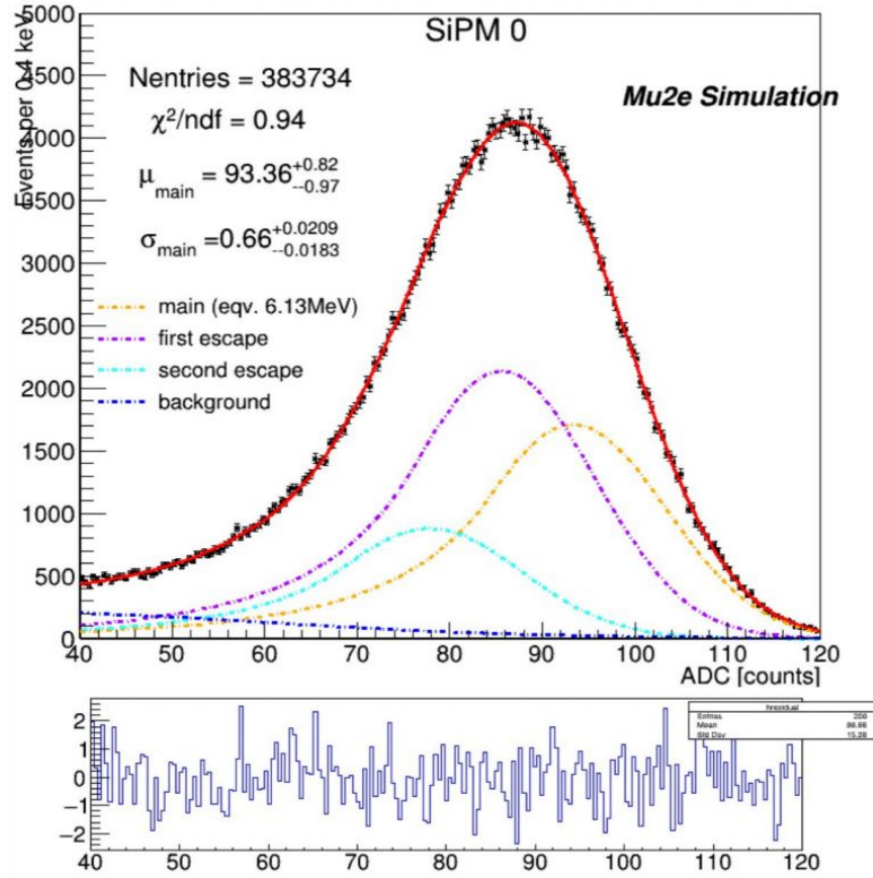


Figure 3.9: Fitting of simulated crystal response to the 6.13 MeV photon used for calibration ; credit: Huma Jafree [43]

process. This process is dominant at low energy ( $< 50$  keV) and its probability is higher for high-Z elements

Figure 3.11 showcases the properties of crystals that were considered for the Mu2e electromagnetic calorimeter. The choice of pure CsI comes from its fast decay time (30 ns for the slow component and 6 ns for the fast component) and affordable price, even though its light output is weaker (less than 5 % of LYSO's light output). Another choice of crystal that is considered for a potential upgrade of the Mu2e experiment is barium fluoride  $\text{BaF}_2$  due to its ultra-fast component (0.9 ns) with a similar light yield as CsI. However, the problem comes from the other  $\text{BaF}_2$  component with a very long decay time of 650 ns which is not compatible with the timing requirement of the Mu2e calorimeter. One of the R&D programs at Caltech is looking at 2 different solutions to remove this slow component while keeping the fast component of  $\text{BaF}_2$ :

1. use yttrium doping to change the crystal structure

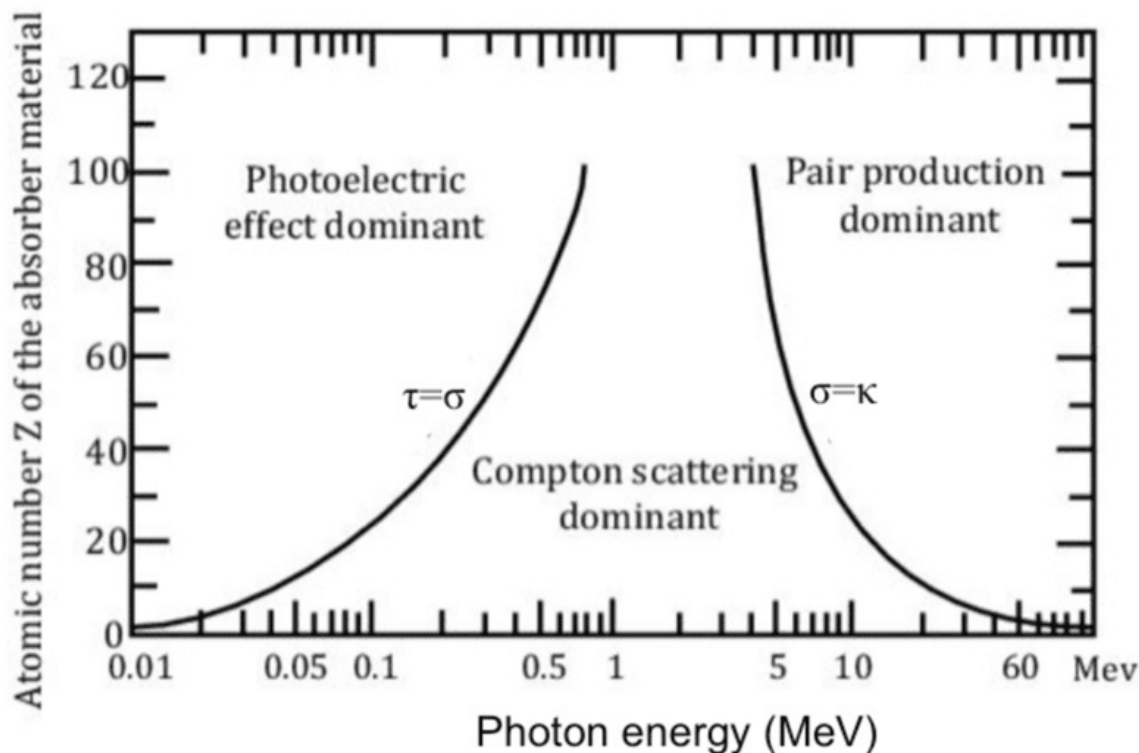


Figure 3.10: The different types of photon interactions as a function of energy and atomic number of stopping material (source: [oncologymedicalphysics.com](http://oncologymedicalphysics.com))

2. use a solar-blind photosensor with low quantum efficiency at the wavelength of the slow component

### 3.3 Crystal quality control

#### 3.3.1 Crystal wrapping

The 1348 pure cesium iodide crystals have been fabricated by two companies: SICCAS in China and Saint-Gobain in France. The companies shipped the crystals to Caltech and INFN for wrapping and quality control.

The crystal wrapping process follows 4 main steps illustrated in Figure 3.12 [44, 45]:

1. the Tyvek wrapping paper is cut to the appropriate size and pre-folded to envelop the crystal
2. two 3D-printed ABS (Acrylonitrile Butadiene Styrene) frames are positioned against both front and back faces of the crystal
3. the frames are glued to the Tyvek paper (and not to the crystal itself)

| Parameter:             | $\rho$          | MP               | $X_0^*$ | $R_M^*$ | $dE/dx^*$ | $\lambda_I^*$ | $\tau_{\text{decay}}$                 | $\lambda_{\text{max}}$               | $n^\dagger$ | Relative light yield                   | Hygro-scopic? | $d(\text{LY})/dT$                     |
|------------------------|-----------------|------------------|---------|---------|-----------|---------------|---------------------------------------|--------------------------------------|-------------|----------------------------------------|---------------|---------------------------------------|
| Units:                 | $\text{g/cm}^3$ | $^\circ\text{C}$ | cm      | cm      | MeV/cm    | cm            | ns                                    | nm                                   |             | % <sup>‡</sup>                         |               | %/ $^\circ\text{C}$ <sup>§</sup>      |
| NaI(Tl)                | 3.67            | 651              | 2.59    | 4.13    | 4.8       | 42.9          | 245                                   | 410                                  | 1.85        | 100                                    | yes           | -0.2                                  |
| BGO                    | 7.13            | 1050             | 1.12    | 2.23    | 9.0       | 22.8          | 300                                   | 480                                  | 2.15        | 21                                     | no            | -0.9                                  |
| BaF <sub>2</sub>       | 4.89            | 1280             | 2.03    | 3.10    | 6.5       | 30.7          | 650 <sup>s</sup><br><0.6 <sup>f</sup> | 300 <sup>s</sup><br>220 <sup>f</sup> | 1.50        | 36 <sup>s</sup><br>4.1 <sup>f</sup>    | no            | -1.9 <sup>s</sup><br>0.1 <sup>f</sup> |
| CsI(Tl)                | 4.51            | 621              | 1.86    | 3.57    | 5.6       | 39.3          | 1220                                  | 550                                  | 1.79        | 165                                    | slight        | 0.4                                   |
| CsI(Na)                | 4.51            | 621              | 1.86    | 3.57    | 5.6       | 39.3          | 690                                   | 420                                  | 1.84        | 88                                     | yes           | 0.4                                   |
| CsI(pure)              | 4.51            | 621              | 1.86    | 3.57    | 5.6       | 39.3          | 30 <sup>s</sup><br>6 <sup>f</sup>     | 310                                  | 1.95        | 3.6 <sup>s</sup><br>1.1 <sup>f</sup>   | slight        | -1.4                                  |
| PbWO <sub>4</sub>      | 8.30            | 1123             | 0.89    | 2.00    | 10.1      | 20.7          | 30 <sup>s</sup><br>10 <sup>f</sup>    | 425 <sup>s</sup><br>420 <sup>f</sup> | 2.20        | 0.3 <sup>s</sup><br>0.077 <sup>f</sup> | no            | -2.5                                  |
| LSO(Ce)                | 7.40            | 2050             | 1.14    | 2.07    | 9.6       | 20.9          | 40                                    | 402                                  | 1.82        | 85                                     | no            | -0.2                                  |
| PbF <sub>2</sub>       | 7.77            | 824              | 0.93    | 2.21    | 9.4       | 21.0          | -                                     | -                                    | -           | Cherenkov                              | no            | -                                     |
| CeF <sub>3</sub>       | 6.16            | 1460             | 1.70    | 2.41    | 8.42      | 23.2          | 30                                    | 340                                  | 1.62        | 7.3                                    | no            | 0                                     |
| LaBr <sub>3</sub> (Ce) | 5.29            | 783              | 1.88    | 2.85    | 6.90      | 30.4          | 20                                    | 356                                  | 1.9         | 180                                    | yes           | 0.2                                   |
| CeBr <sub>3</sub>      | 5.23            | 722              | 1.96    | 2.97    | 6.65      | 31.5          | 17                                    | 371                                  | 1.9         | 165                                    | yes           | -0.1                                  |

\*Numerical values calculated using formulae in this review.

†Refractive index at the wavelength of the emission maximum.

‡Relative light yield measured for samples of 1.5  $X_0$  cube with a Tyvek paper wrapping and a full end face coupled to a photodetector. The quantum efficiencies of the photodetector are taken out.

§Variation of light yield with temperature evaluated at room temperature.

*f* = fast component, *s* = slow component

Figure 3.11: Comparison between different inorganic crystal scintillators (taken from [9])

4. thin aluminum tape is used to light-seal the side of the crystal where the Tyvek does not overlap

in which each CsI crystal is fitted with a 3D-printed plastic frame on both sides

### 3.3.2 Crystal quality control

The quality control process was divided in two parts: a mechanical check and an optical quality control. The mechanical check ensures that the crystal dimensions are within the tolerance. The optical quality control measures the optical properties of the crystal after they are wrapped with a reflective Tyvek layer. The test is performed inside a black box that contains a positron-emitting radioactive source ( $^{22}\text{Na}$ ) and a photomultiplier tube (PMT).

The procedure to measure the optical properties of a crystal is as follow [47]:

1. Install the crystal inside the black box containing a positron-emitting radioactive source ( $^{22}\text{Na}$ ) and a bi-alkali photomultiplier tube

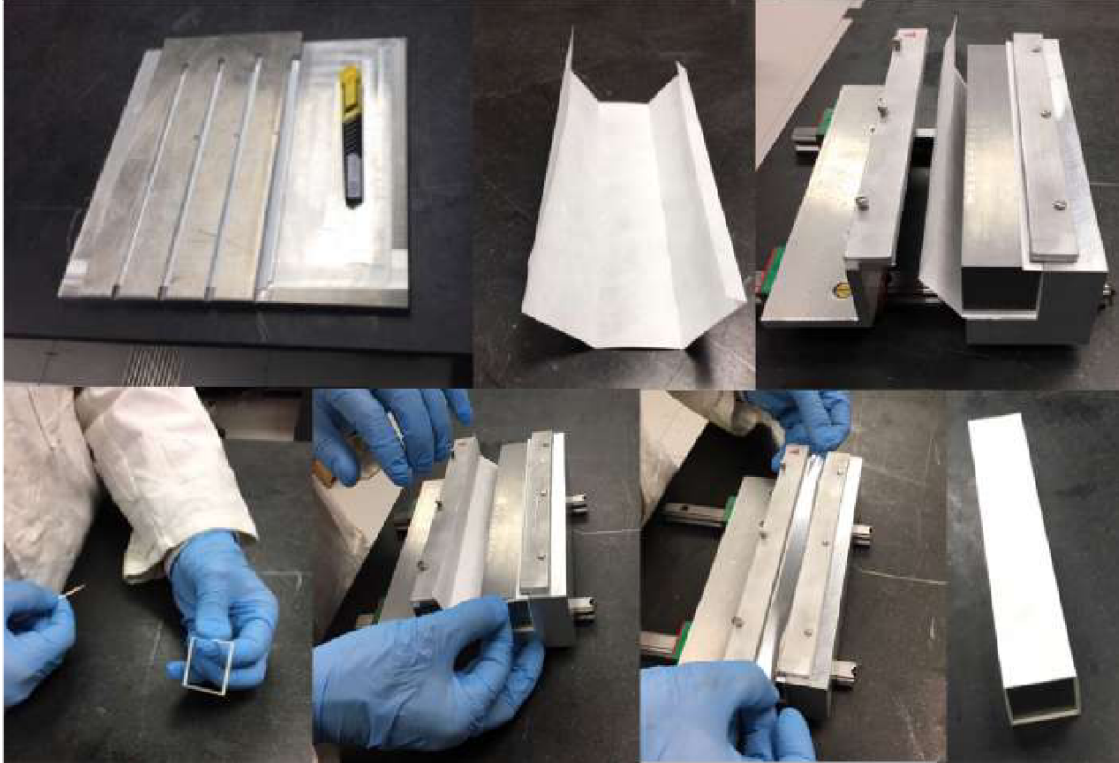


Figure 3.12: Pictures showing the different steps of the crystal wrapping procedure [45]

2. The radioactive source emits positrons that annihilate with electrons to create two back-to-back 511 keV gammas in coincidence
3. We place a collimator and an avalanche photodiode (APD) behind the radioactive source to select the backward-going gamma emitted by the electron-positron annihilation as the seed for the coincidence
4. The forward-going gamma deposits its energy in the crystal, which converts it into light that is captured by the photomultiplier tube
5. We use the time-coincidence between the APD and the PMT measurement to remove the noise
6. This measurement is repeated at multiple positions along the crystal

The PMT measures the energy deposited in the crystal, which should display a peak corresponding to the absorption of the 511 keV photon. This peak is fit with a Gaussian function: its mean is used to derive the light output, and its standard deviation provides the energy resolution.

Several figures of merit are then computed to evaluate the overall quality of the crystal, and the requirement defined by the experiment:

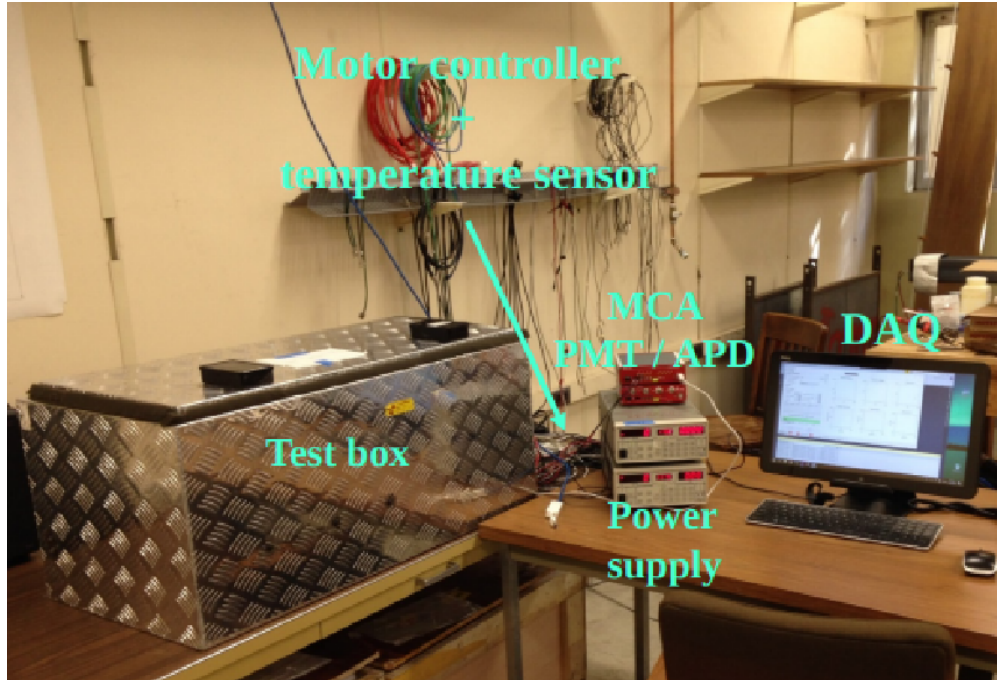


Figure 3.13: Crystal QA station at Caltech [46]

**Energy resolution ( $\text{FWHM} < 45\%$ ):** The resolution of the Gaussian fit function

**Light output ( $> 100$  photoelectrons per MeV with a 200 ns gate):** The number of photoelectrons measured per MeV of energy deposited; we use the knowledge of the peak position being at 511 keV to derive the number of photoelectrons per MeV.

**Light Response Uniformity (LRU) ( $< 5\%$ ):** The rms spread of the measurement along the crystal.

**Fast over Total ( $> 75\%$ ):** The amount of light coming from the fast component (using a 200 ns gate) divided by the total amount of light collected (using a 3000 ns gate).

The plots in Figure 3.15 show the optical properties of all of the crystals tested for the calorimeter.

### 3.3.3 Long-time monitoring

Two crystals have been kept in storage at Caltech to keep track of optical properties changes on a longer time-scale. The study started in 2021 and is still going on. We also studied the impact of partial and full re-wrapping of the crystal in the tyvek paper.

Figure 3.16 presents the evolution of the optical properties of two crystals measured regularly over a long period of time.



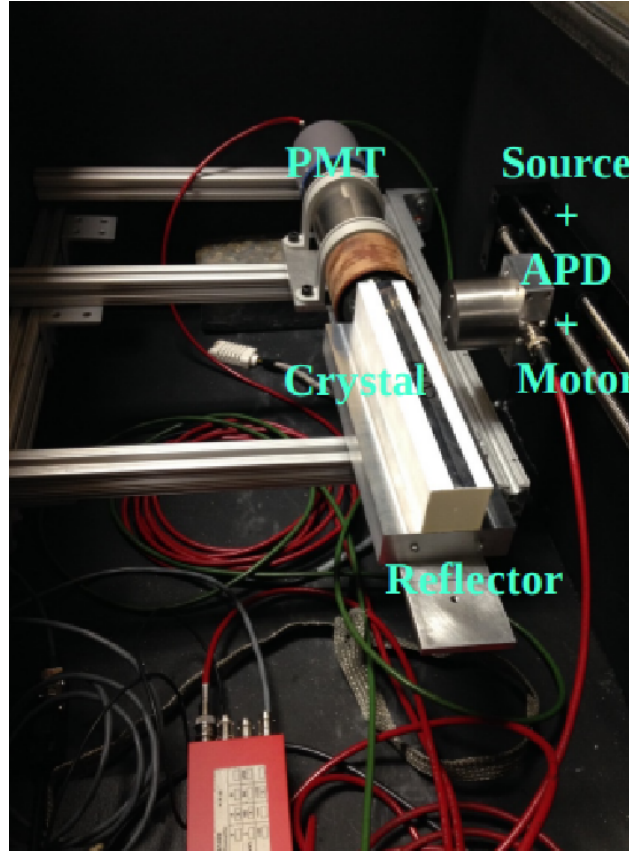


Figure 3.14: Inside the black box of the Crystal QA station at Caltech [46]

We can observe that all of the optical properties of the CsI crystals degrade over time at a different rate. Even though the ratio of fast over total and the light response uniformity have been mostly stable with a small degradation over time, the resolution and the light output have deteriorated at a faster pace.

All the plots display the date when both crystals were fully re-wrapped (February 2020), and when only one of the crystals was partially re-wrapped<sup>5</sup> (December 2022). The re-wraps were performed to test if some of the optical properties of the crystal can be recovered with this simple manipulation. Looking at the light output (Figure 3.16a), the full re-wrapping was able to mostly recover the original light output, but the partial re-wrapping was not effective. The rate of light output reduction is high at the beginning but then stabilizes after 2 years.

### 3.4 DT generator commissioning

The calorimeter energy calibration system requires to irradiate the fluid containing fluorine atoms with a neutron source to obtain the 6.13 MeV gamma rays. The apparatus used is a Deuterium-

<sup>5</sup>a partial re-wrap is preformed by removing the tyvek paper and reusing the same piece to re-wrap the crystal (instead of taking a new one in the case of a full re-wrap)



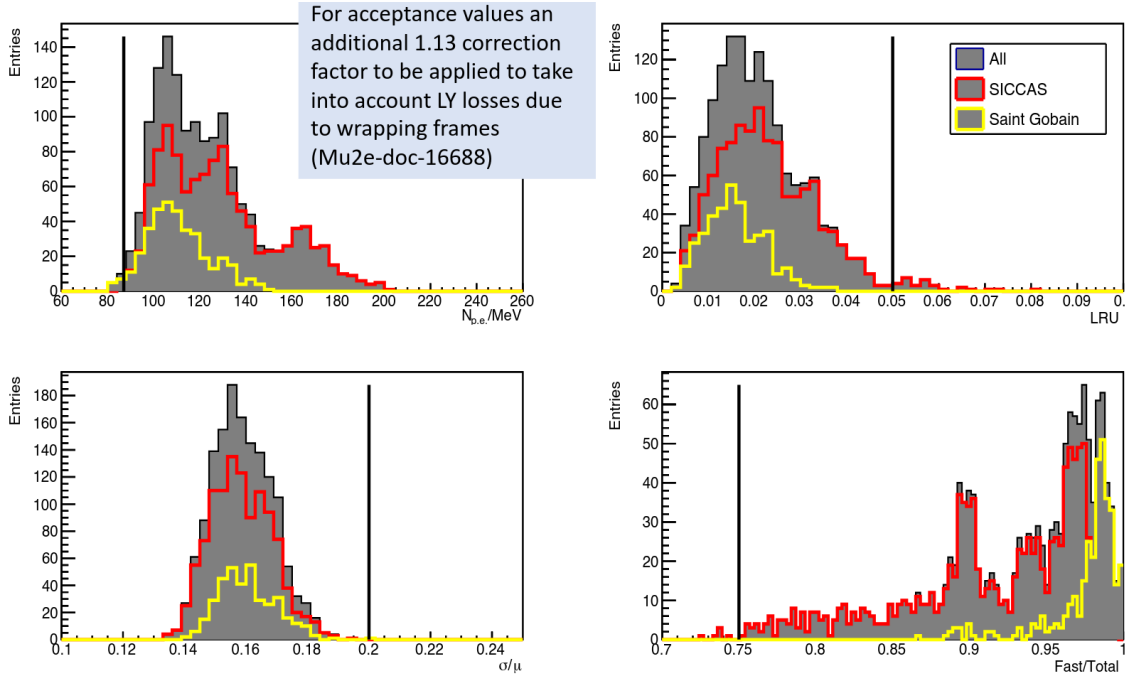


Figure 3.15: Summary of the optical properties of the CsI crystals used in the calorimeter (credit: Simona Giovannella [48])

Tritium (DT) generator manufactured by Starfire Industry<sup>6</sup> in November 2021. It is a compact particle accelerator (see Figure 3.17) that uses an RF ion source to generate a deuterium plasma that is accelerated to 100 keV into a sealed tritium target. The fusion reaction between deuterium and tritium yields 14.1 MeV neutrons at a rate of  $O(10^9)$  neutrons per second.

In November 2022, the DT generator has been commissioned [49] to check the neutron rate and to verify that the shielding used keeps the radiation level within the acceptable range. It is placed at the bottom of a pit that is covered by three layers of radiation shielding: 8 inches of lead, 12 inches of High-Density PolyEthylene (HDPE) and finally a 12-inch thick concrete slab (the ridges in Figure 3.18 indicate the thickness of each shielding layer). The DT generator needs to be run once a month to prevent helium buildup in the tritium target, which would hinder the formation of a stable plasma.

Figure 3.19 shows the operating voltage and current of the DT generator during its commissioning in November 2022. We can observe that the DT generator was not able to produce a stable plasma during the first 10 minutes, leading to multiple trips that are triggered by the software to protect the device when the anode current goes above a certain threshold. Eventually, we were able to run continuously for 35 minutes at an operating voltage of 80 kV (below the nominal operating voltage of 100 kV) to perform the commissioning test.

<sup>6</sup>model nGen 310

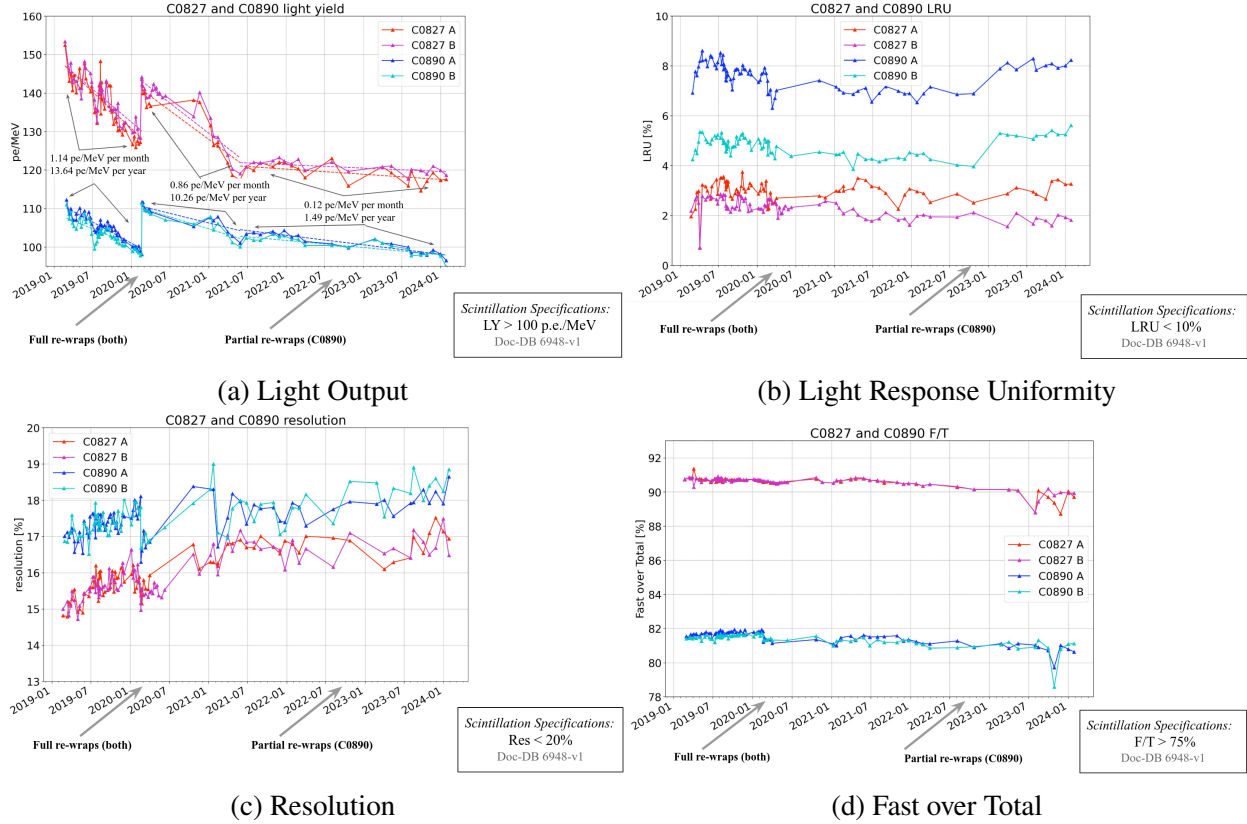


Figure 3.16: Evolution of optical properties of CsI crystals over a long period of time

The commissioning procedure [50] aims to check the neutron generation rate using two different methods, and is conducted while the Fermilab radiation safety team monitors the radiation level measured around the enclosure. The first method is to use a portable neutron counter<sup>7</sup> placed several centimeters from the front of the DT generator. The second method is to irradiate an aluminum foil for more than 20 minutes, and then measure the strength of four different activation photon lines: the  $^{27}_{13}\text{Al}(n, p)^{27}_{12}\text{Mg}$  reaction produces 0.843 MeV and 1.014 MeV gamma rays with a half-life of 9.46 min, and the  $^{27}_{13}\text{Al}(n, \alpha)^{24}_{11}\text{Na}$  reaction produces 1.369 MeV and 2.754 MeV gamma rays with a mean lifetime of 14.96 h [51].

After the aluminum foil is irradiated, it is extracted from the shielded area and sent to the Radionuclide Analysis Factory where a high-purity germanium detector is used to count the number of photons emitted in each line.

The results are shown in Table 3.1 (more details in [49]). The measured rate is consistent within each reaction, but there is a small difference between the two reactions. It should be noted that the calculated rate corresponds to the DT generator running at 80 kV, and using the relative radiation rate measured by the portable neutron at 80 kV and 100 kV, we estimate that the DT generator

<sup>7</sup>HPI model REM500

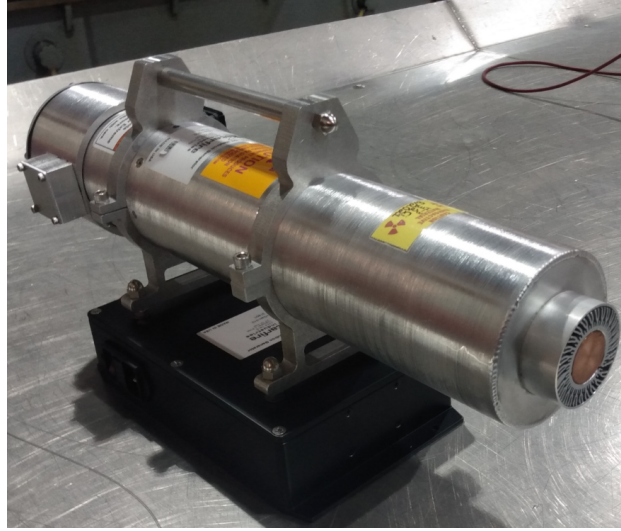


Figure 3.17: Deuterium-Tritium (DT) generator

| Reaction                                            | Mean lifetime [s]  | Photon energy [MeV] | Branching ratio | estimated neutron rate                  |
|-----------------------------------------------------|--------------------|---------------------|-----------------|-----------------------------------------|
| $^{27}_{13}\text{Al}(n, p)^{27}_{12}\text{Mg}$      | 819                | 0.843               | 0.71            | $1.09 \times 10^8 \pm 4.51 \times 10^6$ |
| $^{27}_{13}\text{Al}(n, p)^{27}_{12}\text{Mg}$      | 819                | 1.014               | 0.29            | $1.05 \times 10^8 \pm 4.30 \times 10^6$ |
| $^{27}_{13}\text{Al}(n, \alpha)^{24}_{11}\text{Na}$ | $7.77 \times 10^4$ | 1.369               | 1               | $1.52 \times 10^8 \pm 6.24 \times 10^6$ |
| $^{27}_{13}\text{Al}(n, \alpha)^{24}_{11}\text{Na}$ | $7.77 \times 10^4$ | 2.754               | 1               | $1.50 \times 10^8 \pm 6.26 \times 10^6$ |

Table 3.1: Table summarizing the result of the aluminum foil activation experiment aimed to measure the neutron rate of the DT generator

neutron rate at the nominal operating voltage of 100 kV should be enhanced by a factor 3. This is slightly below the requested rate of  $10^9$  neutrons per second, but it is still sufficient if we increase the time of the calorimeter energy calibration procedure.

### 3.5 Particle identification algorithm (PID)

On the software side, I have been involved in the improvement of the particle identification algorithm called TrkPID. The purpose of this machine learning algorithm is to distinguish between cosmic muons and conversion electrons. As detailed in Section 1.6.3, the trajectory of a high-energy cosmic muon can have the same helix radius as a conversion electron. The main tool that we have to differentiate between the two particles is to look at the shape of the particle shower in the calorimeter, and time difference between the interaction in the tracker and in the calorimeter.

Muons deposit less energy in the calorimeter than electrons because of their high masses which reduces the interactions with photons that generate the electromagnetic shower. In addition, they will travel slower than the electrons so the time difference between their interaction in the tracker and the calorimeter will be higher.



Figure 3.18: DT generator position in a pit, before it is covered with shielding

### 3.5.1 Pre-existing TMVA algorithm

There was already an existing PID algorithm in the Mu2e Offline codebase, built using the ROOT TMVA package. It used a multilayer perceptron architecture with sigmoid activation functions (see the architecture in Figure 3.20).

It had very good performance, with a signal efficiency (the fraction of conversion electrons correctly labeled) of 98.5 % and an Area Under the Receiver Operating Characteristic (ROC) Curve (AUC) of 0.999.

### 3.5.2 New python algorithm

There was a push within the Mu2e collaboration to transition machine learning algorithms from ROOT TMVA to a more modern python tensorflow. The TMVA SOFIE (System for Optimized Fast Inference code Emit) tool enables to convert a tensorflow model into an optimized C++ code (as Mu2e Offline code is mostly in C++).

The new algorithm uses a similar architecture (multilayer perceptron but using ReLU activation function), but the number of inputs has been reduced from 5 to 4, and the number of neurons has increased from 10 to 16.

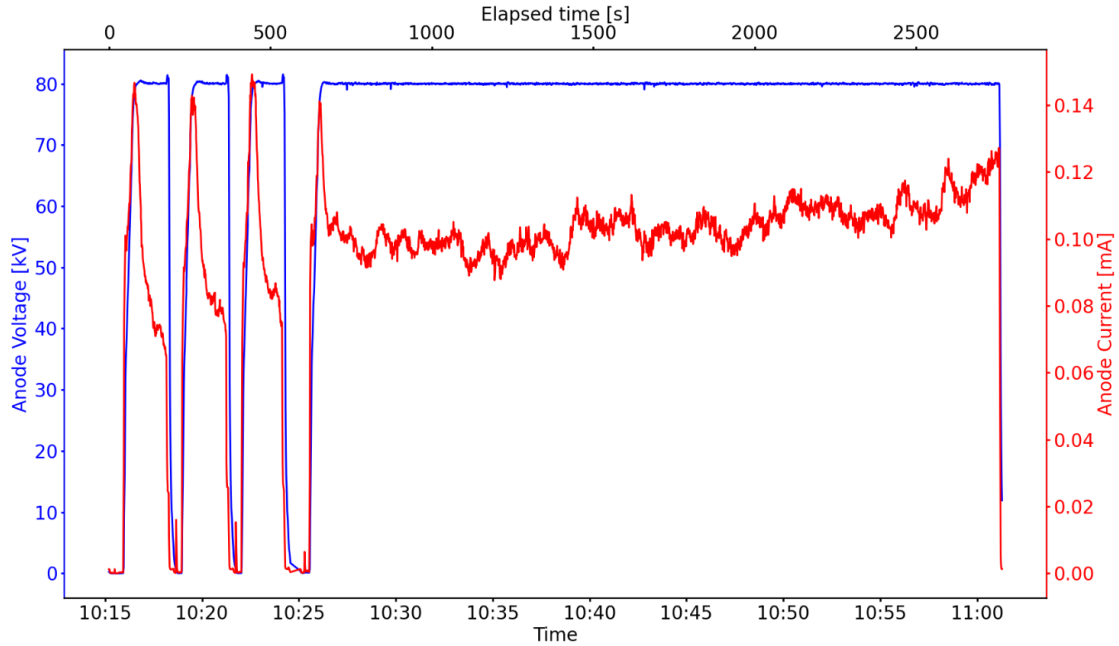


Figure 3.19: Plot of the anode voltage (blue) and anode current (red) of the DT generator during the commissioning test

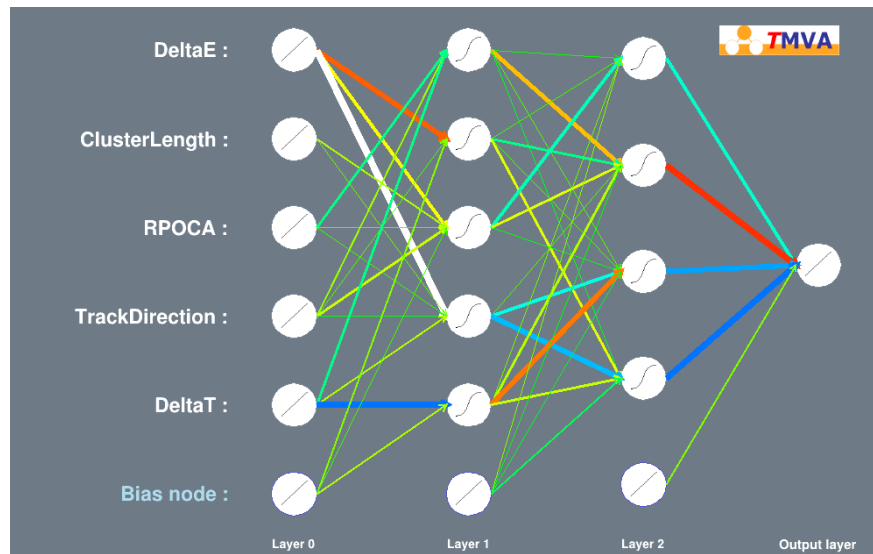


Figure 3.20: Architecture of the pre-existing TrkPID machine learning algorithm

The four training features are:

**DeltaE:** The energy difference between the calorimeter cluster energy and the reconstructed tracker momentum

**RPOCA:** Radius of the Point Of Closest Approach

**TrkDir:** Transverse component of the trajectory

**DeltaT:** Time difference between the tracker hit and the calorimeter cluster

They are shown on Figure 3.21. We can see that DeltaE and DeltaT are the two training features with the biggest discrimination power, as the overlap between the muon and the electron distribution is the least.

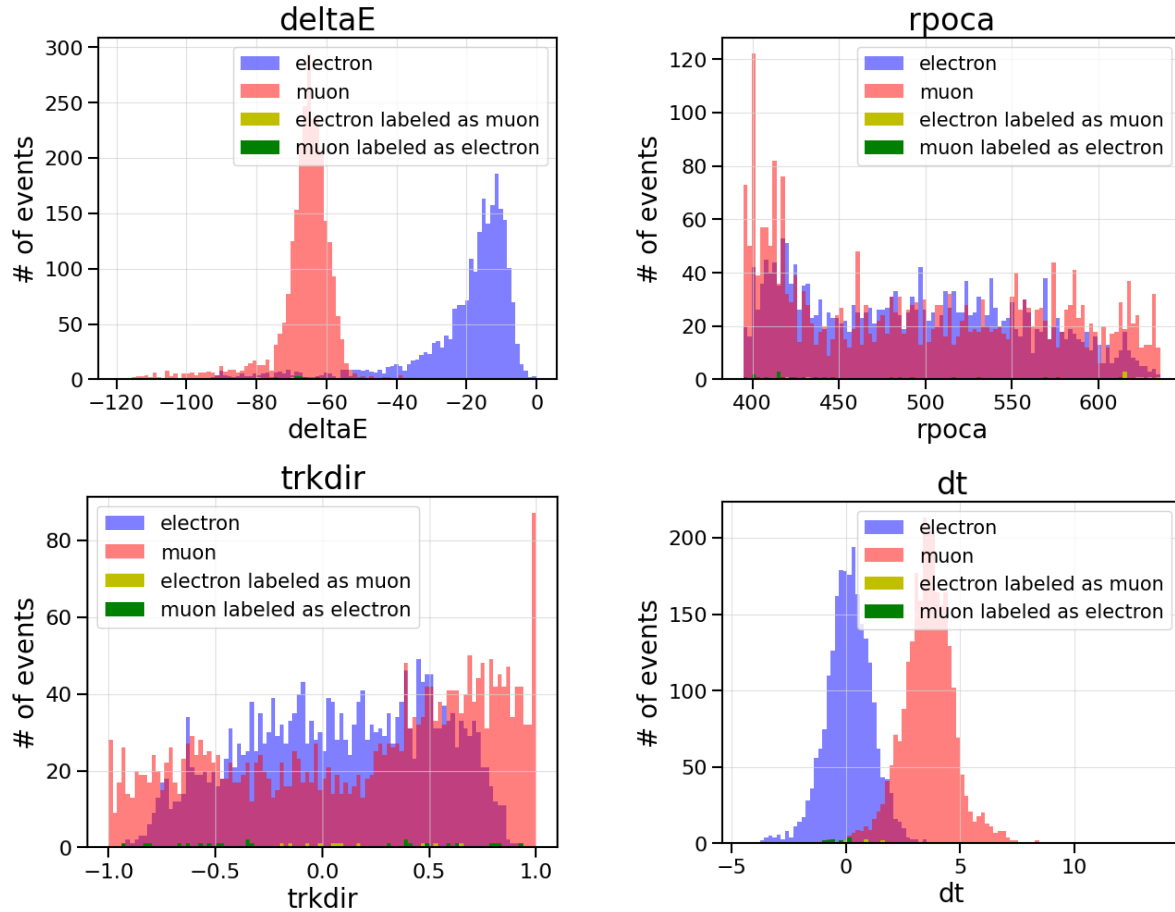


Figure 3.21: Distributions of the four training features of the PID algorithm

### 3.5.3 Performance

The performance of the new algorithm is slightly better, with a signal efficiency of 98.8 % and an AUC of 0.999. We obtain a true positive rate (correctly labeled electrons) of 99.3 %, a true negative rate (correctly labeled muons) of 99.0 %. Figure 3.22 shows the output of the PID algorithm

Figure 3.23 displays the signal efficiency, background rejection, and significance as a function of the threshold value (the value of the model output that separates muons and electrons). This enables us to choose the threshold value of 0.67 that maximizes the significance  $S = \frac{Signal}{\sqrt{Signal+Background}}$ .



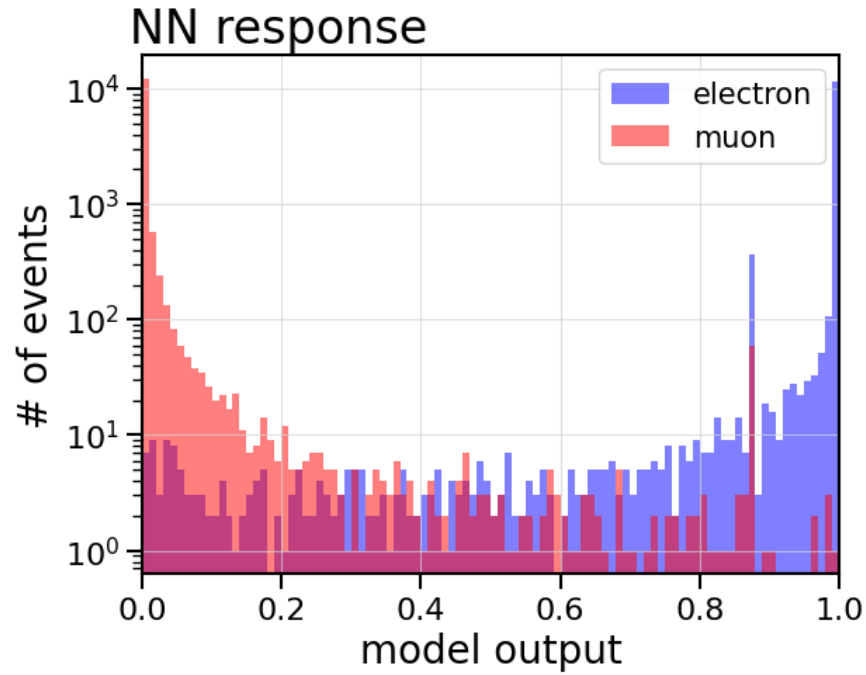


Figure 3.22: Output of the particle identification algorithm

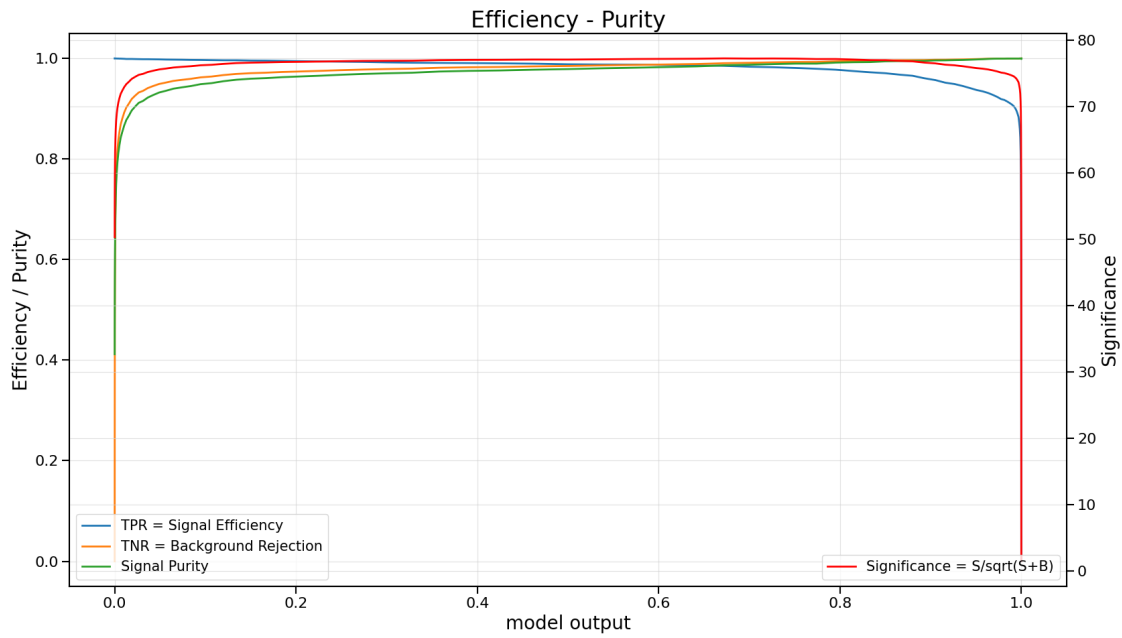


Figure 3.23: Efficiency, purity, and significance of the PID algorithm as a function of the threshold

## *Chapter 4*

### ANALYSIS DEVELOPMENT

The goal of this chapter is to present the methodology and the structure of the software developed to perform the analysis of the Mu2e experimental data. The Mu2e collaboration was originally planning to display their result using a cut-and-count method, however a subset of the collaboration has been wanting to develop a different analysis technique using Maximum Likelihood Estimation (MLE) and provide both a frequentist and a Bayesian. The work presented in this chapter has been performed by the Caltech-LBNL-Northwestern analysis group. It is based on an early version that I developed, which then has been expanded and improved by multiple collaborators. Thus, most of the results and plots displayed in this chapter have not been made by me, as I wanted to showcase the newest version of the analysis instead of an older and more simplistic one.

#### **4.1 Maximum Likelihood Estimation method**

The Maximum Likelihood Estimation (MLE) method is a fitting tool that finds the best value for some parameters to obtain the best fit to the observed data. It is based on maximizing the likelihood function, which corresponds to the observed data having the highest probability of being generated by this function. This method requires a Probability Distribution Function (PDF) with some of its parameters being changed to best fit the data.

In our case, we are trying to fit both the momentum and time distribution of the experimental data, and our choice of PDF need to sum all of our backgrounds and our muon conversion signal. Our floating parameters used to fit to the experimental data are the numbers of events that belong to each background.

One of the main drawbacks of this method is that we need to already know (or guess) the shape of all the PDFs. For known Standard Model backgrounds with theory and previous experimental data available, this is not too complicated, but this can be an issue with Beyond the Standard Model signals. It is possible to add more floating parameters related to the shape of the PDF to account for uncertainties, however the more parameters need to be fitted, the longer it takes, and it can make the fit underconstrained.

## 4.2 Analysis methodology

### 4.2.1 Goal

The goal of this software is to interpret the raw data coming from the Mu2e experiment to produce a single figure of merit: the observed rate of neutrinoless muon conversion.

$$R_{\mu e} = \frac{\Gamma(\mu^- + \text{Al} \rightarrow e^- + \text{Al})}{\Gamma(\mu^- + \text{Al} \rightarrow \nu_\mu + \text{Mg})} \quad (4.1)$$

where  $\Gamma(\mu^- + \text{Al} \rightarrow e^- + \text{Al})$  is the rate of neutrinoless muon conversion to electron and  $\Gamma(\mu^- + \text{Al} \rightarrow \nu_\mu + \text{Mg})$  is the rate of muon capture in the aluminum target. This study is focusing on the numerator term, as another analysis group within the Mu2e collaboration is tasked to provide the denominator term based on experimental measurement.

### 4.2.2 Starting point

The starting point of the analysis is the measurements coming from the tracker and electromagnetic calorimeter. The tracker provides a measurement of the momentum of the charged particles going through it, while the electromagnetic calorimeter collects the energy deposited of particles through the electromagnetic force. Information from both detectors is used to provide the best estimation of the momentum of electrons coming from the stopping target with an energy around 105 MeV.

### 4.2.3 Reconstruction algorithms

The goal of the reconstruction sequence is to use the raw measurements coming from the calorimeter and tracker to estimate the properties of the charged particles that went through the detectors. The energy of the particle can be determined by adding up the energy deposited in the calorimeter crystals, while the tracker can reconstruct the trajectory that the charged particle followed.

Charged particles in a uniform magnetic field exhibit a helical trajectory where the radius of the helix is proportional to its momentum through this kinematic equation:

$$qvB = \frac{\gamma m v^2}{r} \quad (4.2)$$

$$r = \frac{\gamma m v}{qB} \quad (4.3)$$

where  $qvB$  is the magnetic force of a relativistic particle with charge  $q$ , Lorentz factor  $\gamma$ , velocity  $v$  in a magnetic field of strength  $B$ ; and  $\frac{\gamma m v^2}{r}$  is the centripetal force at helix radius  $r$  of a particle of mass  $m$ .

We use a sequence of reconstruction algorithms to:

- clean up the data by removing noise hits in the tracker and calorimeter
- organize tracker hits into groups that correspond to the path of an individual particle
- organize collections of energy deposited in the calorimeter into clusters that correspond to a single particle

We use a Kalman filter algorithm [52] to extract the kinematic properties of the particles based on their tracker hits and associated calorimeter clusters.

- The calorimeter cluster time is used as a seed to find a group of tracker hits that are time-compatible with the cluster
- An initial fit is performed using only these hits to calculate the geometric parameters of the helical trajectory
- After the initial fit has converged, we can use it to find additional tracker hits and calorimeter clusters that were missed; they are added only if they reduce the uncertainty of the fit

At this stage, every event<sup>1</sup> contains a list of tracks that each represent the trajectory of a charged particle.

Then, we use a machine learning algorithm that determines the quality of the track based on the number of tracker hits that are used in the fit, the fit uncertainty, and other parameters.

### 4.3 Analysis software structure

The Mu2e analysis software developed by the Caltech-LBNL-Northwestern analysis group is based on previous work that I built with the purpose to provide preliminary analysis capabilities and to test the different tools that we use. The software package is built in python and uses the zfit package [53] to perform a maximum likelihood estimation. The choice of using zfit in a python environment (instead of RooFit in the ROOT environment) was taken as python is using more cutting-edges tools created by a larger community . The structure of the code is schematized in Figure 4.1.

On one hand, we have a module that imports the data from a ROOT file and convert it into a format that python can read. At the same time, we apply a standard set of cuts on the data to remove unwanted events (see Section 4.4).

On the other hand, we define the expected partial distribution functions (PDFs) of the signal and the backgrounds for the two components that we are interested in (momentum and time distributions). The source of each PDF is detailed in Section 4.5.

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<sup>1</sup>a Mu2e event is defined by the 1695 ns time window between each beam pulse

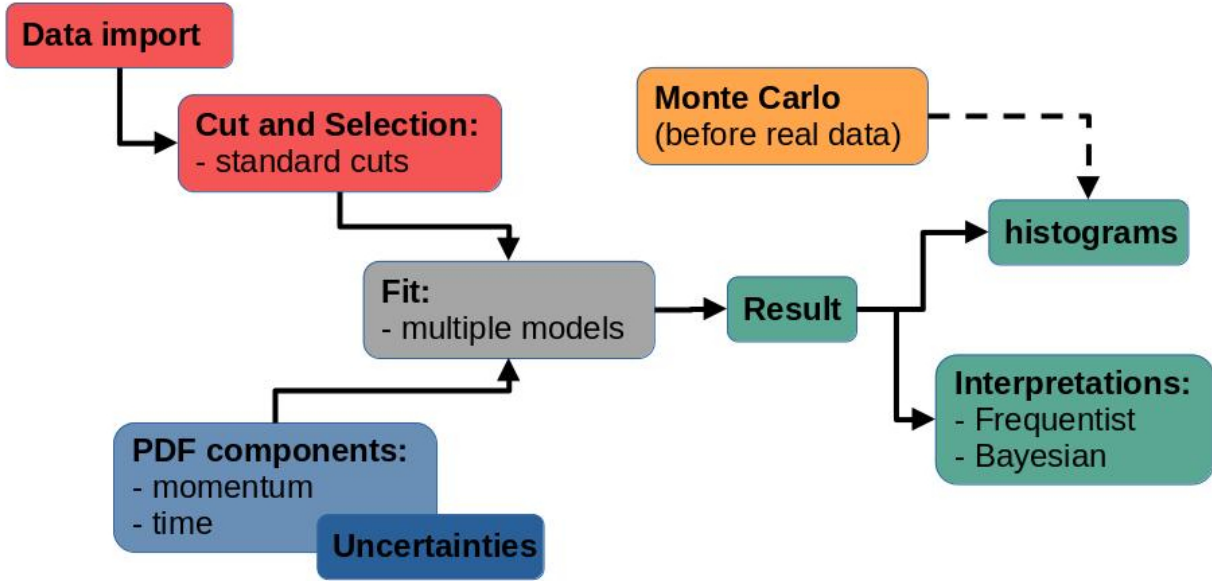


Figure 4.1: Workflow of the Mu2e analysis software

The main part of the code defines the likelihood function and minimizes its logarithm by changing a limited number of floating parameters to best fit the simulation data. The result is the value of these floating parameters that are mostly the number of particles that belong to each background.

We can then interpret the result by quoting significance and limits using a frequentist or a Bayesian approach.

#### 4.4 Dataset selection and cuts

Until Mu2e can produce its own experimental data, we use the Mu2e Offline code to generate simulation data that mimic real data. Multiple simulation campaigns have produced different datasets over the years focused on specific physics studies, such as a singular background. The one that we use, called MDS (Mock Data Sample) aims to provide a realistic simulation of the physics data coming out of the detectors for a mix of all the backgrounds with an added possible signal. Even though it doesn't provide very high statistics for each background as they are mixed in the dataset using their expected rate, it still produces an estimation of the actual data coming from the experiment over an entire month of running. In the rest of this chapter, all the results displayed are based on the MDS2c dataset

This list of cuts is not definitive and will be updated as the experiment get closer to getting experimental data. An example list of cuts with explanation is given in Table 4.1.

The number of events getting rejected by each cut can be seen in Table 4.2.

<sup>1</sup>sid (surface ID) is a number assigned to each surface in the Mu2e simulation

| Constraint on variable                                           | Description                                                                                 |
|------------------------------------------------------------------|---------------------------------------------------------------------------------------------|
| $\text{trk.pdg} = 11$                                            | Track fit use the assumption that the particle is an electron                               |
| $\text{mom.fCoordinates.fZ} > 0$                                 | Downstream track segment                                                                    |
| $\text{trkfit.sid}^1 = 0$                                        | Track intersect the entrance of the tracker                                                 |
| $\text{trkqual.result} > 0.2$                                    | Result of the TrackQual algorithm: track has a good quality                                 |
| $\text{trkpid.result} > 0.6$                                     | Result of the TrackPID algorithm: event is not a cosmic muon                                |
| $\text{trk.nactive} \geq 20$                                     | Minimum number of active hit in the tracker                                                 |
| $\text{trksegspars\_lh.t0err} < 0.9$                             | Uncertainty on t0 is small enough                                                           |
| $ \text{trksegs\_time} - \text{crvcoins.time}  > 150 \text{ ns}$ | Event time is not close to a cosmic ray event vetoed by the CRV                             |
| $\text{trkfit.sid}^1 = 102$                                      | Track upstream extrapolation intersects the stopping target                                 |
| $\text{trkfit.sid}^1 \neq 95$                                    | Track upstream extrapolation does not intersect the Outer Proton Absorber (OPA)             |
| $475 \text{ ns} < \text{trksegs.time} < 1650 \text{ ns}$         | Time at which the track intersect the tracker entrance is within the experiment time window |
| $95 \text{ MeV} < \text{trksegs.mom.mag} < 115 \text{ MeV}$      | Particle momentum within the momentum window                                                |

Table 4.1: List of cuts and selections applied to the dataset

| Cut             | Fraction of background events passing the cut [%] | Fraction of signal events passing the cut [%] |
|-----------------|---------------------------------------------------|-----------------------------------------------|
| electron        | 95.54                                             | 99.54                                         |
| downstream      | 66.75                                             | 99.53                                         |
| trkqual         | 55.42                                             | 87.03                                         |
| active hit      | 98.81                                             | 98.95                                         |
| t0 error        | 87.96                                             | 96.57                                         |
| stopping target | 38.73                                             | 95.06                                         |
| no OPA          | 89.01                                             | 99.99                                         |
| CRV             | 64.56                                             | 85.12                                         |
| Total           | 6.83                                              | 66.36                                         |

Table 4.2: Number of events passing each cut ; the second [resp. third] column shows the fraction of background [resp. signal, i.e conversion electrons] events in the entire dataset that pass each cut independently



The takeaway from this table is that most of the cuts have a very low impact on the conversion electron signal, the two largest one being trkqual and CRV. The cut on the track quality removes tracks that are not well reconstructed by the reconstruction algorithms, and this can be lessened with improvements of the algorithm. The cut from the cosmic ray veto has not been optimized yet so improvement is expected in the coming years, however the cosmic ray flux is irreducible. This set of cuts is still quite effective at removing more than 90 % of background events while cutting back around one third of conversion electron events.

Figure 4.2 [resp. Figure 4.3] shows the momentum and time distribution of background and signal events without [resp. with] cuts applied. Both plots use the MDS2c dataset that contains the equivalent of one month of beam time with one booster batch<sup>2</sup> and a muon conversion rate  $R_{\mu e} = 1 \times 10^{-13}$ . The efficiency of the cosmic ray veto cut is clearly visible on both plots, and the muon conversion signal is more visible in the momentum plot after cuts.

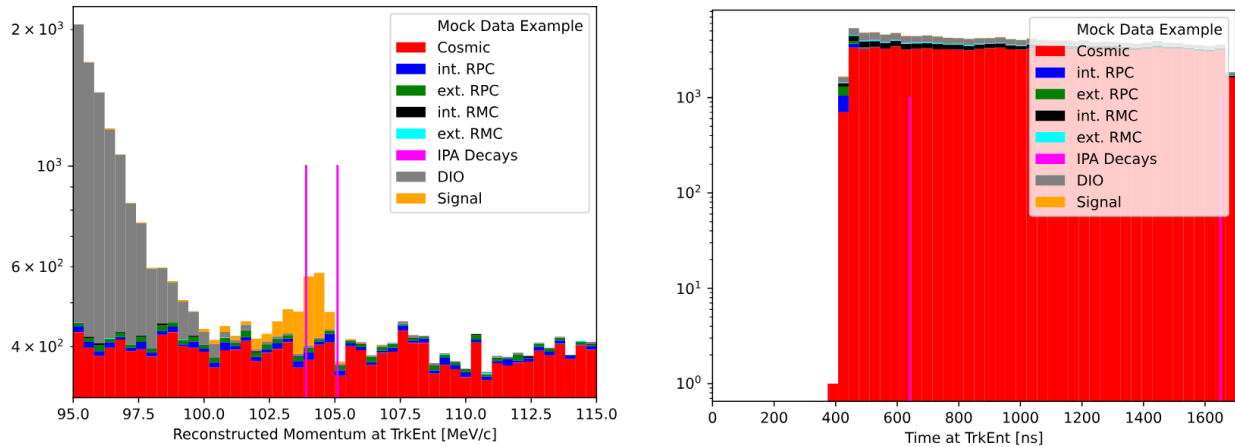


Figure 4.2: Momentum (left) and time (right) distribution of background and signal events before any cut is applied. Credit: S. Middleton [54]

#### 4.5 Definition of the Probability Distribution Functions (PDFs)

Before the experiment measures any of the backgrounds, we need to rely on Monte Carlo simulations, theoretical calculations, and previous experimental measurements to define the partial distribution functions (PDFs) of the signal and the backgrounds. Table 4.3 [resp. Table 4.4] summarizes the shape of the momentum component [resp. time component] of the PDFs that is assumed and the reasoning for the choice. Some of the backgrounds of the experiment are not listed in the table because they are either too small (beam-related backgrounds such as beam electrons and decay-in-flight [22]) or because they cannot be distinguished from conversion electrons at

<sup>2</sup>In Section 2.3 describing the Fermilab accelerator, the booster can transfer one or two proton batches to the recycler ring

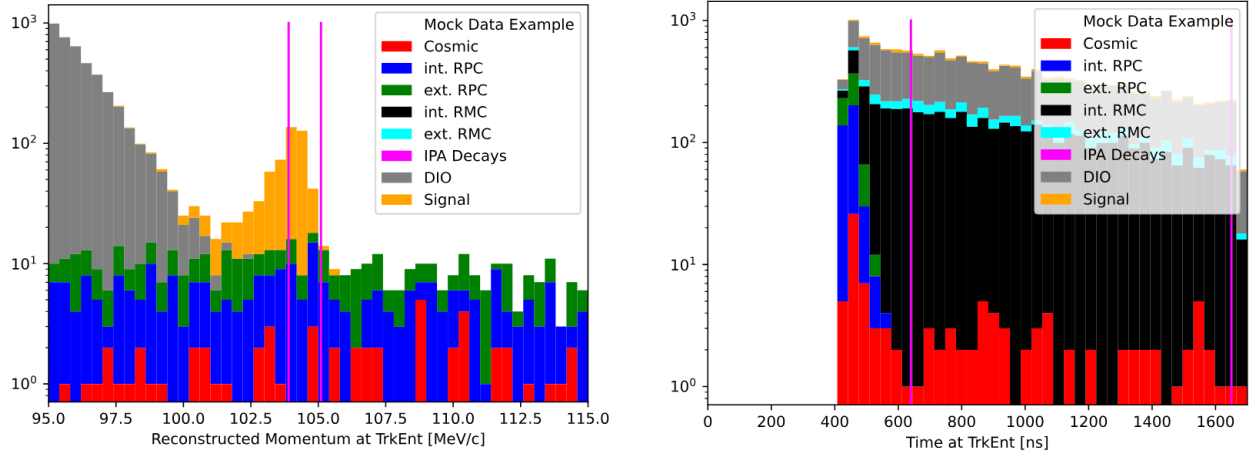


Figure 4.3: Momentum (left) and time (right) distribution of background and signal events after cuts. Credit: S. Middleton

| Background                   | Momentum PDF              | Source type                            | Source   |
|------------------------------|---------------------------|----------------------------------------|----------|
| Conversion electrons         | Dirac peak                | Theory                                 | [55, 56] |
| Decay-In-Orbit (DIO)         | Czarnecki spectrum        | Theory                                 | [20, 57] |
| Cosmic Rays                  | Chebyshev polynomial fit  | Simulation                             | [54]     |
| Radiative Pion Capture (RPC) | Bistirlich spectrum       | Experimental (Mg target instead of Al) | [21]     |
| Momentum resolution          | Double-sided Crystal Ball | Simulation                             | [54]     |
| Detector efficiency          | Chebyshev polynomial fit  | Simulation                             | [54]     |
| Energy loss                  | Landau distribution       | Simulation                             | [54]     |

Table 4.3: Definition of the momentum component of probability distribution functions used for the signal and backgrounds of the Mu2e analysis

the analysis stages so they are removed using hardware (anti-proton window in the middle of the transport solenoid, out-of-time backgrounds attenuated by the beam extinction). A more detailed explanation of each background is available in Section 1.6. Similarly to the list of dataset cuts, this list is not definitive and might change.

The momentum distribution of the cosmic-induced electrons (Figure 4.4 is provided by a simulation using the CORSIKA<sup>3</sup> (COsmic Ray Simulations for KAscade) generator coupled to the Mu2e geometry.

After going through the entire experiment, the spectrum of RPC electrons interacting with the tracker is plotted for both internal and external RPC in Figure 4.5. We can observe a difference in the rate of positrons versus the rate of electrons (even though the shape of their spectrum is basically identical). This comes from real high-energy photons producing additional electrons

<sup>3</sup>CORSIKA website

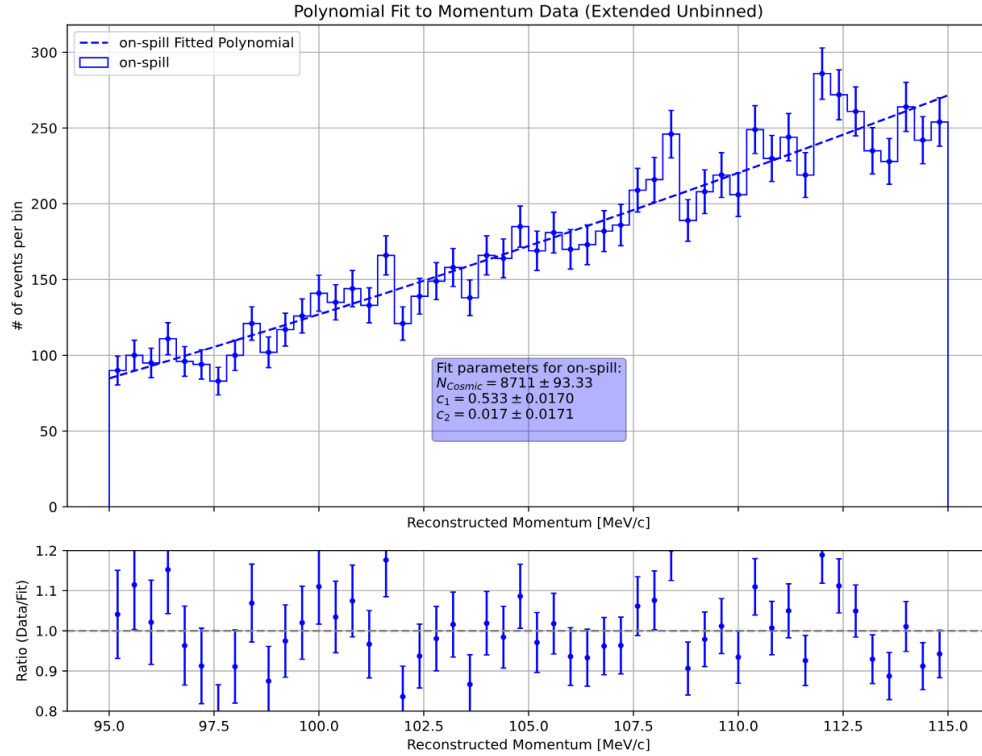


Figure 4.4: Momentum distribution of electrons produced by cosmic ray muons. Credit: S. Middleton [54]

through Compton scattering in the case of external RPC. This effect does not happen in the internal RPC case as the photon is virtual.

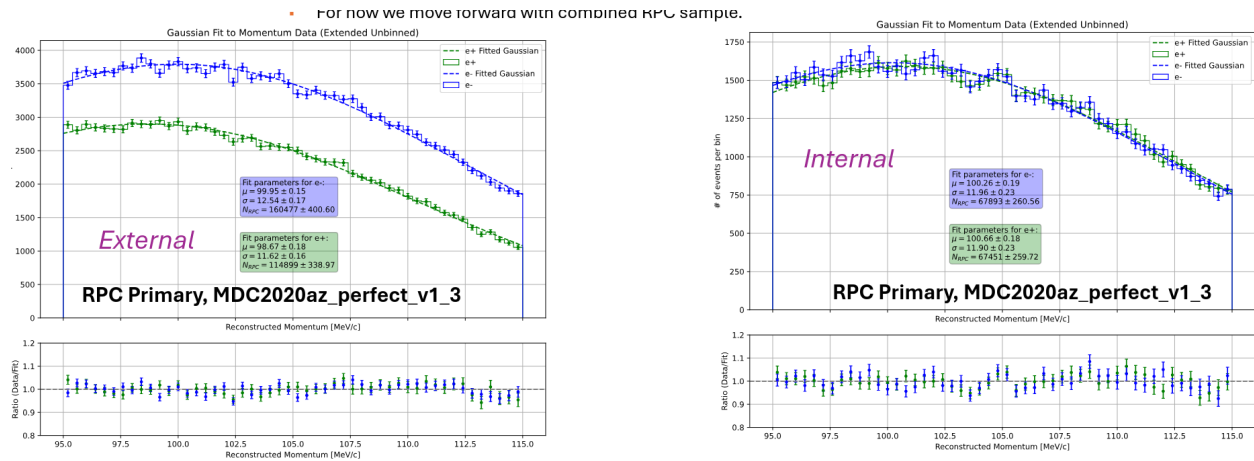


Figure 4.5: Momentum spectrum of electrons and positrons generated by external (left) and internal (right) radiative pion capture, as they would be measured by the tracker

These distributions do not include detector effects unique to Mu2e. Thus, every momentum component needs to be convoluted with the detector efficiency, the momentum resolution, and the

energy loss. Each one of these effects are studied independently using simulations of electrons with a uniform momentum distribution.

The detector efficiency study looks at how many electrons produced in the stopping target reach the entrance of the tracker, as a function of their momentum. The resulting distribution (Figure 4.6) is due to the annular shape of the tracker that makes it efficient only for electrons in a limited momentum range between 80 and 115 MeV.

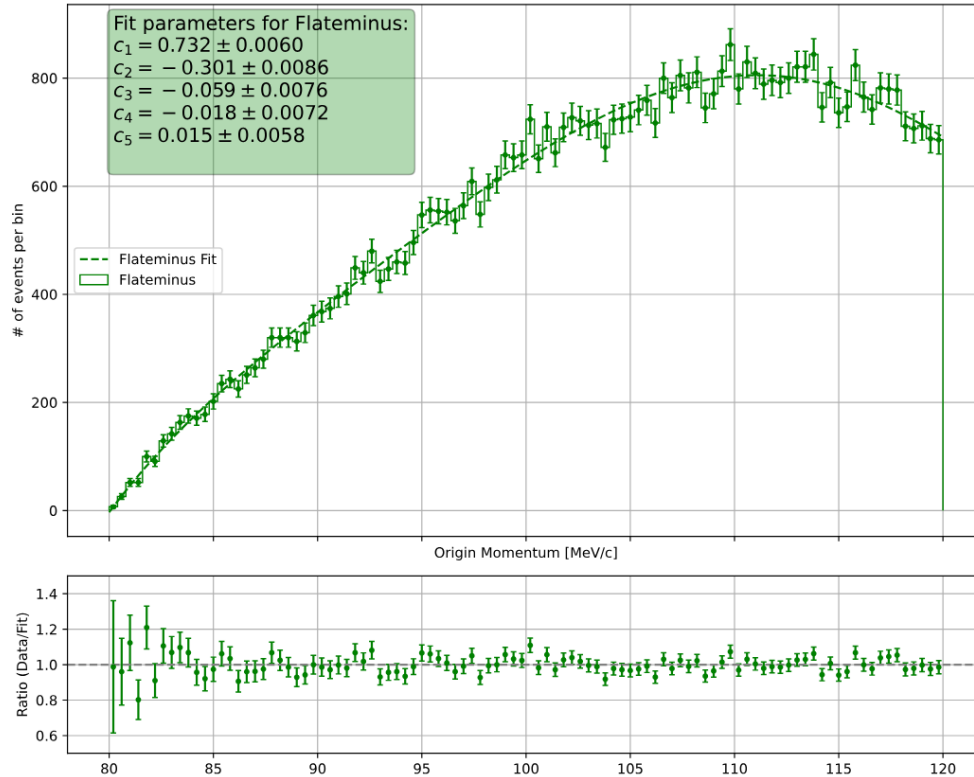


Figure 4.6: Efficiency of the detector as a function of the electron momentum. Credit: S. Middleton [54]

The momentum resolution (Figure 4.7) exhibits the difference between the momentum of the reconstructed track and its true value. The distribution used to fit the simulation data is a double-sided Crystal Ball distribution with  $\sigma = 0.136$  MeV, smaller than the 180 keV resolution requirement for the tracker.

Finally, the energy loss is due to the electron interacting with material mostly in the stopping target and in the tracker. The plot in Figure 4.8 displays the difference of momentum between electron generated in the stopping target and when they reach the middle of the tracker.

<sup>1</sup> $\tau_\mu = 864$  ns is the lifetime of a muon orbiting an aluminum nucleus

<sup>2</sup> $\tau_\pi = 26$  ns is the lifetime of a charged pion

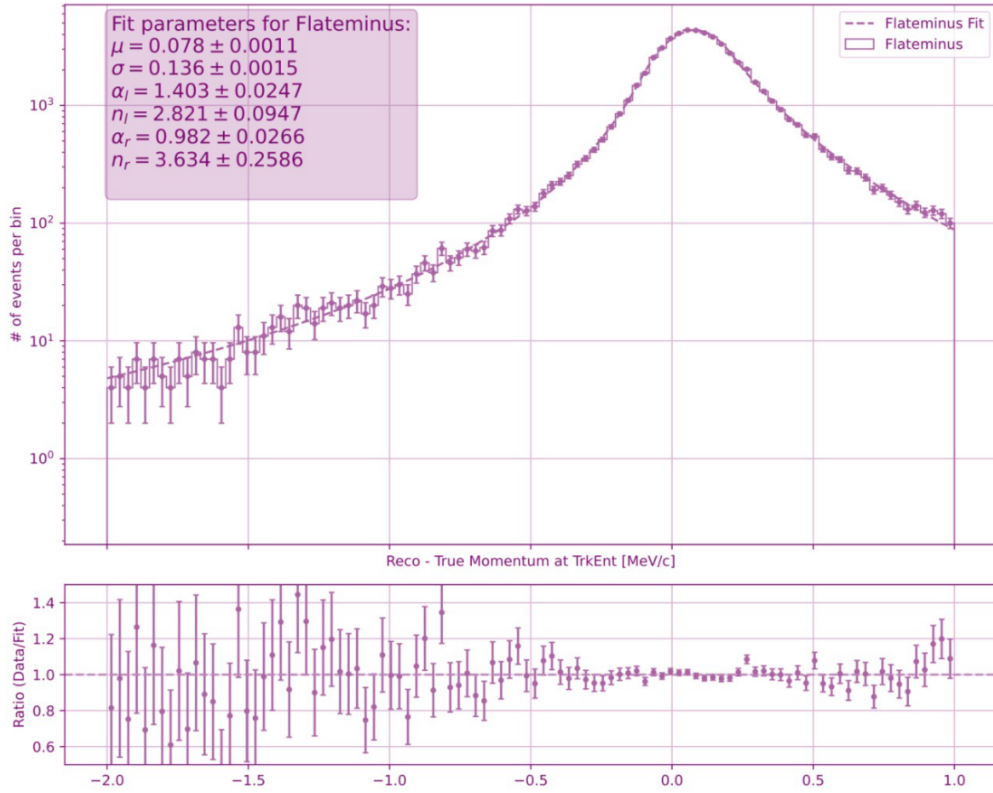


Figure 4.7: Momentum resolution of the detector as a function of the electron momentum. Credit: S. Middleton [54]

| Background                   | Time PDF                       | Source type  | Source |
|------------------------------|--------------------------------|--------------|--------|
| Conversion electrons         | Exponential decay $\tau_\mu^1$ | Experimental | [9]    |
| Decay-In-Orbit (DIO)         | Exponential decay $\tau_\mu^1$ | Experimental | [9]    |
| Cosmic Rays                  | Uniform                        | Theory       |        |
| Radiative Pion Capture (RPC) | Exponential decay $\tau_\pi^2$ | Experimental | [9]    |

Table 4.4: Definition of the time component of probability distribution functions used for the signal and backgrounds of the Mu2e analysis

## 4.6 Preliminary results

### 4.6.1 Example of cut and count

Before performing the maximum likelihood fit, we can already perform a simple cut and count analysis. We use the momentum window  $103.6 < p < 104.9 \text{ MeV}$  and the time window  $640 < t_0 < 1650 \text{ ns}$  optimized for the Mu2e sensitivity update of 2020 [22], and represented in Figure 4.2 and Figure 4.3 by the vertical pink lines.

Figure 4.9 is a 2D histogram of the momentum and time distributions of background (red) and signal (blue) events around the momentum and time window of interest. We observe that the cut and count analysis method does not produce any false positive (background event passing all the cuts),

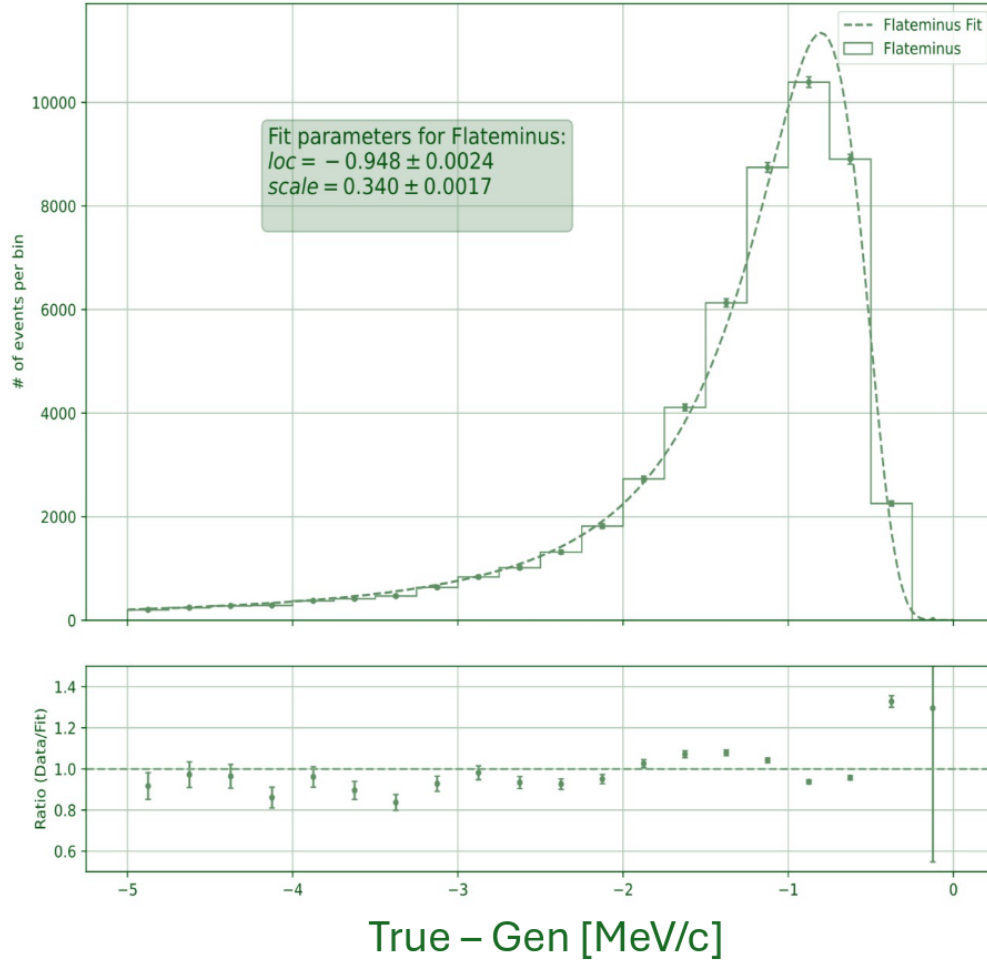


Figure 4.8: Energy loss of electrons measured at the middle of the tracker. Credit: S. Middleton [54]

but it misses a significant number of conversion electrons. This is one of the main advantages of a maximum likelihood analysis, as it uses additional information from the shape of the distributions to better categorize background and signal events.

#### 4.6.2 Maximum likelihood result

The simplest maximum likelihood fit to perform is when all of the backgrounds and signal PDFs parameters are fully constrained, and the only floating parameters are the number of particles belonging to each background. An example of this fit is displayed in Figure 4.10, where the left [resp. right] plot shows the momentum [resp. time] distribution fit for the MDS2c dataset that contains the equivalent of one month of beam time with one booster batch and a muon conversion rate  $R_{\mu e} = 1 \times 10^{-13}$ . The resulting number of conversion electrons calculated from the fit is 422, which is a bit underestimating the true number of 436.

Figure 4.11 shows a similar plot but with a smaller signal at  $R_{\mu e} = 1 \times 10^{-14}$ . In this case, the



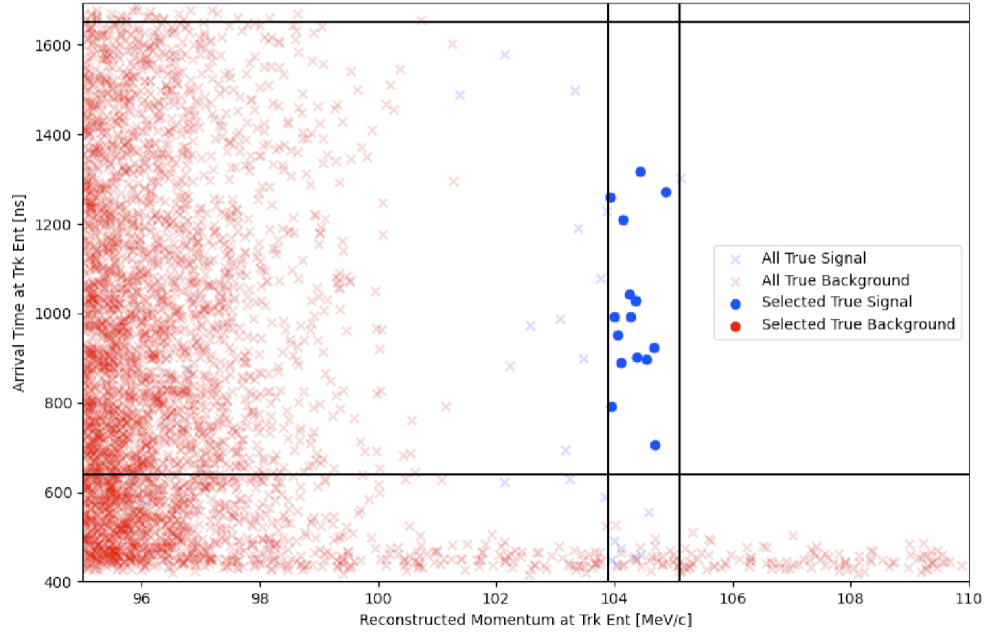


Figure 4.9: 2D histogram of momentum (x-axis) and time (y-axis) distributions of background and signal events. Credit: S. Middleton [54]

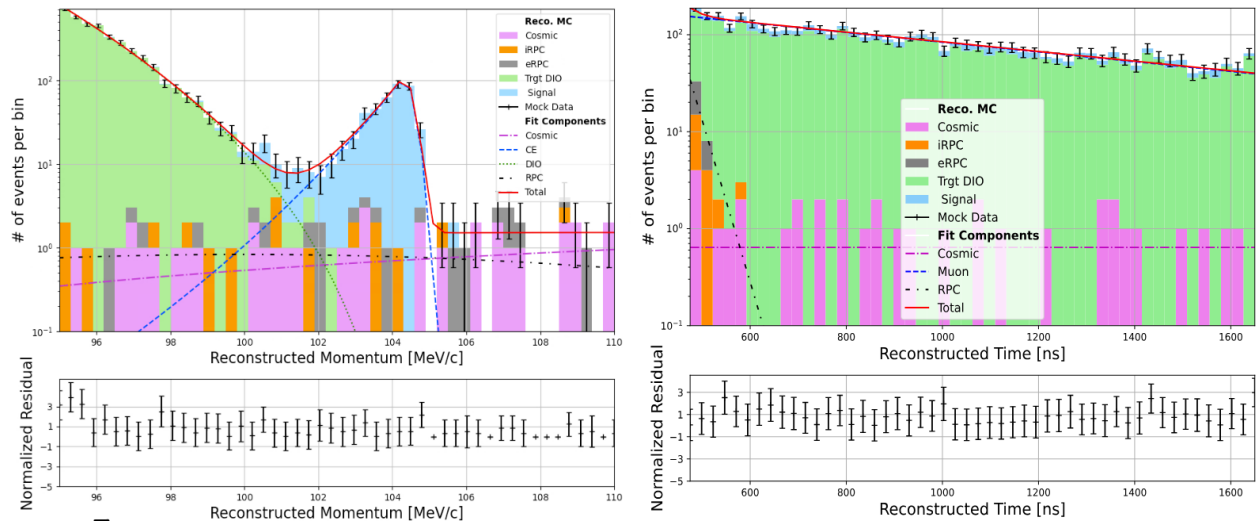


Figure 4.10: Maximum likelihood fit of the MDS2c dataset with  $R_{\mu e} = 1 \times 10^{-13}$ . Credit: S. Middleton [54]

number of conversion electrons calculated from the fit is 39, which is the exact same number as the Monte Carlo truth.

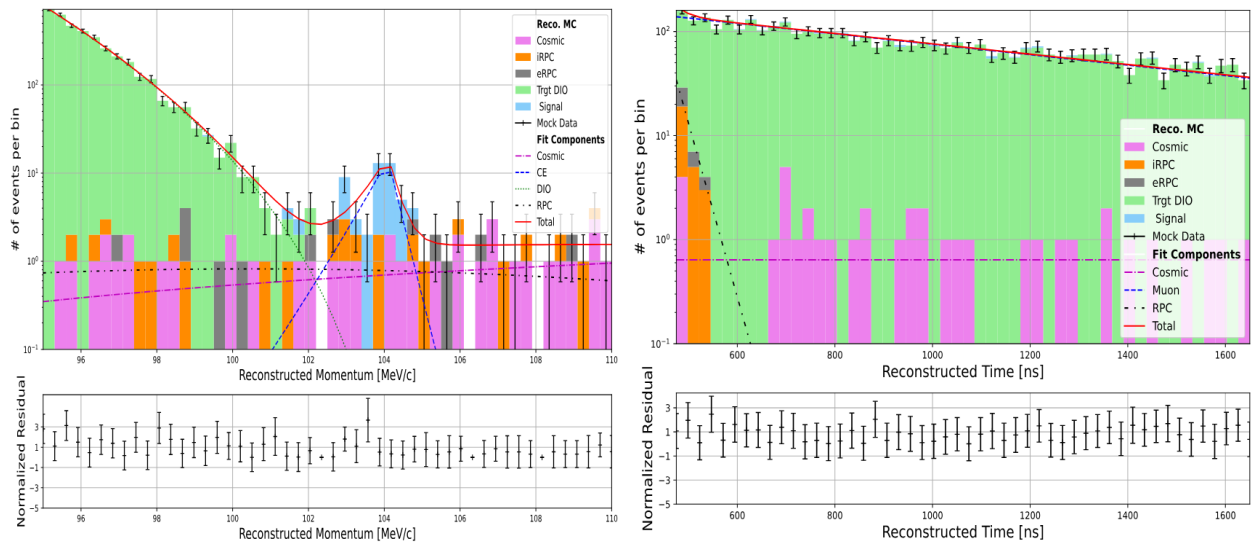


Figure 4.11: Maximum likelihood fit of the MDS2c dataset with  $R_{\mu e} = 1 \times 10^{-14}$ . Credit: S. Middleton [54]

## Chapter 5

### PHENOMENOLOGY WORK

This chapter is derived from the work published here: [14].

Should the decay or conversion experiments find evidence for CLFV decays or  $\mu \rightarrow e$  conversion in aluminum, interest will turn to understanding the effective operators that mediate CLFV at low energies. This can be done by studying the Dalitz plot distributions of polarized muon or tau decays to three leptons [58–60] or by measurements of the conversion rate with other nuclear targets, as the  $(Z, A)$  dependence of the conversion rate is sensitive to the Lorentz structure [61–64]. Future proposed experiments, such as Mu2e-II [65] and a conversion search at the Advanced Muon Facility [66], will provide opportunities to measure  $\mu \rightarrow e$  conversion in other target materials.

The  $\mu \rightarrow e$  conversion process manifestly involves the nuclear physics of the target elements. We discuss herein several aspects of extracting the New Physics from the nuclear physics. In particular, we present a new systematic study of the atomic number dependence of the coherent conversion rate. We utilize the method of Barrett moments [67] to add a substantial amount of muonic X-ray data to previous studies that mainly utilize electron scattering data on nuclear charge distributions. This allows us to take into account the fact that many nuclei have permanent quadrupole deformations, which affects the evaluation of matrix elements of New Physics operators. We also employ a new treatment of the neutron distribution and present a new approach to normalization of experimental and theoretical results.

The study of the  $(Z, A)$  dependence of conversion is most cleanly done with a target consisting of a single stable isotope, as with  $^{27}_{13}\text{Al}$ , the target in both the Mu2e and COMET experiments. Potential higher  $Z$  targets such as Ti have many stable isotopes and are typically not readily available as separated isotopes in sufficient quantity to meet experimental conversion sensitivity requirements. Therefore, in Sec. 5.2 we discuss conversion rates for both targets composed of individual isotopes and targets with natural elemental abundance. Section 5.3 addresses the question of the historical approach to the presentation of experimental limits on  $\mu \rightarrow e$  conversion. The usual approach, in analogy to the concept of a decay branching fraction, is to normalize the conversion rate to the rate of muon capture on a particular nucleus, and therefore to present limits on this ratio, referred to as  $R_{\mu e}$ :

$$R_{\mu e}(Z, A) = \frac{\Gamma(\mu^- + N(Z, A) \rightarrow e^- + N(Z, A))}{\Gamma(\mu^- + N(Z, A) \rightarrow \text{all captures})}. \quad (5.1)$$

We introduce an alternative normalization, which hews more closely to what a given experiment actually measures and better separates the lepton physics and the nuclear physics, removing extraneous contributions to the  $Z, A$  dependence of conversion.

Section 5.4 is a discussion of the practicalities involved in choosing future targets.

### 5.1 Review of existing literature

Should CLFV be observed in  $\mu \rightarrow e$  conversion in the upcoming round of experiments, interest will turn to identifying the Lorentz structure of the CLFV coupling, which can be accessed by a sufficiently precise measurement of the atomic number dependence of the conversion rate [61, 62, 64, 68].

The most widely cited treatment of the atomic number dependence of coherent  $\mu \rightarrow e$  conversion is that of Kitano, *et al.*[61], extended by Cirigliano *et al.*[62], which includes 55 isotopes whose charge distribution, measured using elastic electron scattering, were compiled by De Vries *et al.*[69]. These measurements are parameterized using a variety of models for the nuclear charge distribution: harmonic oscillator, two and three-parameter spherical Fermi, two and three-parameter Gaussian, as well as model-independent sum-of-Gaussians, and Fourier-Bessel expansion treatments where available. The spin-independent contribution to the coherent conversion rate has an  $A^2$  enhancement and is in most models dominant. Three types of effective operators, scalar, vector and dipole, contribute to coherent conversion. The rate of  $\mu \rightarrow e$  conversion is calculated using the overlap integrals between the  $\mu$  and  $e$  Dirac wave functions and nucleon densities for these three cases. While some direct measurements of neutron distributions are explored in Refs.[61, 62], for their main results the neutron and proton distributions are assumed to be identical, which means that the overlap integral related to the neutron distribution is equal to the overlap integral related to the proton distribution scaled by  $N/Z$ .

The recent calculations of Haxton *et al.* [70][71] improve these analyses for a selected number of nuclei by employing nuclear-level effective field theory to determine the matrix elements. Effective field theory has also been exploited to refine the interpretation of experimental CLFV limits in terms of New Physics couplings [72].

The Kitano *et al.* and Cirigliano *et al.* studies present the  $Z$ -dependence of the conversion rates for 55 isotopes, that have had their muon capture lifetime measured [73], in the form of a ratio:  $R_{\mu e}^Z/R_{\mu e}^{Al}$ . The  $Z$ -dependence of this ratio has a great deal of structure, largely due to the influence of “magic numbers” associated with closed shells in the nuclear shell model on the nuclear size and shape. The influence of shell structure on the nuclear size, and thus the evaluation of the New Physics matrix elements for the largely coherent conversion process is unavoidable. The additional structure in the  $Z$  dependence, introduced by the division by the muon capture rate, a

non-coherent Standard Model process, can, however, be avoided. This formulation is traceable in part to the original conversion normalization proposal of Weinberg and Feinberg [74]. The question of normalization of the conversion rate will be discussed in Sec. 5.3.

### 5.1.1 Treatment of the neutron distribution

Kitano *et al.* [61] used measured neutron distributions when possible. These measurements, derived from charged pion, proton or alpha particle scattering, were available for only 16 nuclei. Their primary method of including neutrons in determining the  $(Z, A)$  dependence of conversion was therefore to scale the overlap integral related to the proton distribution by a factor of  $N/Z$ . Particularly in heavy nuclei, protons and neutrons populate levels with different quantum numbers and are thus in different shells. This can produce rather different shapes and sizes for protons and neutrons, especially for nuclei at the edge of the valley of stability. In particular quadrupole deformations, as measured by  $B(E2)$  (the electric quadrupole transition probabilities) determined by Coulomb excitation and by muonic X-ray hyperfine structure, show a different dependence for protons and neutrons [75]. We have therefore resorted to a model calculation to account for these details. To improve on simple  $N/Z$  scaling, we account for the fact that neutron distributions are typically larger than proton distributions by using a comprehensive set of calculations employing the deformed relativistic Hartree-Bogoliubov theory in continuum (DRHBc) [76, 77] to estimate the size and shape of the neutron distributions. This approach more accurately accounts for the fact that in most nuclei, particularly those in the region of large permanent quadrupole deformation ( $Z = 60 - 80$ ), neutrons are in different shells than protons. Zhang *et al.* [78] have used the DRHBc theory [76, 77] for even-even nuclei ranging from  $Z = 8$  to  $Z = 120$  to determine individual neutron and proton distributions, accounting for quadrupole deformation. This work has recently been extended to other even-nuclei [79], but it has not been included in the results we are showing here.

### 5.1.2 The effects of quadrupole deformation

Many nuclei, especially those with protons or neutrons far from a closed shell, are non-spherical, having permanent quadrupole or higher multipole shapes. We address the effect of these deformations on the calculation of  $\mu \rightarrow e$  conversion rates. The conversion  $\mu \rightarrow e$  occurs primarily from the  $1S$  state, so conversion rates can be calculated using only the radial Dirac equation with an equivalent spherically symmetric charge (or neutron) distribution. However, characterizing the average over non-spherical distributions with a derived *rms* radius does not account for the effective smearing at the outer edge of a nucleus due, for example, to a quadrupole deformation.

The effective nuclear charge or neutron distribution skin thickness enters into the evaluation of the CLFV matrix elements. The relative importance of the skin thickness in determining the matrix

element depends on the atomic number (*c.f.*  $N/Z$ ) and the quadrupole deformation. We calculate the CLFV matrix elements using a Dirac equation with spherical symmetry, the angular integration accounting for the effect of the quadrupole deformation, whether oblate or prolate. This produces an effect largely concentrated at the nuclear surface, increasing the effective skin thickness of the charge distribution. The  $N/Z$  ratio increases with atomic number; the excess neutrons producing a “neutron skin”, a larger effective skin thickness for the neutrons, as well as effects on the charge distribution, *e.g.* isotope shifts in electronic or muonic atom spectra. These effects are further modulated by both proton and neutron shell structure, particularly around magic number closed shells.

The case of  $^{27}\text{Al}$  is of particular interest, as it is the target for the Mu2e and COMET experiments.  $^{27}\text{Al}$  has a large quadrupole moment (146.6 mb) [80]. Most shell model calculations conclude that this nucleus has a prolate shape, with  $\beta = 0.39$ , although Dehnhard [81] argues for an oblate ground state deformation. The sign of the quadrupole deformation does not enter into the calculation of the relevant integrals in the solution of the Dirac equation.

### 5.1.3 The isotopes of neodymium

Neodymium has five significant stable isotopes whose charge distributions have been measured in both electron scattering [82] and muonic X-ray spectra [83]. This provides an opportunity to explore some of the subtleties encountered in combining these different determinations of the nuclear charge distribution. There are measurements on five even-even neodymium isotopes:  $A=142, 144, 146, 148$ , and  $150$ , which range from spherical to deformed. This allows us to explore the interplay of the effect of a quadrupole deformation on the effective skin thickness, as well as the differences between the two techniques, as shown in Fig. 5.1.

The values of the quadrupole deformation  $\beta$ , determined largely from  $B(E2)$  measurements [75], show a steady increase with neutron number, culminating at  $N = 90$  (shown in Fig. 5.2). The value of  $\beta$  in the three-parameter fits to the charge distribution is held fixed for both the muonic X-ray and electron scattering cases.

The calculations of Zhang *et al.* using the DRHBc theory show that the *rms* charge radius of these Nd isotopes grows as  $A^{1/3}$ , while the neutron radius grows quicker, as the neutrons are in a higher shell and further from a shell closure. This is our primary motivation for using the Zhang *et al.* calculations to evaluate the  $S(n)$  and  $V(n)$  overlap integrals, rather than scaling the neutron distributions by  $N/Z$  as has been the practice in [61][62]. Related calculations by Zhang *et al.* [84] also reproduce the behavior of the quadrupole deformation in the Nd isotopes as a function of neutron number.



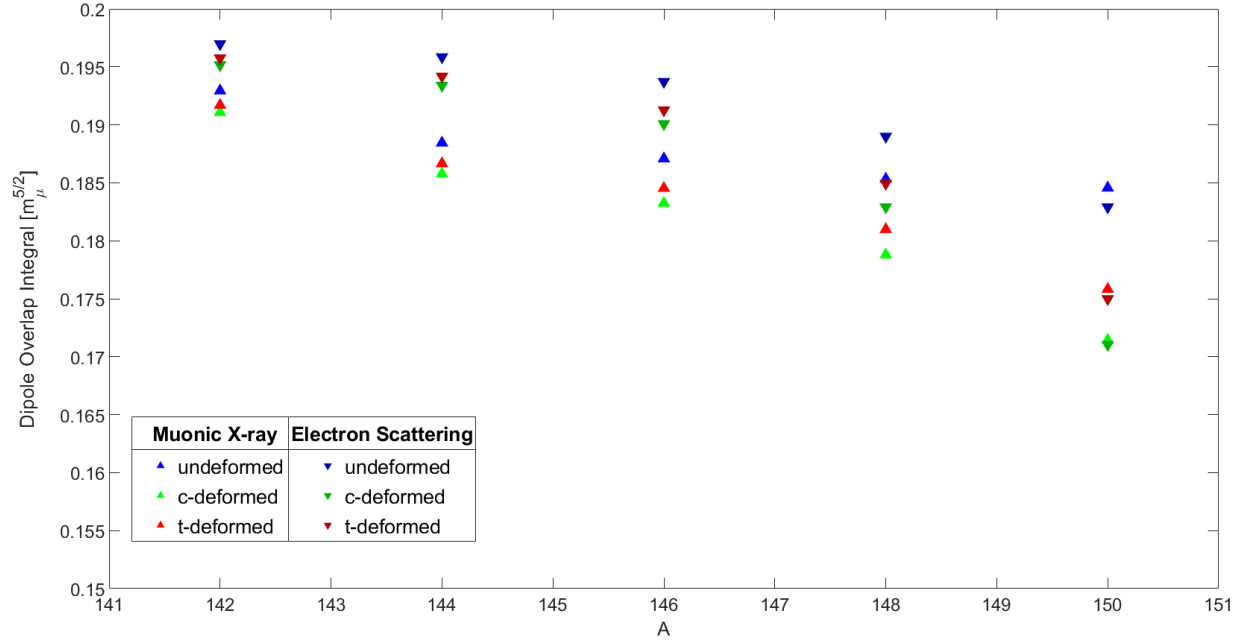


Figure 5.1: The dipole overlap integral for five even-even isotopes of Nd as determined using muonic X-ray data [83] and electron scattering data [82] and three treatments of the charge distribution (detailed in Sec. 5.2.2).

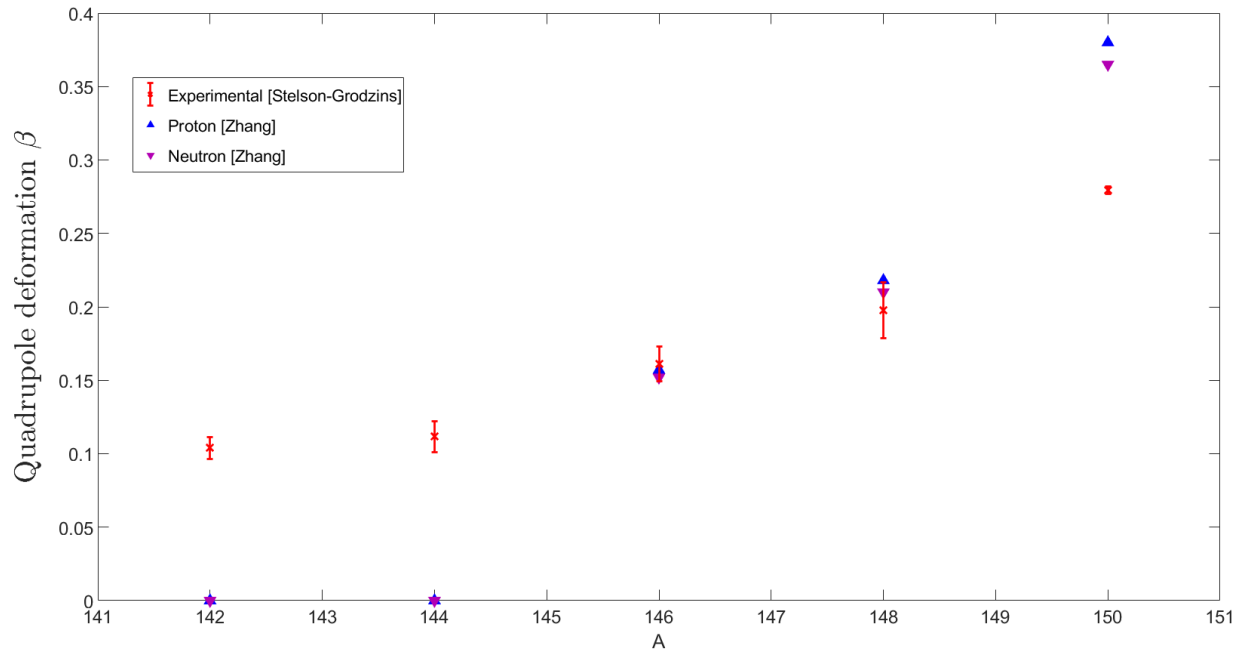


Figure 5.2: Quadrupole deformation of five even-even isotopes of Nd determined from  $B(E2)$  measurements in Coulomb excitation [75] (with experimental uncertainty), and calculated for the charge and neutron distributions in the model of Zhang *et al.* [78].

#### 5.1.4 Goal of this study

Our new determination of the atomic number dependence of the coherent conversion rate employs the method of Barrett moments [67] to add the many muonic X-ray measurements of nuclear charge distributions to the electron scattering data used in previous studies. The muonic X-ray data encompass measurements of many strongly-deformed nuclei, using the resolved hyperfine structure in the X-ray transitions to measure the nuclear quadrupole moment shape, typically parameterized by a three-parameter Fermi distribution.

Our treatment of the  $A$  and  $Z$  dependence of conversion differs from previous treatments in several ways:

- While previous studies have mainly used electron-scattering-based nuclear size determinations, we include the many measurements of nuclear charge distributions determined using muonic X-rays. This substantially enlarges the sample size, particularly in the regime above  $Z = 60$ , where many nuclei have substantial quadrupole deformations. We combine the elastic electron scattering and muonic X-ray data using the method of Barrett moments, and devise a procedure to incorporate the effect of permanent  $Y_{20}$  deformations on the effective nuclear skin thickness. By this approach, we can include the conversion rates for a total of 236 isotopes.
- Rather than using a neutron distribution equal to the proton charge distributions, the primary method used in previous treatments, we use the deformed relativistic Hartree-Bogoliubov theory in continuum (DRHBc) [78] for the neutron distributions and compare with other approaches. This model, bench-marked against a wide variety of experimental determinations for even-even nuclei, allows us to include a wider variety of nuclei and to explore isotopic effects on the conversion rate.
- We present the  $\mu \rightarrow e$  conversion rates for the coherent New Physics process normalized to the total muon lifetime, rather than to the muon capture rate.

## 5.2 Atomic number dependence of $\mu \rightarrow e$ conversion

### 5.2.1 Theoretical background

In the following study, we concentrate on the dominant spin-independent coherent conversion process in which the final and initial state of the nucleus is identical and the coherent conversion rate is enhanced by  $A^2$ .

The lepton flavor-violating coherent conversion rate of a muon into an electron is given by Kitano *et al.* [61] as:

$$\Gamma_{conv} = 2G_F^2 \left| A_R^* D + \tilde{g}_{LS}^{(p)} S^{(p)} + \tilde{g}_{LS}^{(n)} S^{(n)} + \tilde{g}_{LV}^{(p)} V^{(p)} + \tilde{g}_{LV}^{(n)} V^{(n)} \right|^2 + 2G_F^2 \left| A_L^* D + \tilde{g}_{RS}^{(p)} S^{(p)} + \tilde{g}_{RS}^{(n)} S^{(n)} + \tilde{g}_{RV}^{(p)} V^{(p)} + \tilde{g}_{RV}^{(n)} V^{(n)} \right|^2 \quad (5.2)$$

where  $G_F$  is the Fermi constant, and  $A_{R,L}^*$  and  $\tilde{g}$  are dimensionless coupling constants that describe the strength of each component of the Lagrangian.  $D$ ,  $S$  and  $V$  are the overlap integrals for dipole, scalar, and vector interactions respectively. The  $L$  and  $R$  subscripts indicate left-handed and right-handed components and the  $(n)$  and  $(p)$  superscripts denote the neutron and proton terms respectively.

The overlap integrals are defined as:

$$\begin{aligned} D &= \frac{4}{\sqrt{2}} m_\mu \int_0^\infty (-E(r)) (g_e^- f_\mu^- + f_e^- g_\mu^-) r^2 dr \\ S^{(p)} &= \frac{1}{2\sqrt{2}} \int_0^\infty Z \rho^{(p)}(r) (g_e^- g_\mu^- - f_e^- f_\mu^-) r^2 dr \\ S^{(n)} &= \frac{1}{2\sqrt{2}} \int_0^\infty (A - Z) \rho^{(n)}(r) (g_e^- g_\mu^- - f_e^- f_\mu^-) r^2 dr \\ V^{(p)} &= \frac{1}{2\sqrt{2}} \int_0^\infty Z \rho^{(p)}(r) (g_e^- g_\mu^- + f_e^- f_\mu^-) r^2 dr \\ V^{(n)} &= \frac{1}{2\sqrt{2}} \int_0^\infty (A - Z) \rho^{(n)}(r) (g_e^- g_\mu^- + f_e^- f_\mu^-) r^2 dr \end{aligned}$$

where  $f$  and  $g$  are the lower and upper components of the radial solution of the Dirac equation describing a muon orbiting a nucleus and converting to an electron. The functions  $f_\mu$  and  $(f_e)$  are the muon (electron) wavefunction [85]. The terms  $\rho^{(n)}$  and  $\rho^{(p)}$  describe the neutron and proton densities in the nuclei respectively. The electric field,  $E(r)$ , is derived using Gauss' Law:

$$E(r) = \frac{Ze}{r^2} \int_0^r r'^2 \rho^{(p)}(r') dr'. \quad (5.3)$$

The muon and electron wavefunctions in the vicinity of the  $^{27}\text{Al}$  nucleus are shown in Fig. 5.3. The conversion occurs overwhelmingly from the  $1S$  state; we therefore integrate over polar and azimuthal angles to account for the effect of quadrupole deformations.

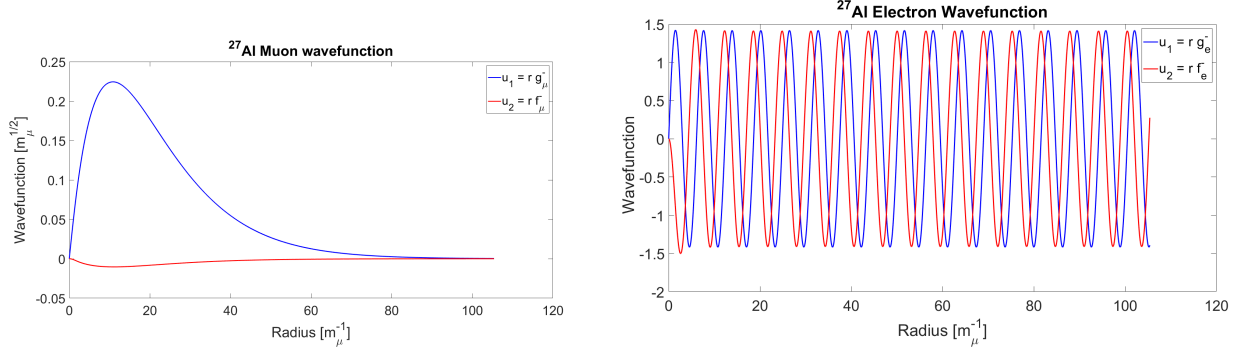


Figure 5.3: The two components of the wavefunctions of the muon (top) and the electron (bottom) in the vicinity of the Al nucleus.

## 5.2.2 Methodology

### Combining electron scattering and muonic X-ray measurements

To combine measurements of nuclear charge distribution obtained from electron scattering and muonic X-rays we use the method developed by Barrett [67]. Electron scattering experiments derive information on the nuclear charge distribution from the energy and angular distribution of the scattered electron, mapping the momentum transfer of the electron to the Fourier transform of the charge distribution [69]. These treatments typically keep only the first term in the  $q^2$  expansion.

Muonic X-ray experiments use the energy of X-rays emitted in the atomic cascade of muonic atoms to determine the size and shape of the nucleus. Due to the strong overlap of the muon wavefunction with the nucleus, the energy of the  $3D - 2P$  and  $2P - 1S$  transitions is highly sensitive to nuclear size parameters. Analysis of the hyperfine structure allows for the (model-dependent) determination of permanent quadrupole charge distributions. This method typically provides a more precise measurement of the quadrupole deformation of nuclei than electron scattering experiments.

While for light nuclei the  $2P - 1S$  transition energy of a muonic atom can be matched to a single mean square radius  $\langle r^2 \rangle$ , this is not true for heavier nuclei, where nuclear distributions with the same RMS radius can generate quite different transition energies. Barrett [67] introduced a different moment, shared by all nuclear distributions, yielding the same transition energy. The Barrett moment is defined as:

$$\langle r^k e^{-\alpha r} \rangle = \frac{4\pi}{Ze} \int_0^\infty \rho(r) r^k e^{-\alpha r} r^2 dr, \quad (5.4)$$

where  $k$  and  $\alpha$ , which are  $Z$ -dependent, are given in [67].

We define the Barrett radius  $R_{k\alpha}$  from the implicit equation [86]:

$$\frac{3}{(R_{k\alpha})^3} \int_0^{R_{k\alpha}} \rho(r) r^k e^{-\alpha r} r^2 dr = \langle r^k e^{-\alpha r} \rangle. \quad (5.5)$$

In both electron scattering and muonic X-ray analyses, the nuclear charge distribution has often been described using a 2-parameter Fermi distribution (2pF):

$$\rho(r) = \frac{\rho_0}{1 + \exp \left[ \frac{r-c}{a} \right]}, \quad (5.6)$$

where  $c$  is the radius at the half maximum and  $t = 4a \ln(3)$  is the skin thickness, defined as the region in which the charge density falls from 90% to 10% of the central value. This model is central to our Barrett moment-centered treatment.

We can see an example of the computation of the Barrett moment from two different datasets for neodymium in Table 5.1. The Barrett moments derived from the two types of experiments are seen to be in good agreement, supporting our approach to combining the electron scattering and muonic X-ray of measurements in determining the  $Z$  dependence of the conversion rate.

### Quadrupole deformation

In order to compute the overlap integral, we need to solve the Dirac equation to obtain the muon and electron wavefunctions (as described in Sec. 5.2.1). We used an existing code [87] to solve the Dirac equation for a muonic atom in the potential of a spherically-symmetric 2-parameter Fermi distribution. For approximately spherical nuclei ( $Z < 60$  and  $Z > 80$ ), we can directly apply this solver, whereas for deformed nuclei we first need to get an equivalent spherically-symmetric distribution.

The method used to include the effect of nuclear quadrupole deformation on the matrix elements is as follows:

- employ a deformed 3-parameter Fermi distribution<sup>1</sup>:

$$\rho(r, \theta) = \frac{\rho_0}{1 + \exp \left[ \frac{r-c(1+\beta Y_{20}(\theta))}{a} \right]} \quad (5.7)$$

where we take parameters  $c$ ,  $t = 4a \ln(3)$  and  $\beta$  from available literature detailed in Sec. 5.2.2.

- We convert this to a spherically-symmetric 2-parameter Fermi distribution by removing the quadrupole deformation  $\beta$  and adjusting the skin thickness  $t$  to provide a constant Barrett

moment (defined in Eq. 5.4). This equivalent 2-parameter Fermi distribution is then used to solve the Dirac equation.

Using the  $t$  parameter to match the Barrett moment effectively smears out the nuclear surface, accounting for the integration of the  $Y_{20}$  deformation over angles.

One could modify the  $c$  parameter rather than the  $t$  parameter to match the Barrett moment. This produces a small difference in the overlap integrals (see example for Nd in Fig. 5.1).

## Dataset

Our calculations employ a compilation of data from different sources, which we list in the footnotes of the tables in Appendix A. When there are different sources for data on an isotope, we use the data from the compilation listing the largest number of isotopes.

- Nuclear charge distribution parameters:

The majority of  $c$  and  $t$  values we employ come from the Fricke *et al.* [86] (Table III.A and III.C) compilation of muonic X-ray and electron scattering experimental data. For several specific isotopes that were not included in [86], muonic X-ray measurements were added [88–92]. When muonic X-ray measurements do not exist, we use the compilation of electron scattering experimental data from de Vries *et al.* [69]. When the only information available is the *rms* charge radius<sup>2</sup>, we use data from Angeli *et al.* [93].

For quadrupole deformation in the deformed region ( $60 \leq Z \leq 80$ ), we use the Zhang *et al.* [78] model that calculates separate quadrupole deformations only for even-even proton and neutron distributions. For the other deformed nuclei, we use the model of Möller *et al.* [94] for deformed isotopes. This employs a Finite-Range Drop Model (FRDM) to compute ground-state quadrupole deformations, as well as many other nuclear properties.

- Barrett moment parameters:

There are two extensive compilations of the Barrett parameters  $k$  and  $\alpha$ : Barrett *et al.* [67] and Fricke *et al.* [86]. The latter is fitted to the experimental muonic X-ray measurements that we also use, but it is not available for every isotope, whereas the former is theoretical but can be applied to every elements. As we only compute Barrett moments in deformed nuclei ( $60 \leq Z \leq 80$ ), we decided to use the incomplete Fricke compilation. For isotopes that are not available, we chose to interpolate using neighboring elements. We decided not to use the Barrett compilation as there is a significant difference of up to 15% with the Fricke

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<sup>1</sup>This is not to be confused with the spherical three-parameter Fermi distribution often used in electrons scattering from heavy nuclei.



compilation. It is worth noting that even with this significant discrepancy between the two datasets, the difference in the computed overlap integrals is smaller than 0.25%.

- Neutron distribution:

We use the Zhang *et al.* [78] DRHBc model to separately evaluate the proton and the neutron nuclear distributions. This model treats only even-even nuclei, avoiding the additional single particle effects on both charge and neutron distributions seen in even-odd and odd-even nuclei. It provides different quadrupole deformation for the neutron and proton distributions.

## Uncertainties

We consider two sources of systematic uncertainties: the treatment of the quadrupole deformation  $\beta$  and the radius at half maximum  $c$  in the Fermi distribution.

We take the quadrupole deformation error from Stelson and Grodzins [75], where uncertainty on  $B(E2)$  is converted into uncertainty on  $\beta$  assuming a uniform ellipsoidal charge distribution. The uncertainty on  $c$  is taken directly from Fricke *et al.* [86].

Across all isotopes, the relative uncertainty on  $c$  does not exceed 2%, while the relative uncertainty on  $\beta$  can be up to 20%. We therefore propagated only the uncertainty in  $\beta$  to the Barrett moment and ignored the  $c$  uncertainty.

The resulting relative uncertainty on the Barrett moment on all the available elements never exceeded 1%; we show the values for the neodymium isotopes in Table 5.1 and Fig. 5.2 as an example.

It should be noted that different sources for nuclear distribution parameters can have significant impact on the resulting overlap integral values. We have tried to keep most of our data coming from a single compilation [86] to limit this variation, but we had to add additional sources for missing data (visible in the footnotes of the tables in Appendix A).

### 5.2.3 Results

Appendix A contains all the results and parameters used in this study. It is divided in two tables, Table A.1 shows the results for nuclei that we approximate as spherically symmetric, and Table A.2 for the deformed nuclei ( $60 \leq Z \leq 80$ ). The components of the 2-parameters Fermi distributions of each isotope is provided, as well as the values of the Barrett parameters for deformed nuclei.

The resulting overlap integrals calculated on the 236 stable isotopes with natural abundance above 1% are displayed in Fig. 5.4. The plot compares the results of Heeck *et al.* [64]; our new results are

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<sup>2</sup>If the available literature does not provide a 2-parameter Fermi distribution - some electron scattering measurements use a Fourier-Bessel expansion -, we use a least square method to fit the distribution to a 2pF assuming a fixed value of  $t = 2.3$  fm

in general agreement. The main difference appears in the deformed nuclei region ( $60 \leq Z \leq 80$ ), where our values are higher due to our explicit treatment of the effect of the deformation on the matrix elements. This results in a smoother behavior of the overlap integral value after  $Z = 60$ , furthering our attempts to isolate the New Physics CLFV interaction from nuclear effects.

There are a couple of outliers, for example  $^{159}_{65}\text{Tb}$  and  $^{165}_{67}\text{Ho}$ , that display smaller value compared to previous work, with significant difference in the case of  $^{159}_{65}\text{Tb}$ . The discrepancy can be attributed to the origin of the nuclear distribution data, as these nuclei are not part of the main compilation of nuclear data used [86]. For  $^{159}_{65}\text{Tb}$ , choosing experimental data from deWit *et al.* [89] compared to extrapolating 2pF parameters from the rms radius given in Angeli *et al.* [93] accounts for the difference.

Figure 5.5 shows the overlap integrals weighted by natural abundance, in comparison with work from Kitano *et al.* [61]. The latter does not use natural abundance weighting but only displays one isotope per element. Again, the main difference between the two datasets is in the deformed nuclei region.

From the overlap integrals, we can compute the conversion rate using Eq. 5.2 for all the elements, and we obtain the sensitivity of different target materials normalized to the conversion rate in  $^{27}\text{Al}$ . The relative sensitivity is defined as the conversion rate normalized by the muon capture rate [62]:

$$\frac{R_{\mu e}(Z)}{R_{\mu e}(\text{Al})} = \frac{\frac{\Gamma_{\text{conv}}(Z)}{\Gamma_{\text{capture}}(Z)}}{\frac{\Gamma_{\text{conv}}(\text{Al})}{\Gamma_{\text{capture}}(\text{Al})}} \quad (5.8)$$

In Fig. 5.6, our result is compared to that of Cirigliano *et al.* [62].

Four physics models are considered: dipole ( $D$ ), scalar ( $S$ ) and two vector type ( $V^{(\gamma)}$  and  $V^{(Z)}$ ).  $V^{(\gamma)}$  describes the scenarios where the transition charge radius operator gives the dominant contribution to the CLFV Lagrangian, and  $V^{(Z)}$  describes the case where the dominant operator is assumed to be an effective Z-penguin [95].

Figure 5.7 removes the normalization relative to muon capture and shows the conversion rates in each material relative to that in  $^{27}\text{Al}$ . The objective is to separate the coherent muon-to-electron conversion process from the incoherent muon capture process. The motivation for this presentation of our results is detailed in Sec. 5.3.

### 5.3 Normalization and $(Z, A)$ Dependence of the Conversion Rate

The conventional approach to the normalization of  $\mu \rightarrow e$  conversion experiments, quoting the conversion rate (experimental limit or theory prediction) normalized to the measured rate of  $\mu$

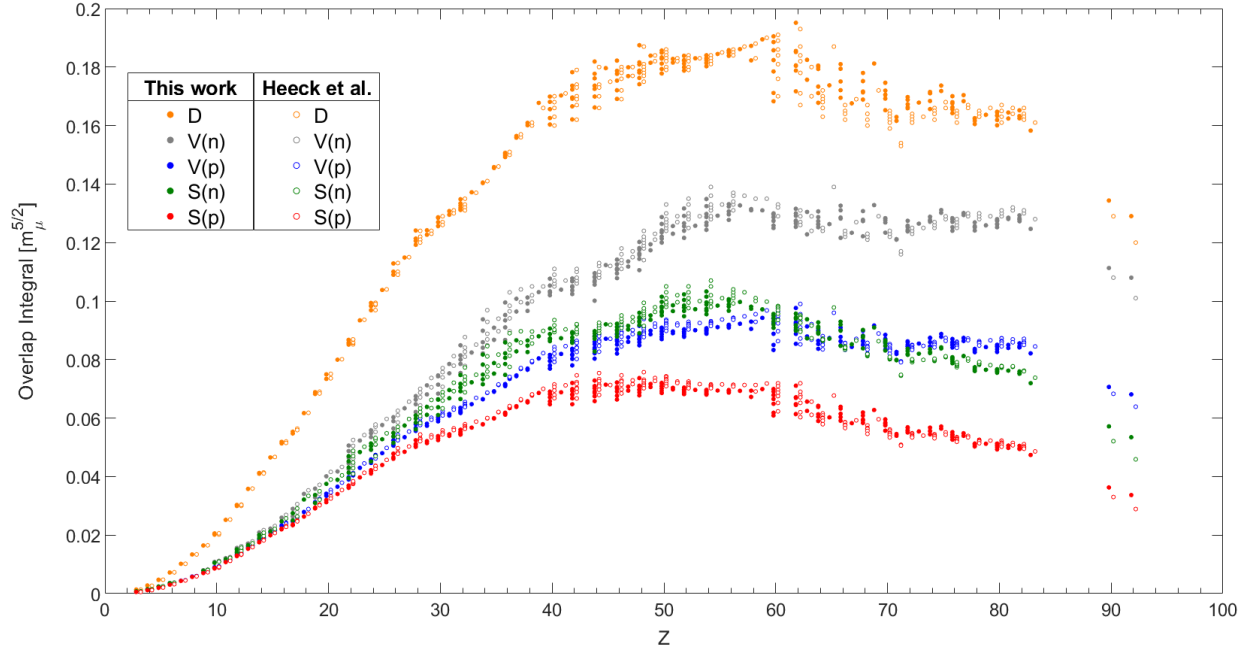


Figure 5.4: The overlap integrals for dipole, vector and scalar couplings as a function of atomic number for isotopes having a natural abundance  $> 1\%$ , for the compilation of Heeck *et al.* [64] and this work. For clarity, we shift the result of Heeck *et al.* by  $+\frac{1}{2}$  unit on the x-axis.

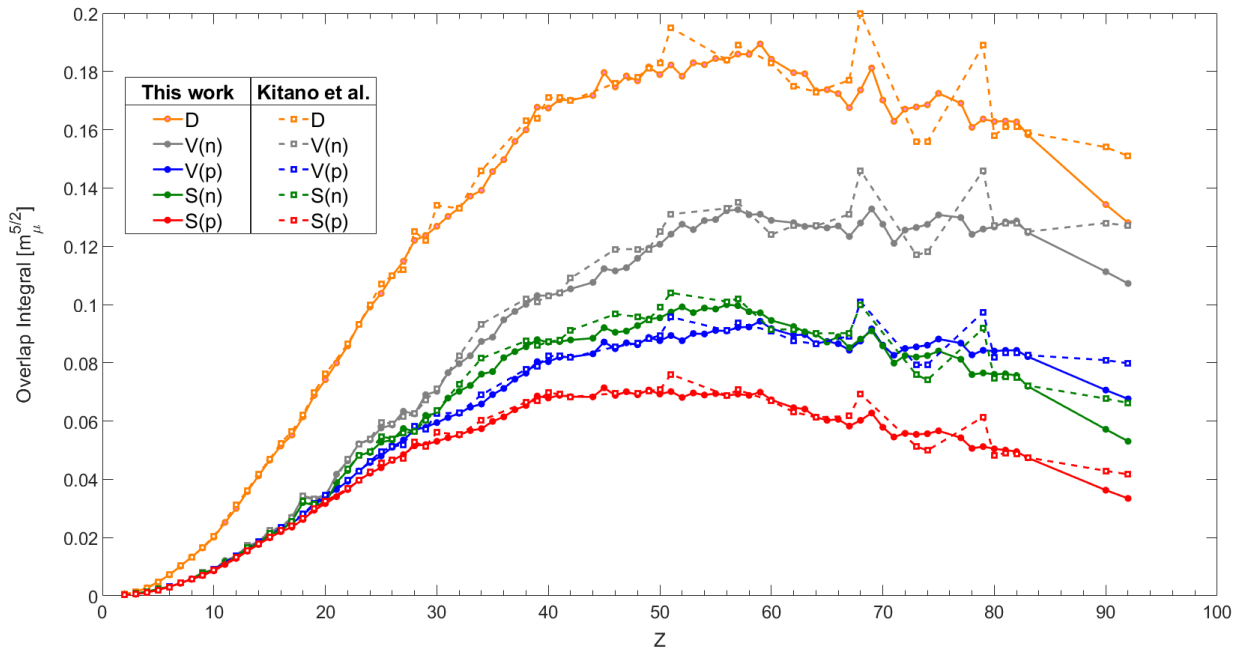


Figure 5.5: The overlap integrals for dipole, vector and scalar couplings as a function of atomic number for each element, weighted by natural abundance, for the compilation of Kitano *et al.* [61, 62] and this work.

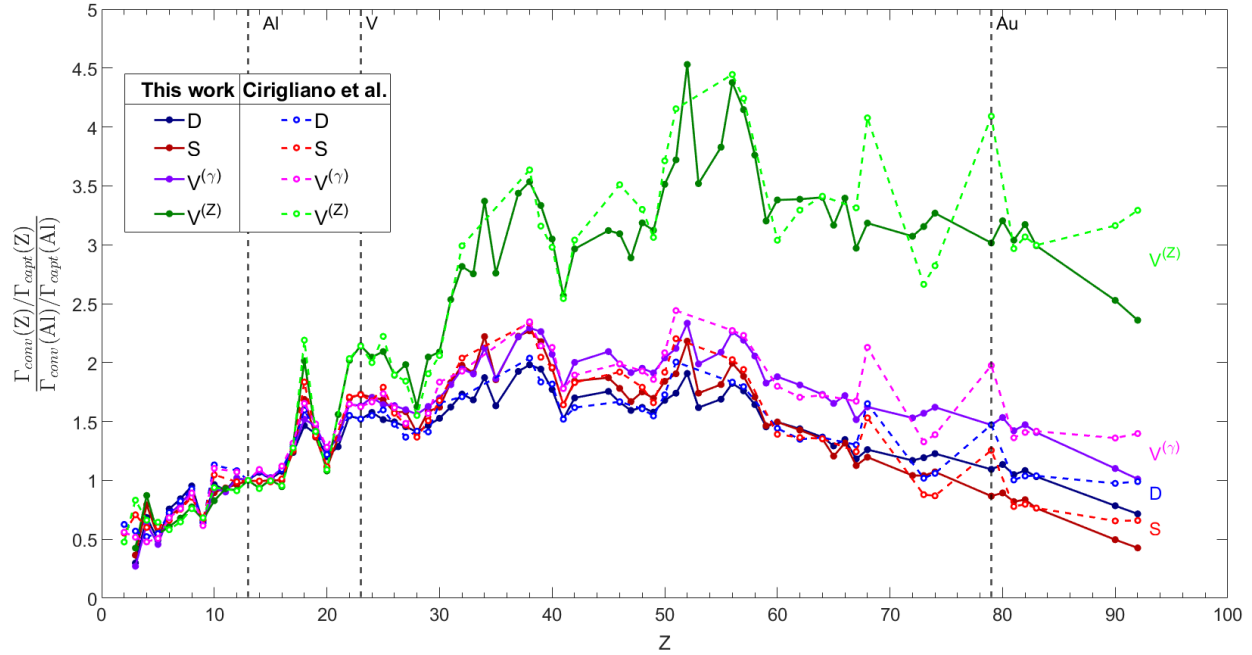


Figure 5.6: Comparison with of our results on sensitivity as a function of  $Z$  with those of Cirigliano *et al.*[62]. The conversion rates are normalized to the muon capture rate and are relative to the rate for aluminum (see Eq. 5.8).

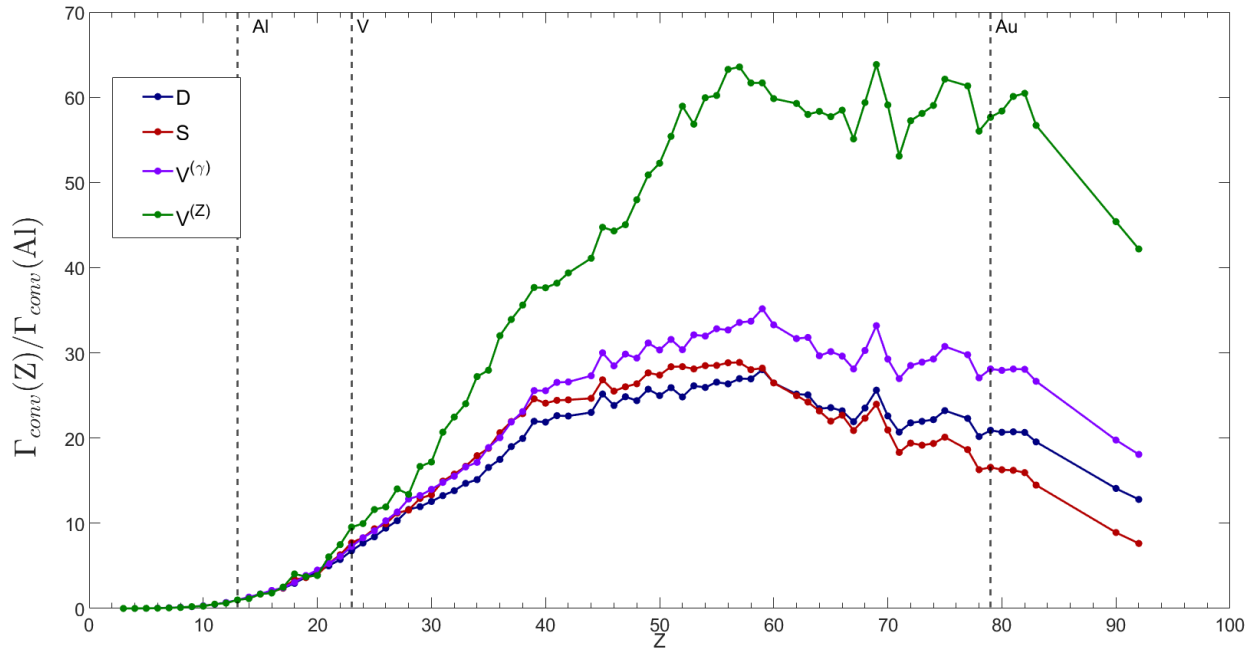


Figure 5.7: Our calculation of the experimental sensitivity of CLFV experiments as a function of atomic number. The conversion rates are not normalized to the muon capture rate, but are relative to the rate for aluminum (see Eq. 5.9).

Table 5.1: Comparison of muonic X-ray and electron scattering determinations of two-parameter Fermi distributions in neodymium isotopes.  $\beta$  comes directly from  $B(E2)$  measurement in [75]. The Barrett parameters values for Nd are  $\alpha = 0.130$  and  $k = 2.175$  [67].

| Isotope                  | c (fm)            | t (fm)            | $\beta$ [75]      | <i>rms</i> radius (fm) | Barrett moment   | Barrett radius $R_{k\alpha}$ (fm) |
|--------------------------|-------------------|-------------------|-------------------|------------------------|------------------|-----------------------------------|
| Muonic X-ray[83]         |                   |                   |                   |                        |                  |                                   |
| $^{142}\text{Nd}$        | $5.80 \pm 0.03$   | $2.32 \pm 0.08$   | $0.104 \pm 0.02$  | $4.91 \pm 0.08$        | $15.99 \pm 0.03$ | $6.27 \pm 0.01$                   |
| $^{144}\text{Nd}$        | $5.85 \pm 0.03$   | $2.27 \pm 0.08$   | $0.123 \pm 0.02$  | $4.94 \pm 0.08$        | $16.11 \pm 0.04$ | $6.31 \pm 0.01$                   |
| $^{146}\text{Nd}$        | $5.82 \pm 0.03$   | $2.42 \pm 0.08$   | $0.151 \pm 0.02$  | $4.98 \pm 0.08$        | $16.26 \pm 0.06$ | $6.34 \pm 0.02$                   |
| $^{148}\text{Nd}$        | $5.84 \pm 0.03$   | $2.40 \pm 0.08$   | $0.197 \pm 0.04$  | $5.00 \pm 0.08$        | $16.38 \pm 0.13$ | $6.38 \pm 0.03$                   |
| $^{150}\text{Nd}$        | $5.86 \pm 0.03$   | $2.35 \pm 0.08$   | $0.279 \pm 0.005$ | $5.04 \pm 0.08$        | $16.58 \pm 0.01$ | $6.43 \pm 0.01$                   |
| Electron Scattering [82] |                   |                   |                   |                        |                  |                                   |
| $^{142}\text{Nd}$        | $5.7045 \pm 0.03$ | $2.539 \pm 0.013$ | $0.104 \pm 0.02$  | $4.92 \pm 0.08$        | $15.98 \pm 0.03$ | $6.27 \pm 0.01$                   |
| $^{144}\text{Nd}$        | $5.6634 \pm 0.03$ | $2.696 \pm 0.013$ | $0.123 \pm 0.02$  | $4.96 \pm 0.08$        | $16.11 \pm 0.04$ | $6.31 \pm 0.01$                   |
| $^{146}\text{Nd}$        | $5.6600 \pm 0.03$ | $2.760 \pm 0.013$ | $0.151 \pm 0.02$  | $4.99 \pm 0.08$        | $16.24 \pm 0.06$ | $6.34 \pm 0.02$                   |
| $^{148}\text{Nd}$        | $5.6871 \pm 0.03$ | $2.798 \pm 0.022$ | $0.197 \pm 0.04$  | $5.04 \pm 0.08$        | $16.47 \pm 0.13$ | $6.40 \pm 0.03$                   |
| $^{150}\text{Nd}$        | $5.7185 \pm 0.03$ | $2.861 \pm 0.031$ | $0.279 \pm 0.005$ | $5.13 \pm 0.08$        | $16.86 \pm 0.01$ | $6.50 \pm 0.01$                   |

capture on a given nucleus, has been in place for more than seventy years. We will discuss the shortcomings of this convention and propose a revised presentation of  $\mu \rightarrow e$  conversion results that addresses our concerns.

The first limit on  $\mu \rightarrow e$  conversion, by Lagarrigue and Peyrou [96], using cosmic ray muons stopped in copper and tin targets in a Wilson cloud chamber, employed previous measurements of the muon lifetime (dominated by muon capture in this regime) in copper and antimony [97] as normalization. The first accelerator experiment, using a copper target [98], also normalized to the (directly measured) rate of muon capture.

The choice to normalize to the muon capture rate is not precisely analogous to the idea of a branching fraction (the number of decays into a particular mode, divided by all decays), which would be to divide the conversion rate in the field of a particular nucleus by all possible fates of the muon ( $\mu \rightarrow e$  conversion, decay in orbit or nuclear capture). This normalization is essentially a historical convention initially codified by the work of Weinberg and Feinberg in 1959 [74]. All results or predictions on muon-to-electron conversion have henceforth been presented in the form  $R_{\mu \rightarrow e}$  (Eq. 5.1).

Compilations of the history of experimental limits on CLFV processes typically present the 90% confidence level limits for decays and conversion on the same plot. This analogy ignores the fact that decay and conversion experiments are normalized differently. The decay limits are reported as true branching fractions, while the conversion rate limits are on the fraction of muon captures resulting in the production of a mono-energetic electron, which does not account for all fates of a muon in a muonic atom. Indeed, the lifetime of such a muon is determined in varying proportions

by the conversion rate, a BSM process, by the nuclear capture rate, an incoherent Standard Model process, and by the lifetime of the decay-in-orbit muon, which is modified from the free decay rate by the atomic binding energy, the so-called Huff factor (0.993 for aluminum, 0.981 for titanium and 0.850 for gold) [99].

It is clear from these points that a revised approach is desirable. In particular, one would like to avoid the spurious introduction of nuclear effects into the presentation of a conversion result to the greatest extent possible to facilitate a conceptually cleaner comparison with results from decay experiments.

Normalizing an experimental conversion result requires determination of the number of stopped muons within the sensitive time window of the experiment. This involves muon decay as well as nuclear muon capture. In the upcoming Mu2e experiment downstream detectors count  $2P - 1S$  muonic X-rays or other transitions and delayed  $\gamma$ -rays from muon capture to infer the stopped muon rate. This measured rate is then used to normalize the conversion rate limit or observation.

Table 5.2: Muon capture rates on  $^{27}\text{Al}$  leading to Mg, Na and Ne final states (from [100]).

| Reaction                                                 | Observed<br>$\gamma$ -ray<br>yield | Estimated<br>ground-state<br>transition | Missing<br>yields | Total<br>yield |
|----------------------------------------------------------|------------------------------------|-----------------------------------------|-------------------|----------------|
| $^{27}\text{Al}(\mu^-, \nu)^{27}\text{Mg}$               | 10(1)                              | 0                                       | 3                 | 13             |
| $^{27}\text{Al}(\mu^-, \nu n)^{26}\text{Mg}$             | 53(5)                              | 4                                       | 4                 | 61             |
| $^{27}\text{Al}(\mu^-, \nu 2n)^{25}\text{Mg}$            | 7(1)                               | 3                                       | 2                 | 12             |
| $^{27}\text{Al}(\mu^-, \nu 3n)^{24}\text{Mg}$            | 2                                  | 3                                       | 1                 | 6              |
| $^{27}\text{Al}(\mu^-, \nu p x n)^{26-23}\text{Na}$      | 2                                  | 2                                       | 1                 | 5              |
| $^{27}\text{Al}(\mu^-, \nu \alpha x n)^{23-21}\text{Ne}$ | 1                                  | 2                                       | 0                 | 3              |
| Total                                                    | 75(5)                              | 14                                      | 11                | 100            |

Table 5.2 lists the muon capture reactions in  $^{27}\text{Al}$ , which produce states of Mg, Na, and Ne [100]. Note that only 13% of captures result in the  $^{27}\text{Mg}$  ground state. The majority of captures result in neutron emission, with the nucleus left in either ground or excited states. The detailed calculation of the relevant nuclear matrix elements is quite complex, which is the reason the experimentally measured value of the total  $\mu$  capture rate is used in deriving a conversion experiment's single event sensitivity. Knowledge of the number of stopped muons within the sensitive time window of the experiment is fundamental to normalization of the result.

The experimental measurement of the total muon lifetime, with its associated uncertainties, thus unavoidably involves the calculation of the experimental efficiency and therefore the calculation

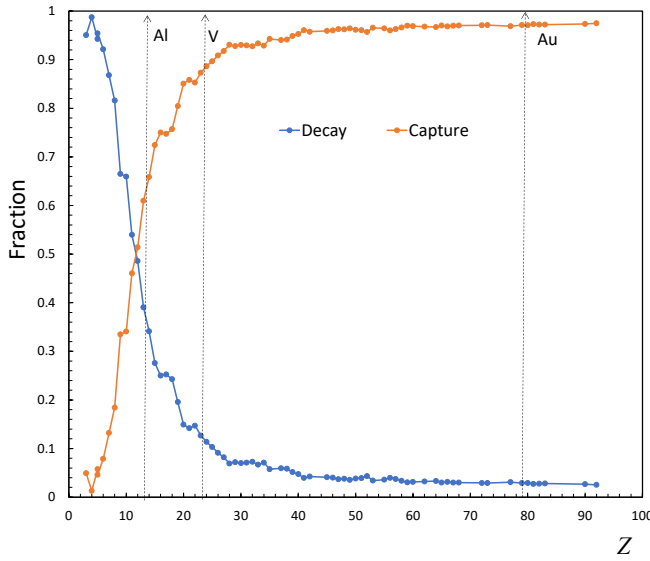


Figure 5.8: The fraction of muon decay in orbit in a muonic atom compared to the  $\mu^-$  capture rate as a function of  $Z$ . Experimental values are taken from the Measday compilation [73], a survey experiment [99] or a specific previous experiment (Ref. [100] for  $^{27}\text{Al}$ ).

of the  $\mu \rightarrow e$  conversion rate. Since the overlap of the muon atomic wave function with the nuclear proton and neutron distribution influences the effective lifetime, the New Physics and the Standard Model nuclear physics are inextricably mixed: the measured rate (or limit on the rate) manifestly depends on the muon capture lifetime. The muon nuclear capture rate *grosso modo* follows Wheeler’s [101]  $Z_{\text{eff}}^4$  law, but in detail shows the effect of nuclear shell structure on nuclear size. The convention of quoting a “capture fraction”, thereby exaggerates the effect of nuclear shell model structure, complicating the isolation of New Physics from nuclear effects.

An explicit example can be found in equation (3) in the report of the SINDRUM II limit on the conversion rate in lead (Pb) [102], where the denominator in the calculation of  $B_{\mu e}$  is  $f_{\text{capt}} N_{\text{stop}} \epsilon_{\text{tot}}$ . Since  $f_{\text{capt}}$  for Pb is 0.95, the normalization to  $\mu$  capture is only slightly different from the normalization to muon stops. For lighter nuclei, however, for example, aluminum,  $f_{\text{capt}}$  is 0.61, so the change in normalization amounts to 64%. Further, since the  $\mu$  capture rate as a function of atomic number reflects nuclear shell structure as well the details of the low-lying levels of individual nuclei, and is primarily an incoherent process, its use introduces extraneous nuclear physics into consideration of the  $Z$  dependence of the coherent New Physics process of  $\mu$  to  $e$  conversion.

From a theoretical perspective, a model calculation of the rate of conversion effectively yields an absolute rate (more specifically, a rate characterized by  $G_F^2$  and a mass-scale coupling factor). The conventional normalization involves a hybrid ratio of the calculated rate of the coherent conversion



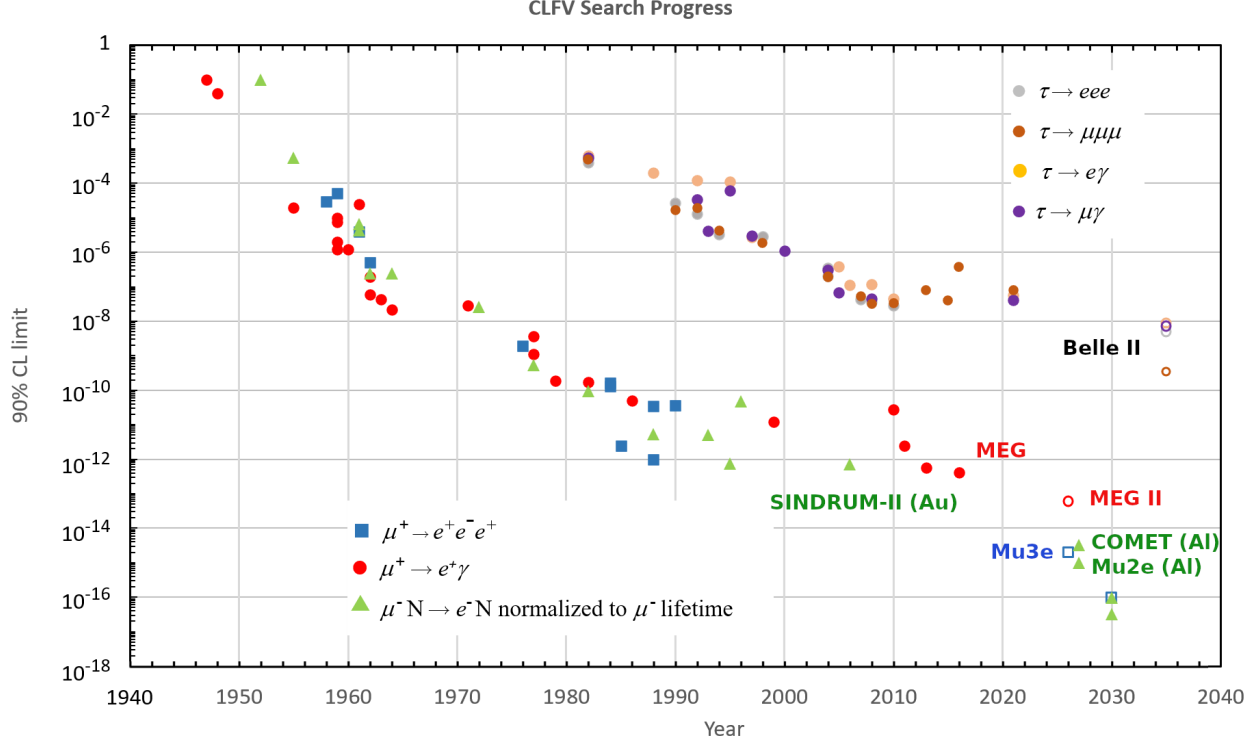


Figure 5.9: Chronology of 90% confidence limits on  $\mu \rightarrow e\gamma$ ,  $\mu \rightarrow 3e$ ,  $\mu$  to  $e$  conversion,  $\tau \rightarrow e\gamma$ ,  $\tau \rightarrow \mu\gamma$  and  $\tau \rightarrow 3e$ , including predicted limits for current experiments. The  $\mu$  to  $e$  conversion results are normalized to the total muon lifetime, not the heretofore conventional  $\mu$  capture rate. Unfilled symbols represent the goals of experiments currently in preparation. Further improvement in search sensitivity is possible with new stopped muon beams under study for decades hence.

process divided by the experimental measurement of a partially incoherent muon capture process. This has not mattered in any practical sense up to this point, but makes conceptual comparisons with decay experiments unnecessarily difficult. We should remove this inconsistency before we begin to compare measured  $\mu \rightarrow e$  conversion rates for different nuclei to explore the Lorentz structure of the conversion process.

Crivellin *et al.* [113] write the conversion rate, **not** the conversion ratio, as

$$\Gamma_{conv} = \frac{m_\mu^5}{4\Lambda^4} |eC_L^D D_N + 4(G_F m_\mu m_p \tilde{C}_{(p)}^{SL} S_N^{(p)} + \tilde{C}_{(p)}^{VR} V_N^{(p)} + p \rightarrow n)|^2 + L \leftrightarrow R, \quad (5.9)$$

involving the proton and neutron fields, but otherwise similar to the muon decay rates ( $C$  are dimensionless Wilson coefficients and  $\Lambda$  is the effective mass scale).

The historical normalization of this process to the muon capture rate conflates the actual sensitivity of a conversion experiment with the nuclear physics of muon capture. In the background-free

Table 5.3: Atomic number-dependent adjustment of  $\mu \rightarrow e$  conversion limits to normalization to muon stops rather than captures.

| Year | Reference | Nucleus | 90% CL Limit<br>Normalized to<br>$\mu$ Capture | 90% CL Limit<br>Normalized to<br>$\mu$ Stops |
|------|-----------|---------|------------------------------------------------|----------------------------------------------|
| 1952 | [96]      | Sn, Sb  | $1.0 \times 10^{-1}$                           | $1.0 \times 10^{-1}$                         |
| 1955 | [98]      | Cu      | $5.0 \times 10^{-4}$                           | $5.4 \times 10^{-4}$                         |
| 1961 | [103]     | Cu      | $4.0 \times 10^{-6}$                           | $4.3 \times 10^{-6}$                         |
| 1961 | [104]     | Cu      | $5.9 \times 10^{-6}$                           | $6.4 \times 10^{-6}$                         |
| 1962 | [105]     | Cu      | $2.2 \times 10^{-7}$                           | $2.4 \times 10^{-7}$                         |
| 1964 | [106]     | Cu      | $2.2 \times 10^{-7}$                           | $2.4 \times 10^{-7}$                         |
| 1972 | [107]     | Cu      | $2.6 \times 10^{-8}$                           | $2.8 \times 10^{-8}$                         |
| 1977 | [108]     | S       | $4.0 \times 10^{-10}$                          | $5.3 \times 10^{-10}$                        |
| 1982 | [109]     | S       | $7.0 \times 10^{-11}$                          | $9.3 \times 10^{-11}$                        |
| 1988 | [110]     | Ti      | $4.6 \times 10^{-12}$                          | $5.4 \times 10^{-12}$                        |
| 1993 | [111]     | Ti      | $4.3 \times 10^{-12}$                          | $5.0 \times 10^{-12}$                        |
| 1995 | [112]     | Ti      | $6.5 \times 10^{-13}$                          | $7.6 \times 10^{-13}$                        |
| 1996 | [102]     | Pb      | $4.6 \times 10^{-11}$                          | $4.7 \times 10^{-11}$                        |
| 2006 | [11]      | Au      | $7.0 \times 10^{-13}$                          | $7.2 \times 10^{-13}$                        |

case the experimental sensitivity depends only on the number of conversion electrons in the signal window over the sensitive time of the experiment, which is also true of a rare decay experiment. Why then should we insert an extraneous muon capture factor into the many theoretical comparisons of conversion vs. decay sensitivity against particular models?

The limits normalized to muon stops and muon capture are listed in Table 5.3. Fig. 5.7 presents our calculation of the  $(Z, A)$  dependence of the CLFV matrix elements without the muon capture normalization, demonstrating the much-reduced extraneous structure heretofore introduced by normalization to the muon capture rate.

Figure 5.9 shows the existing  $\mu \rightarrow e$  conversion and decay experimental limits. Here we normalize the conversion results to muon stops, removing the historical muon capture normalization, making the comparison with decay experiments more consistent.

#### 5.4 Possible Target Considerations

Coherent muon-to-electron conversion in a nucleus results in the emission of a mono-energetic electron with an energy  $E_{\mu e}$  that is nucleus-dependent (104.97 MeV for aluminum (Al)), with

radiative corrections calculated in Ref. [114]. The dominant intrinsic background in a conversion search is electrons from decay-in-orbit. The momentum spectrum of these electrons has a long recoil tail with significant radiative corrections [115, 116] and an endpoint close to the conversion electron signal. Another background source are electrons from radiative pion capture, produced when pions in the muon beamline stop in the target. These pions are captured into the orbit of the nucleus, resulting in the emission of a photon,  $\pi^- + N(A, Z) \rightarrow \gamma^{(*)} + N(A, Z - 1)$ , followed by an asymmetric ( $\gamma \rightarrow e^+ e^-$ ) conversion producing electrons with energies nearly up to the charged pion mass ( $139 \text{ MeV}/c^2$ ). The upcoming Mu2e and COMET experiments mitigate pion backgrounds by using pulsed beams and by exploiting the short pion lifetime ( $\sim 26 \text{ ns}$  at rest), delaying the data-taking window by a few hundred ns. Since the time distribution of the conversion electron depends on the mean lifetime of the muonic atom and is nucleus-dependent (see Table 5.4), this has implications for which target materials can be studied. Cosmic ray-induced backgrounds must also be vetoed, but have a small dependence on stopping target design [22].

Table 5.4 details four potential target materials: titanium, vanadium, lithium, and gold. Figure 5.8 shows the variation of the average capture and decay fractions with atomic number. Heavier nuclei have smaller decay fractions and larger capture fractions, which is beneficial, as it results in fewer decay background electrons for the same number of stopped muons.

Table 5.4: Elements and their characteristics (atomic number ( $Z$ ), density ( $\rho$ ), lifetime ( $\tau_{mean}$ ), and relative average fraction of decay ( $f_{dec.}$ ) to capture ( $f_{capt.}$ ) along with their naturally occurring abundance ( $Ab.$ ) for given isotopes ( $I.$ ), and their nuclear spins ( $s$ )). The experimental values for capture and decay fractions are taken from the Measday compilation [73], a survey experiment [99] or a specific previous experiment (Ref. [100] for  $^{27}\text{Al}$ ).

| Element | $Z$ | $\rho$<br>[g/cm <sup>3</sup> ] | $\tau_{mean}$<br>[ns] | $f_{dec.}$<br>[%] | $f_{capt.}$<br>[%] | $I.$              | $Ab.$<br>[%] | $s$   |
|---------|-----|--------------------------------|-----------------------|-------------------|--------------------|-------------------|--------------|-------|
| Li      | 3   | 0.534                          | 2175                  | 99                | 1                  | $^6\text{Li}$     | 7.6          | 1     |
|         |     |                                |                       |                   |                    | $^7\text{Li}$     | 92.4         | $3/2$ |
| Al      | 13  | 2.11                           | 864                   | 39                | 61                 | $^{27}\text{Al}$  | 100          | $5/2$ |
| Ti      | 22  | 4.51                           | 329                   | 15                | 85                 | $^{46}\text{Ti}$  | 8.25         | 0     |
|         |     |                                |                       |                   |                    | $^{47}\text{Ti}$  | 7.44         | $5/2$ |
|         |     |                                |                       |                   |                    | $^{48}\text{Ti}$  | 73.72        | 0     |
|         |     |                                |                       |                   |                    | $^{49}\text{Ti}$  | 5.41         | $7/2$ |
|         |     |                                |                       |                   |                    | $^{50}\text{Ti}$  | 5.18         | 0     |
| V       | 23  | 6.11                           | 284                   | 13                | 87                 | $^{50}\text{V}$   | 0.25         | 6     |
|         |     |                                |                       |                   |                    | $^{51}\text{V}$   | 99.75        | $7/2$ |
| Au      | 79  | 19.3                           | 73                    | 3                 | 97                 | $^{197}\text{Au}$ | 100          | $3/2$ |

We have considered only coherent contributions from dipole, scalar, and vector interaction, as these conversion rates are enhanced by  $A^2$ . Spin-dependent (SD) contributions, which do not have this coherent enhancement, have been studied in Refs. [68, 71, 117, 118]. The dipole, scalar, and vector operators contribute to the Spin-independent (SI) rate, while axial, tensor, and pseudoscalar operators contribute to the SD rate. The SD rate depends on the distribution of spin in the nucleus [119], and therefore requires detailed modeling of the target nucleus. In most models, SI conversion dominates due to this  $A^2$  enhancement, but this is not true in all models. For example, Ref. [120] describes how the SD interaction induced by ALP- $\pi^0$  mixing is the leading contribution to  $\mu \rightarrow e$  conversion in models where axion-like particles (ALPs) induce the conversion. Consequently, the spin of the target nuclei is important in unraveling the Lorentz structure of the New Physics.

From a single Al conversion measurement, we will not know the form of the coupling. Figs. 5.6 and 5.7 show that if conversion is measured in Al, both titanium (Ti) and vanadium (V) have the advantage of providing good separation in the relative conversion rates produced by the dipole, scalar, and vector interactions. This makes them useful for determining the type of physics responsible. From a practical point of view, Table 5.4 shows that the mean lifetime of a muonic Ti or V atom is not so short that pion-induced backgrounds would overwhelm the conversion signal. Ti and V have smaller average decay fractions than Al, meaning lower decay backgrounds for the same number of stopped muons. For these reasons Ti and V are viable target choices for the next generation of conversion measurements. Natural titanium has several stable isotopes with different spins and separated isotopes of Ti are not readily available in the quantities needed for a target of  $\sim 200$  g. Employing a natural Ti target introduces odd-nucleon isotopes which could produce a non-zero SD response. These SD contributions could be distinguished from the coherent SI response [70], however, this mixing of isotopes complicates the unraveling of SD and SI conversion rates. Vanadium is an attractive alternative; it provides the same physics benefits (increased survival fraction, similar muonic lifetime, *etc.*) with the advantage that it has a single stable isotope,  $^{51}\text{V}$  (spin  $\frac{7}{2}$ ), with  $> 99\%$  abundance.

Figures 5.6 and 5.7 present gold (Au) as an obvious choice. Au has several additional physics benefits, Table 5.4 shows that there is one stable isotope and that the relative fraction of decay to capture in Au is small, meaning on average 3 % of muons will undergo decay, a significant reduction from 39 % in Al. Unfortunately, Au has a mean muonic atom lifetime of just 73 ns so it would not be feasible to use a Au target in a Mu2e or COMET style design due to the enforced time selection required to remove pion-induced backgrounds. If pion contamination could be eliminated using a Fixed Field Alternating-gradient machine such as in the proposed Advanced Muon Facility [66], measuring conversion in Au could be feasible.

Comparing conversion in light targets with very different neutron-to-proton ratios (for example

lithium (Li) and Al) could allow us to distinguish operators involving neutrons from those involving protons [117]. Additionally, Ref. [68] suggests that a conversion measurement in lighter nuclei, such as Li, would be of interest for detecting SD conversion since the SD rate is relatively suppressed by  $1/A^2$  compared to the SI rate. As a result, the ratio  $\omega_{conv,SD}/\omega_{conv,SI}$  is larger in lighter nuclei. A Li foil-style target is feasible [121]. However, the disadvantage here is that the muonic lifetime in Li is close to the free muon lifetime. As a result, the survival fraction is small and the relative decay fraction would be much larger than in Al, meaning more decay background for the same number of stopped muons. Since Li has a much lower density,  $\sim 4$  times less than Al, stopping the same number of muons would require a much larger target volume and due to the much smaller survival fraction, reaching the same sensitivity as aluminum would require a much longer running time.

All the target materials presented here have physics advantages and the specific target chosen will depend on, and influence, the experimental design of any future facility, which is beyond the scope of this paper.

## CONCLUSION

This thesis described the theoretical background and the experimental setup of the Mu2e experiment. More particularly, the Caltech group made several contributions to the electromagnetic calorimeter, such as the preparation and measurement of the scintillating crystals, the successful commissioning of the Deuterium-Tritium neutron generator, and the improvement of the particle identification machine learning algorithm that categorizes electrons generated by cosmic ray and conversion electrons with an accuracy greater than 99 %. In addition, a maximum likelihood method has been implemented to perform the data analysis of the experiment. It can perform two dimensional (momentum and time) fitting of the signal and several backgrounds (DIO, cosmic, RPC), and preliminary results show that the predicted number of events is quite close to the Monte Carlo truth. Finally, an improved calculation of the muon conversion rate in  $^{236}\text{U}$  isotopes has been performed. It includes the effect of quadrupole deformation by using data from muonic X-ray experiments, and the impact of neutron distribution estimation.

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## Appendix A

### TABLE OF OVERLAP INTEGRALS

The results obtained using the method described herein for the 236 stable isotopes with natural abundance  $> 1\%$ .

The description of the columns is as follows:

|                                                        |                                                    |
|--------------------------------------------------------|----------------------------------------------------|
| <b>Isotope:</b> Isotope and nucleon number             | $\beta$ : Permanent quadrupole deformation         |
| $Z$ : Proton number                                    | $\alpha$ and $k$ : Barrett parameters (Sec. 5.2.2) |
| $N$ : Neutron number                                   | $R_{k\alpha}$ : Barrett radius [fm] (Sec. 5.2.2)   |
| $c$ : Radius at half maximum [fm]                      | $D, S(p), V(p), S(n), V(n)$ :                      |
| $t_{eq}$ : Equivalent skin thickness [fm] (Sec. 5.2.2) | Overlap integrals [ $m_\mu^{5/2}$ ] (Sec. 5.2.1)   |

Table A.1: Table of overlap integrals for nuclei assumed spherical

| Isotope             | $Z$ | $N$ | $c$   | $t$ | $D$     | $S(p)$  | $V(p)$  | $S(n)$  | $V(n)$  |
|---------------------|-----|-----|-------|-----|---------|---------|---------|---------|---------|
| ${}^6\text{Li}^a$   | 3   | 3   | 2.13  | 2.3 | 0.00131 | 0.00055 | 0.00055 | 0.00055 | 0.00055 |
| ${}^7\text{Li}^a$   | 3   | 4   | 1.75  | 2.3 | 0.00137 | 0.00058 | 0.00058 | 0.00077 | 0.00078 |
| ${}^9\text{Be}$     | 4   | 5   | 1.789 | 2.3 | 0.00277 | 0.00117 | 0.00118 | 0.00146 | 0.00147 |
| ${}^{10}\text{B}$   | 5   | 5   | 1.928 | 2.3 | 0.00468 | 0.00198 | 0.002   | 0.00198 | 0.002   |
| ${}^{11}\text{B}^a$ | 5   | 6   | 1.82  | 2.3 | 0.00475 | 0.00201 | 0.00203 | 0.00241 | 0.00244 |
| ${}^{12}\text{C}$   | 6   | 6   | 2.001 | 2.3 | 0.0072  | 0.00306 | 0.0031  | 0.00306 | 0.0031  |
| ${}^{13}\text{C}$   | 6   | 7   | 1.996 | 2.3 | 0.0072  | 0.00306 | 0.0031  | 0.00357 | 0.00362 |
| ${}^{14}\text{N}$   | 7   | 7   | 2.151 | 2.3 | 0.01018 | 0.00434 | 0.00441 | 0.00434 | 0.00441 |
| ${}^{16}\text{O}$   | 8   | 8   | 2.413 | 2.3 | 0.01338 | 0.00571 | 0.00582 | 0.00571 | 0.00582 |
| ${}^{19}\text{F}$   | 9   | 10  | 2.776 | 2.3 | 0.01644 | 0.007   | 0.00717 | 0.00778 | 0.00797 |
| ${}^{20}\text{Ne}$  | 10  | 10  | 2.959 | 2.3 | 0.02016 | 0.00859 | 0.00883 | 0.00859 | 0.00883 |
| ${}^{22}\text{Ne}$  | 10  | 12  | 2.871 | 2.3 | 0.02057 | 0.00877 | 0.00901 | 0.01053 | 0.01081 |
| ${}^{23}\text{Na}$  | 11  | 12  | 2.939 | 2.3 | 0.02521 | 0.01077 | 0.0111  | 0.01175 | 0.01211 |
| ${}^{24}\text{Mg}$  | 12  | 12  | 3.045 | 2.3 | 0.02996 | 0.01281 | 0.01325 | 0.01281 | 0.01325 |
| ${}^{25}\text{Mg}$  | 12  | 13  | 2.998 | 2.3 | 0.03031 | 0.01297 | 0.0134  | 0.01405 | 0.01452 |
| ${}^{26}\text{Mg}$  | 12  | 14  | 3.007 | 2.3 | 0.03024 | 0.01294 | 0.01337 | 0.01509 | 0.0156  |
| ${}^{27}\text{Al}$  | 13  | 14  | 3.055 | 2.3 | 0.03579 | 0.01533 | 0.0159  | 0.01651 | 0.01712 |



| Isotope            | $Z$ | $N$ | $c$   | $t$    | $D$     | $S(p)$  | $V(p)$  | $S(n)$  | $V(n)$  |
|--------------------|-----|-----|-------|--------|---------|---------|---------|---------|---------|
| $^{28}\text{Si}$   | 14  | 14  | 3.154 | 2.3    | 0.04118 | 0.01764 | 0.01837 | 0.01764 | 0.01837 |
| $^{29}\text{Si}$   | 14  | 15  | 3.148 | 2.3    | 0.04124 | 0.01767 | 0.0184  | 0.01893 | 0.01971 |
| $^{30}\text{Si}$   | 14  | 16  | 3.172 | 2.3    | 0.04099 | 0.01755 | 0.01828 | 0.02006 | 0.02089 |
| $^{31}\text{P}$    | 15  | 16  | 3.265 | 2.3    | 0.04655 | 0.01994 | 0.02084 | 0.02127 | 0.02223 |
| $^{32}\text{S}$    | 16  | 16  | 3.382 | 2.3    | 0.05187 | 0.0222  | 0.02331 | 0.0222  | 0.02331 |
| $^{34}\text{S}$    | 16  | 18  | 3.418 | 2.3    | 0.05134 | 0.02196 | 0.02306 | 0.0247  | 0.02594 |
| $^{35}\text{Cl}^b$ | 17  | 18  | 3.344 | 2.6718 | 0.05534 | 0.02364 | 0.02493 | 0.02503 | 0.0264  |
| $^{37}\text{Cl}^b$ | 17  | 20  | 3.38  | 2.6762 | 0.05473 | 0.02336 | 0.02464 | 0.02748 | 0.02899 |
| $^{40}\text{Ar}$   | 18  | 22  | 3.642 | 2.3    | 0.0617  | 0.02632 | 0.0279  | 0.03217 | 0.03409 |
| $^{39}\text{K}$    | 19  | 20  | 3.654 | 2.3    | 0.06886 | 0.0294  | 0.03126 | 0.03095 | 0.03291 |
| $^{41}\text{K}$    | 19  | 22  | 3.682 | 2.3    | 0.06825 | 0.02912 | 0.03098 | 0.03372 | 0.03587 |
| $^{40}\text{Ca}$   | 20  | 20  | 3.722 | 2.3    | 0.07495 | 0.03198 | 0.03414 | 0.03198 | 0.03414 |
| $^{44}\text{Ca}$   | 20  | 24  | 3.784 | 2.3    | 0.0734  | 0.03126 | 0.03341 | 0.03752 | 0.0401  |
| $^{45}\text{Sc}$   | 21  | 24  | 3.828 | 2.3    | 0.07996 | 0.03404 | 0.03653 | 0.03891 | 0.04175 |
| $^{46}\text{Ti}$   | 22  | 24  | 3.92  | 2.3    | 0.0851  | 0.03616 | 0.03899 | 0.03945 | 0.04254 |
| $^{47}\text{Ti}$   | 22  | 25  | 3.904 | 2.3    | 0.08559 | 0.03639 | 0.03923 | 0.04135 | 0.04457 |
| $^{48}\text{Ti}$   | 22  | 26  | 3.898 | 2.3    | 0.08576 | 0.03647 | 0.0393  | 0.0431  | 0.04645 |
| $^{49}\text{Ti}$   | 22  | 27  | 3.871 | 2.3    | 0.08661 | 0.03686 | 0.03971 | 0.04524 | 0.04873 |
| $^{50}\text{Ti}$   | 22  | 28  | 3.866 | 2.3    | 0.08675 | 0.03693 | 0.03978 | 0.047   | 0.05062 |
| $^{51}\text{V}$    | 23  | 28  | 3.91  | 2.3    | 0.09342 | 0.03973 | 0.04298 | 0.04837 | 0.05232 |
| $^{50}\text{Cr}$   | 24  | 26  | 4.004 | 2.3    | 0.09829 | 0.04171 | 0.04534 | 0.04518 | 0.04912 |
| $^{52}\text{Cr}$   | 24  | 28  | 3.974 | 2.3    | 0.09936 | 0.0422  | 0.04585 | 0.04924 | 0.05349 |
| $^{53}\text{Cr}$   | 24  | 29  | 4     | 2.3    | 0.09841 | 0.04176 | 0.0454  | 0.05046 | 0.05486 |
| $^{54}\text{Cr}$   | 24  | 30  | 4.042 | 2.3    | 0.09687 | 0.04105 | 0.04466 | 0.05131 | 0.05583 |
| $^{55}\text{Mn}$   | 25  | 30  | 4.073 | 2.3    | 0.1038  | 0.04396 | 0.04802 | 0.05276 | 0.05763 |
| $^{54}\text{Fe}$   | 26  | 28  | 4.055 | 2.3    | 0.11286 | 0.04785 | 0.05242 | 0.05153 | 0.05645 |
| $^{56}\text{Fe}$   | 26  | 30  | 4.12  | 2.3    | 0.11005 | 0.04655 | 0.05107 | 0.05371 | 0.05893 |
| $^{57}\text{Fe}$   | 26  | 31  | 4.144 | 2.3    | 0.109   | 0.04607 | 0.05057 | 0.05493 | 0.0603  |
| $^{59}\text{Co}$   | 27  | 32  | 4.196 | 2.3    | 0.11488 | 0.04847 | 0.05346 | 0.05745 | 0.06335 |
| $^{58}\text{Ni}$   | 28  | 30  | 4.177 | 2.3    | 0.12412 | 0.05242 | 0.05797 | 0.05616 | 0.06211 |
| $^{60}\text{Ni}$   | 28  | 32  | 4.233 | 2.3    | 0.12136 | 0.05115 | 0.05664 | 0.05845 | 0.06474 |
| $^{61}\text{Ni}$   | 28  | 33  | 4.249 | 2.3    | 0.12056 | 0.05078 | 0.05626 | 0.05984 | 0.06631 |

| Isotope            | $Z$ | $N$ | $c$   | $t$ | $D$     | $S(p)$  | $V(p)$  | $S(n)$  | $V(n)$  |
|--------------------|-----|-----|-------|-----|---------|---------|---------|---------|---------|
| $^{62}\text{Ni}$   | 28  | 34  | 4.277 | 2.3 | 0.11922 | 0.05016 | 0.05561 | 0.0609  | 0.06753 |
| $^{63}\text{Cu}$   | 29  | 34  | 4.338 | 2.3 | 0.12419 | 0.05212 | 0.05809 | 0.06111 | 0.0681  |
| $^{65}\text{Cu}$   | 29  | 36  | 4.367 | 2.3 | 0.12268 | 0.05143 | 0.05736 | 0.06384 | 0.0712  |
| $^{64}\text{Zn}$   | 30  | 34  | 4.405 | 2.3 | 0.12865 | 0.05385 | 0.06033 | 0.06103 | 0.06837 |
| $^{66}\text{Zn}$   | 30  | 36  | 4.435 | 2.3 | 0.12699 | 0.05308 | 0.05952 | 0.0637  | 0.07143 |
| $^{67}\text{Zn}^c$ | 30  | 37  | 4.408 | 2.3 | 0.12846 | 0.05376 | 0.06023 | 0.0663  | 0.07429 |
| $^{68}\text{Zn}$   | 30  | 38  | 4.46  | 2.3 | 0.12563 | 0.05246 | 0.05887 | 0.06645 | 0.07457 |
| $^{69}\text{Ga}$   | 31  | 38  | 4.507 | 2.3 | 0.13075 | 0.05448 | 0.06143 | 0.06678 | 0.0753  |
| $^{71}\text{Ga}$   | 31  | 40  | 4.528 | 2.3 | 0.12952 | 0.05392 | 0.06084 | 0.06957 | 0.0785  |
| $^{70}\text{Ge}$   | 32  | 38  | 4.569 | 2.3 | 0.13483 | 0.05601 | 0.0635  | 0.06651 | 0.07541 |
| $^{72}\text{Ge}$   | 32  | 40  | 4.593 | 2.3 | 0.13338 | 0.05534 | 0.0628  | 0.06918 | 0.0785  |
| $^{73}\text{Ge}$   | 32  | 41  | 4.605 | 2.3 | 0.13263 | 0.055   | 0.06244 | 0.07047 | 0.08    |
| $^{74}\text{Ge}$   | 32  | 42  | 4.619 | 2.3 | 0.13182 | 0.05463 | 0.06204 | 0.07171 | 0.08143 |
| $^{76}\text{Ge}$   | 32  | 44  | 4.629 | 2.3 | 0.13117 | 0.05433 | 0.06173 | 0.07471 | 0.08488 |
| $^{75}\text{As}$   | 33  | 42  | 4.653 | 2.3 | 0.13719 | 0.05675 | 0.06475 | 0.07222 | 0.08241 |
| $^{76}\text{Se}$   | 34  | 42  | 4.716 | 2.3 | 0.14051 | 0.05791 | 0.06647 | 0.07154 | 0.08211 |
| $^{77}\text{Se}$   | 34  | 43  | 4.716 | 2.3 | 0.1405  | 0.05791 | 0.06647 | 0.07324 | 0.08406 |
| $^{78}\text{Se}$   | 34  | 44  | 4.718 | 2.3 | 0.14036 | 0.05785 | 0.0664  | 0.07486 | 0.08593 |
| $^{80}\text{Se}$   | 34  | 46  | 4.718 | 2.3 | 0.1404  | 0.05787 | 0.06642 | 0.07829 | 0.08986 |
| $^{82}\text{Se}$   | 34  | 48  | 4.718 | 2.3 | 0.1404  | 0.05786 | 0.06641 | 0.08169 | 0.09376 |
| $^{79}\text{Br}$   | 35  | 44  | 4.752 | 2.3 | 0.1455  | 0.05983 | 0.06901 | 0.07521 | 0.08675 |
| $^{81}\text{Br}$   | 35  | 46  | 4.747 | 2.3 | 0.14581 | 0.05997 | 0.06916 | 0.07882 | 0.09089 |
| $^{80}\text{Kr}$   | 36  | 44  | 4.802 | 2.3 | 0.14923 | 0.06117 | 0.07094 | 0.07476 | 0.08671 |
| $^{82}\text{Kr}$   | 36  | 46  | 4.794 | 2.3 | 0.14979 | 0.06143 | 0.07122 | 0.07849 | 0.091   |
| $^{83}\text{Kr}$   | 36  | 47  | 4.785 | 2.3 | 0.15045 | 0.06172 | 0.07154 | 0.08059 | 0.0934  |
| $^{84}\text{Kr}$   | 36  | 48  | 4.788 | 2.3 | 0.15021 | 0.06162 | 0.07142 | 0.08215 | 0.09523 |
| $^{86}\text{Kr}$   | 36  | 50  | 4.782 | 2.3 | 0.15068 | 0.06183 | 0.07165 | 0.08587 | 0.09951 |
| $^{85}\text{Rb}$   | 37  | 48  | 4.811 | 2.3 | 0.15587 | 0.06382 | 0.07431 | 0.08279 | 0.09641 |
| $^{87}\text{Rb}$   | 37  | 50  | 4.804 | 2.3 | 0.15642 | 0.06407 | 0.07458 | 0.08658 | 0.10079 |
| $^{86}\text{Sr}$   | 38  | 48  | 4.85  | 2.3 | 0.16011 | 0.06537 | 0.07652 | 0.08257 | 0.09665 |
| $^{87}\text{Sr}$   | 38  | 49  | 4.84  | 2.3 | 0.1609  | 0.06573 | 0.07691 | 0.08476 | 0.09917 |
| $^{88}\text{Sr}$   | 38  | 50  | 4.84  | 2.3 | 0.16094 | 0.06574 | 0.07692 | 0.08651 | 0.10121 |

| Isotope             | $Z$ | $N$ | $c$   | $t$    | $D$     | $S(p)$  | $V(p)$  | $S(n)$  | $V(n)$  |
|---------------------|-----|-----|-------|--------|---------|---------|---------|---------|---------|
| $^{89}\text{Y}^b$   | 39  | 50  | 4.76  | 2.5092 | 0.16775 | 0.0686  | 0.0804  | 0.08795 | 0.10307 |
| $^{90}\text{Zr}$    | 40  | 50  | 4.901 | 2.3    | 0.16991 | 0.06904 | 0.0816  | 0.0863  | 0.10201 |
| $^{91}\text{Zr}$    | 40  | 51  | 4.929 | 2.3    | 0.1681  | 0.06822 | 0.08071 | 0.08698 | 0.10291 |
| $^{92}\text{Zr}$    | 40  | 52  | 4.958 | 2.3    | 0.1656  | 0.06709 | 0.07948 | 0.08722 | 0.10332 |
| $^{94}\text{Zr}$    | 40  | 54  | 4.995 | 2.3    | 0.16258 | 0.06572 | 0.07799 | 0.08873 | 0.10529 |
| $^{96}\text{Zr}$    | 40  | 56  | 5.021 | 2.3    | 0.16036 | 0.06473 | 0.0769  | 0.09062 | 0.10766 |
| $^{93}\text{Nb}$    | 41  | 52  | 4.985 | 2.3    | 0.17029 | 0.06882 | 0.08193 | 0.08729 | 0.10391 |
| $^{92}\text{Mo}$    | 42  | 50  | 4.975 | 2.3    | 0.17823 | 0.07201 | 0.086   | 0.08572 | 0.10238 |
| $^{94}\text{Mo}$    | 42  | 52  | 5.026 | 2.3    | 0.1736  | 0.06992 | 0.0837  | 0.08656 | 0.10363 |
| $^{95}\text{Mo}$    | 42  | 53  | 5.041 | 2.3    | 0.17231 | 0.06933 | 0.08307 | 0.08749 | 0.10482 |
| $^{96}\text{Mo}$    | 42  | 54  | 5.071 | 2.3    | 0.1696  | 0.06811 | 0.08172 | 0.08757 | 0.10507 |
| $^{97}\text{Mo}$    | 42  | 55  | 5.076 | 2.3    | 0.16919 | 0.06793 | 0.08152 | 0.08895 | 0.10675 |
| $^{98}\text{Mo}$    | 42  | 56  | 5.105 | 2.3    | 0.16656 | 0.06674 | 0.08022 | 0.08899 | 0.10696 |
| $^{100}\text{Mo}$   | 42  | 58  | 5.156 | 2.3    | 0.16209 | 0.06474 | 0.07802 | 0.08941 | 0.10774 |
| $^{96}\text{Ru}$    | 44  | 50  | 5.085 | 2.3    | 0.18189 | 0.07284 | 0.08811 | 0.08277 | 0.10012 |
| $^{98}\text{Ru}$    | 44  | 54  | 5.128 | 2.3    | 0.17771 | 0.07096 | 0.08603 | 0.08709 | 0.10559 |
| $^{99}\text{Ru}$    | 44  | 55  | 5.145 | 2.3    | 0.17613 | 0.07025 | 0.08525 | 0.08781 | 0.10656 |
| $^{100}\text{Ru}$   | 44  | 56  | 5.171 | 2.3    | 0.17362 | 0.06913 | 0.084   | 0.08798 | 0.10691 |
| $^{101}\text{Ru}$   | 44  | 57  | 5.183 | 2.3    | 0.17254 | 0.06864 | 0.08347 | 0.08892 | 0.10813 |
| $^{102}\text{Ru}$   | 44  | 58  | 5.211 | 2.3    | 0.16992 | 0.06747 | 0.08217 | 0.08894 | 0.10831 |
| $^{104}\text{Ru}$   | 44  | 60  | 5.252 | 2.3    | 0.16617 | 0.0658  | 0.08031 | 0.08972 | 0.10952 |
| $^{103}\text{Rh}^c$ | 45  | 58  | 5.176 | 2.3    | 0.17963 | 0.07142 | 0.08713 | 0.09205 | 0.11231 |
| $^{102}\text{Pd}$   | 46  | 56  | 5.216 | 2.3    | 0.18221 | 0.07216 | 0.08857 | 0.08785 | 0.10782 |
| $^{104}\text{Pd}$   | 46  | 58  | 5.251 | 2.3    | 0.17869 | 0.07059 | 0.08682 | 0.089   | 0.10946 |
| $^{105}\text{Pd}$   | 46  | 59  | 5.261 | 2.3    | 0.17767 | 0.07013 | 0.08631 | 0.08995 | 0.1107  |
| $^{106}\text{Pd}$   | 46  | 60  | 5.285 | 2.3    | 0.17536 | 0.0691  | 0.08516 | 0.09014 | 0.11108 |
| $^{108}\text{Pd}$   | 46  | 62  | 5.318 | 2.3    | 0.17207 | 0.06764 | 0.08352 | 0.09117 | 0.11257 |
| $^{110}\text{Pd}$   | 46  | 64  | 5.349 | 2.3    | 0.16911 | 0.06633 | 0.08206 | 0.09228 | 0.11416 |
| $^{107}\text{Ag}$   | 47  | 60  | 5.301 | 2.3    | 0.17992 | 0.07073 | 0.08758 | 0.09029 | 0.1118  |
| $^{109}\text{Ag}$   | 47  | 62  | 5.331 | 2.3    | 0.1769  | 0.06938 | 0.08607 | 0.09153 | 0.11354 |
| $^{106}\text{Cd}$   | 48  | 58  | 5.288 | 2.3    | 0.18746 | 0.07367 | 0.0915  | 0.08902 | 0.11056 |
| $^{110}\text{Cd}$   | 48  | 62  | 5.344 | 2.3    | 0.18161 | 0.07107 | 0.08857 | 0.0918  | 0.11441 |

| Isotope           | $Z$ | $N$ | $c$   | $t$ | $D$     | $S(p)$  | $V(p)$  | $S(n)$  | $V(n)$  |
|-------------------|-----|-----|-------|-----|---------|---------|---------|---------|---------|
| $^{111}\text{Cd}$ | 48  | 63  | 5.351 | 2.3 | 0.18088 | 0.07075 | 0.08821 | 0.09285 | 0.11577 |
| $^{112}\text{Cd}$ | 48  | 64  | 5.371 | 2.3 | 0.1788  | 0.06983 | 0.08717 | 0.0931  | 0.11623 |
| $^{113}\text{Cd}$ | 48  | 65  | 5.378 | 2.3 | 0.17811 | 0.06952 | 0.08683 | 0.09414 | 0.11758 |
| $^{114}\text{Cd}$ | 48  | 66  | 5.395 | 2.3 | 0.17628 | 0.06871 | 0.08592 | 0.09447 | 0.11813 |
| $^{116}\text{Cd}$ | 48  | 68  | 5.416 | 2.3 | 0.17414 | 0.06776 | 0.08485 | 0.096   | 0.12021 |
| $^{113}\text{In}$ | 49  | 64  | 5.379 | 2.3 | 0.18388 | 0.07167 | 0.08986 | 0.0936  | 0.11737 |
| $^{115}\text{In}$ | 49  | 66  | 5.402 | 2.3 | 0.18146 | 0.0706  | 0.08865 | 0.09509 | 0.11941 |
| $^{116}\text{Sn}$ | 50  | 66  | 5.417 | 2.3 | 0.18565 | 0.07204 | 0.0909  | 0.09509 | 0.11999 |
| $^{117}\text{Sn}$ | 50  | 67  | 5.424 | 2.3 | 0.18491 | 0.07171 | 0.09054 | 0.09609 | 0.12132 |
| $^{118}\text{Sn}$ | 50  | 68  | 5.439 | 2.3 | 0.1833  | 0.071   | 0.08973 | 0.09655 | 0.12203 |
| $^{119}\text{Sn}$ | 50  | 69  | 5.443 | 2.3 | 0.18287 | 0.07081 | 0.08951 | 0.09771 | 0.12353 |
| $^{120}\text{Sn}$ | 50  | 70  | 5.459 | 2.3 | 0.18119 | 0.07007 | 0.08867 | 0.09809 | 0.12414 |
| $^{122}\text{Sn}$ | 50  | 72  | 5.476 | 2.3 | 0.17935 | 0.06925 | 0.08775 | 0.09973 | 0.12637 |
| $^{124}\text{Sn}$ | 50  | 74  | 5.491 | 2.3 | 0.1778  | 0.06857 | 0.08698 | 0.10149 | 0.12873 |
| $^{121}\text{Sb}$ | 51  | 70  | 5.496 | 2.3 | 0.18278 | 0.07036 | 0.08963 | 0.09657 | 0.12302 |
| $^{123}\text{Sb}$ | 51  | 72  | 5.508 | 2.3 | 0.18153 | 0.06981 | 0.089   | 0.09855 | 0.12565 |
| $^{122}\text{Te}$ | 52  | 70  | 5.537 | 2.3 | 0.18387 | 0.07042 | 0.09033 | 0.0948  | 0.1216  |
| $^{124}\text{Te}$ | 52  | 72  | 5.55  | 2.3 | 0.18238 | 0.06977 | 0.08958 | 0.0966  | 0.12404 |
| $^{125}\text{Te}$ | 52  | 73  | 5.553 | 2.3 | 0.18212 | 0.06966 | 0.08946 | 0.09779 | 0.12558 |
| $^{126}\text{Te}$ | 52  | 74  | 5.562 | 2.3 | 0.18112 | 0.06922 | 0.08895 | 0.0985  | 0.12659 |
| $^{128}\text{Te}$ | 52  | 76  | 5.573 | 2.3 | 0.17991 | 0.06869 | 0.08835 | 0.10039 | 0.12912 |
| $^{130}\text{Te}$ | 52  | 78  | 5.583 | 2.3 | 0.17878 | 0.06819 | 0.08778 | 0.10229 | 0.13167 |
| $^{127}\text{I}$  | 53  | 74  | 5.593 | 2.3 | 0.18299 | 0.06963 | 0.09005 | 0.09721 | 0.12573 |
| $^{128}\text{Xe}$ | 54  | 74  | 5.63  | 2.3 | 0.18405 | 0.06967 | 0.09074 | 0.09548 | 0.12435 |
| $^{129}\text{Xe}$ | 54  | 75  | 5.632 | 2.3 | 0.18392 | 0.06962 | 0.09068 | 0.09669 | 0.12594 |
| $^{130}\text{Xe}$ | 54  | 76  | 5.641 | 2.3 | 0.18282 | 0.06914 | 0.09013 | 0.09731 | 0.12684 |
| $^{131}\text{Xe}$ | 54  | 77  | 5.638 | 2.3 | 0.18314 | 0.06928 | 0.09028 | 0.09879 | 0.12874 |
| $^{132}\text{Xe}$ | 54  | 78  | 5.646 | 2.3 | 0.18228 | 0.0689  | 0.08985 | 0.09953 | 0.12979 |
| $^{134}\text{Xe}$ | 54  | 80  | 5.654 | 2.3 | 0.18139 | 0.06852 | 0.08941 | 0.1015  | 0.13245 |
| $^{136}\text{Xe}$ | 54  | 82  | 5.664 | 2.3 | 0.18025 | 0.06802 | 0.08883 | 0.10328 | 0.13489 |
| $^{133}\text{Cs}$ | 55  | 78  | 5.671 | 2.3 | 0.18447 | 0.06942 | 0.09109 | 0.09845 | 0.12918 |
| $^{134}\text{Ba}$ | 56  | 78  | 5.707 | 2.3 | 0.18538 | 0.0694  | 0.09171 | 0.09667 | 0.12774 |

| Isotope           | $Z$ | $N$ | $c$   | $t$ | $D$     | $S(p)$  | $V(p)$  | $S(n)$  | $V(n)$  |
|-------------------|-----|-----|-------|-----|---------|---------|---------|---------|---------|
| $^{135}\text{Ba}$ | 56  | 79  | 5.703 | 2.3 | 0.18576 | 0.06956 | 0.0919  | 0.09814 | 0.12964 |
| $^{136}\text{Ba}$ | 56  | 80  | 5.711 | 2.3 | 0.18485 | 0.06917 | 0.09144 | 0.09881 | 0.13063 |
| $^{137}\text{Ba}$ | 56  | 81  | 5.71  | 2.3 | 0.18494 | 0.06921 | 0.09149 | 0.10011 | 0.13233 |
| $^{138}\text{Ba}$ | 56  | 82  | 5.72  | 2.3 | 0.18382 | 0.06872 | 0.09092 | 0.10063 | 0.13313 |
| $^{139}\text{La}$ | 57  | 82  | 5.742 | 2.3 | 0.18613 | 0.06931 | 0.09225 | 0.09971 | 0.13271 |
| $^{140}\text{Ce}$ | 58  | 82  | 5.774 | 2.3 | 0.18723 | 0.06937 | 0.09297 | 0.09807 | 0.13144 |
| $^{142}\text{Ce}$ | 58  | 84  | 5.815 | 2.3 | 0.18229 | 0.06724 | 0.09048 | 0.09738 | 0.13103 |
| $^{141}\text{Pr}$ | 59  | 82  | 5.795 | 2.3 | 0.18947 | 0.06991 | 0.09426 | 0.09716 | 0.13101 |
| $^{203}\text{Tl}$ | 81  | 122 | 6.602 | 2.3 | 0.16445 | 0.05061 | 0.08501 | 0.07622 | 0.12804 |
| $^{205}\text{Tl}$ | 81  | 124 | 6.617 | 2.3 | 0.16241 | 0.04979 | 0.08396 | 0.07622 | 0.12853 |
| $^{204}\text{Pb}$ | 82  | 122 | 6.617 | 2.3 | 0.16521 | 0.05052 | 0.08556 | 0.07516 | 0.12729 |
| $^{206}\text{Pb}$ | 82  | 124 | 6.631 | 2.3 | 0.16325 | 0.04974 | 0.08455 | 0.07521 | 0.12785 |
| $^{207}\text{Pb}$ | 82  | 125 | 6.637 | 2.3 | 0.16248 | 0.04943 | 0.08415 | 0.07536 | 0.12828 |
| $^{208}\text{Pb}$ | 82  | 126 | 6.637 | 2.3 | 0.16247 | 0.04943 | 0.08414 | 0.07595 | 0.12929 |
| $^{209}\text{Bi}$ | 83  | 126 | 6.687 | 2.3 | 0.15828 | 0.04738 | 0.08213 | 0.07193 | 0.12468 |

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<sup>a</sup>Landolt-Börnstein (only rms radius) [88]

<sup>b</sup>deVries et al.[69]

<sup>c</sup>Angeli et al.[93]

Table A.2: Table of overlap integrals for deformed nuclei

| Isotope             | Z  | N   | c     | $t_{eq}$ | $\beta$ | $\alpha$           | k                  | $R_{k\alpha}$ | D      | $S(p)$ | $V(p)$ | $S(n)$ | $V(n)$ |
|---------------------|----|-----|-------|----------|---------|--------------------|--------------------|---------------|--------|--------|--------|--------|--------|
| $^{142}\text{Nd}$   | 60 | 82  | 5.825 | 2.3      | 0       | 0.124              | 2.243              | 6.284         | 0.1905 | 0.0699 | 0.095  | 0.0956 | 0.1298 |
| $^{143}\text{Nd}$   | 60 | 83  | 5.84  | 2.303    | 0.032   | 0.124              | 2.243              | 6.3           | 0.1885 | 0.0691 | 0.094  | 0.0956 | 0.13   |
| $^{144}\text{Nd}$   | 60 | 84  | 5.864 | 2.3      | 0       | 0.124              | 2.243              | 6.32          | 0.1857 | 0.0679 | 0.0925 | 0.095  | 0.1296 |
| $^{145}\text{Nd}$   | 60 | 85  | 5.881 | 2.341    | 0.109   | 0.124              | 2.243              | 6.351         | 0.1824 | 0.0665 | 0.0908 | 0.0942 | 0.1287 |
| $^{146}\text{Nd}$   | 60 | 86  | 5.902 | 2.383    | 0.154   | 0.124              | 2.243              | 6.386         | 0.1785 | 0.0649 | 0.0888 | 0.0931 | 0.1274 |
| $^{148}\text{Nd}$   | 60 | 88  | 5.944 | 2.46     | 0.213   | 0.124              | 2.243              | 6.454         | 0.1711 | 0.0618 | 0.085  | 0.0909 | 0.125  |
| $^{150}\text{Nd}$   | 60 | 90  | 5.882 | 2.758    | 0.371   | 0.138              | 2.346              | 6.52          | 0.1683 | 0.0609 | 0.0833 | 0.092  | 0.1258 |
| $^{144}\text{Sm}$   | 62 | 82  | 5.862 | 2.298    | 0       | 0.138              | 2.319              | 6.315         | 0.1951 | 0.0711 | 0.0976 | 0.094  | 0.1291 |
| $^{147}\text{Sm}$   | 62 | 85  | 5.945 | 2.275    | 0.14    | 0.138              | 2.319              | 6.382         | 0.1855 | 0.0669 | 0.0927 | 0.0917 | 0.1272 |
| $^{148}\text{Sm}$   | 62 | 86  | 6.008 | 2.176    | 0.156   | 0.135              | 2.295              | 6.405         | 0.1806 | 0.0646 | 0.0902 | 0.0898 | 0.1254 |
| $^{149}\text{Sm}$   | 62 | 87  | 5.981 | 2.29     | 0.183   | 0.136              | 2.304              | 6.421         | 0.1804 | 0.0648 | 0.0902 | 0.0909 | 0.1265 |
| $^{150}\text{Sm}$   | 62 | 88  | 5.856 | 2.607    | 0.222   | 0.125              | 2.221              | 6.431         | 0.1851 | 0.0671 | 0.0922 | 0.0957 | 0.1315 |
| $^{152}\text{Sm}$   | 62 | 90  | 5.869 | 2.741    | 0.309   | 0.133              | 2.288              | 6.499         | 0.1788 | 0.0645 | 0.0888 | 0.0944 | 0.13   |
| $^{154}\text{Sm}$   | 62 | 92  | 5.966 | 2.619    | 0.345   | 0.133              | 2.288              | 6.535         | 0.1717 | 0.0614 | 0.0854 | 0.0917 | 0.1275 |
| $^{151}\text{Eu}$   | 63 | 88  | 6.037 | 2.357    | 0.215   | 0.136              | 2.301              | 6.497         | 0.1757 | 0.0625 | 0.0879 | 0.0872 | 0.1228 |
| $^{153}\text{Eu}$   | 63 | 90  | 5.935 | 2.532    | 0.249   | 0.136              | 2.307              | 6.471         | 0.1825 | 0.0656 | 0.0913 | 0.0938 | 0.1305 |
| $^{154}\text{Gd}$   | 64 | 90  | 5.963 | 2.626    | 0.291   | 0.136              | 2.295              | 6.533         | 0.18   | 0.0641 | 0.0898 | 0.0908 | 0.1273 |
| $^{155}\text{Gd}$   | 64 | 91  | 6.02  | 2.403    | 0.249   | 0.14               | 2.332              | 6.498         | 0.1805 | 0.0642 | 0.0905 | 0.0912 | 0.1287 |
| $^{156}\text{Gd}$   | 64 | 92  | 6.009 | 2.658    | 0.341   | 0.137              | 2.311              | 6.589         | 0.1733 | 0.0613 | 0.0864 | 0.0889 | 0.1252 |
| $^{157}\text{Gd}$   | 64 | 93  | 6.01  | 2.475    | 0.271   | 0.135              | 2.292              | 6.516         | 0.1793 | 0.0638 | 0.0899 | 0.0927 | 0.1306 |
| $^{158}\text{Gd}$   | 64 | 94  | 6.023 | 2.678    | 0.35    | 0.137              | 2.31               | 6.608         | 0.1711 | 0.0604 | 0.0853 | 0.0894 | 0.1262 |
| $^{160}\text{Gd}$   | 64 | 96  | 6.061 | 2.645    | 0.358   | 0.132              | 2.268              | 6.629         | 0.1678 | 0.059  | 0.0837 | 0.089  | 0.1263 |
| $^{159}\text{Tb}^d$ | 65 | 94  | 6.2   | 1.984    | 0.3     | 0.137 <sup>e</sup> | 2.304 <sup>e</sup> | 6.521         | 0.1738 | 0.0602 | 0.0873 | 0.0871 | 0.1263 |
| $^{160}\text{Dy}^c$ | 66 | 94  | 6.092 | 2.712    | 0.338   | 0.139              | 2.306              | 6.682         | 0.1695 | 0.0591 | 0.0849 | 0.0847 | 0.1216 |
| $^{161}\text{Dy}$   | 66 | 95  | 6.038 | 2.564    | 0.271   | 0.139              | 2.306              | 6.574         | 0.181  | 0.0639 | 0.091  | 0.0919 | 0.1311 |
| $^{162}\text{Dy}$   | 66 | 96  | 6.042 | 2.725    | 0.347   | 0.139              | 2.307              | 6.642         | 0.1751 | 0.0615 | 0.0877 | 0.0899 | 0.1282 |
| $^{163}\text{Dy}$   | 66 | 97  | 6.044 | 2.587    | 0.283   | 0.139              | 2.31               | 6.589         | 0.1794 | 0.0632 | 0.0902 | 0.0929 | 0.1326 |
| $^{164}\text{Dy}$   | 66 | 98  | 6.058 | 2.753    | 0.358   | 0.138              | 2.308              | 6.67          | 0.1721 | 0.0603 | 0.0863 | 0.0899 | 0.1286 |
| $^{165}\text{Ho}^c$ | 67 | 98  | 6.12  | 2.78     | 0.284   | 0.14               | 2.314              | 6.735         | 0.1676 | 0.0583 | 0.0843 | 0.0852 | 0.1233 |
| $^{164}\text{Er}^c$ | 68 | 96  | 6.14  | 2.702    | 0.331   | 0.143              | 2.32               | 6.719         | 0.1713 | 0.0592 | 0.0862 | 0.0838 | 0.1222 |
| $^{166}\text{Er}$   | 68 | 98  | 6.098 | 2.742    | 0.351   | 0.143              | 2.331              | 6.698         | 0.1752 | 0.0609 | 0.0882 | 0.088  | 0.1275 |
| $^{167}\text{Er}$   | 68 | 99  | 6.108 | 2.622    | 0.297   | 0.142              | 2.319              | 6.659         | 0.178  | 0.0619 | 0.0898 | 0.0901 | 0.1308 |
| $^{168}\text{Er}$   | 68 | 100 | 6.121 | 2.764    | 0.359   | 0.141              | 2.316              | 6.728         | 0.1716 | 0.0595 | 0.0865 | 0.0876 | 0.1273 |
| $^{170}\text{Er}$   | 68 | 102 | 6.144 | 2.765    | 0.358   | 0.141              | 2.32               | 6.749         | 0.1689 | 0.0583 | 0.0851 | 0.0876 | 0.1278 |
| $^{169}\text{Tm}^f$ | 69 | 100 | 6.126 | 2.567    | 0.298   | 0.141 <sup>e</sup> | 2.295 <sup>e</sup> | 6.652         | 0.1812 | 0.0628 | 0.0916 | 0.091  | 0.1328 |
| $^{170}\text{Yb}$   | 70 | 100 | 6.212 | 2.675    | 0.357   | 0.141 <sup>e</sup> | 2.305 <sup>e</sup> | 6.773         | 0.1705 | 0.058  | 0.0861 | 0.0831 | 0.1234 |
| $^{171}\text{Yb}$   | 70 | 101 | 6.214 | 2.535    | 0.299   | 0.141 <sup>e</sup> | 2.305 <sup>e</sup> | 6.721         | 0.1746 | 0.0596 | 0.0884 | 0.0859 | 0.1276 |
| $^{172}\text{Yb}$   | 70 | 102 | 6.227 | 2.657    | 0.349   | 0.141 <sup>e</sup> | 2.305 <sup>e</sup> | 6.779         | 0.1692 | 0.0575 | 0.0856 | 0.0858 | 0.1277 |
| $^{173}\text{Yb}$   | 70 | 103 | 6.234 | 2.539    | 0.3     | 0.141 <sup>e</sup> | 2.305 <sup>e</sup> | 6.741         | 0.172  | 0.0585 | 0.0871 | 0.086  | 0.1281 |
| $^{174}\text{Yb}$   | 70 | 104 | 6.2   | 2.72     | 0.336   | 0.141 <sup>e</sup> | 2.305 <sup>e</sup> | 6.779         | 0.1706 | 0.0581 | 0.0861 | 0.0866 | 0.1283 |
| $^{176}\text{Yb}$   | 70 | 106 | 6.271 | 2.61     | 0.328   | 0.141 <sup>e</sup> | 2.305 <sup>e</sup> | 6.801         | 0.1652 | 0.0557 | 0.0834 | 0.0847 | 0.1269 |
| $^{175}\text{Lu}^c$ | 71 | 104 | 6.313 | 2.627    | 0.289   | 0.14 <sup>e</sup>  | 2.314 <sup>e</sup> | 6.847         | 0.1629 | 0.0545 | 0.0826 | 0.0799 | 0.121  |

| Isotope             | $Z$ | $N$ | $c$   | $t_{eq}$ | $\beta$ | $\alpha$            | $k$                | $R_{k\alpha}$ | $D$    | $S(p)$ | $V(p)$ | $S(n)$ | $V(n)$ |
|---------------------|-----|-----|-------|----------|---------|---------------------|--------------------|---------------|--------|--------|--------|--------|--------|
| $^{176}\text{Lu}^c$ | 71  | 105 | 6.329 | 2.605    | 0.278   | 0.14 <sup>c</sup>   | 2.314 <sup>c</sup> | 6.853         | 0.1616 | 0.0539 | 0.0819 | 0.0798 | 0.1212 |
| $^{176}\text{Hf}$   | 72  | 104 | 6.288 | 2.643    | 0.305   | 0.1388              | 2.274              | 6.828         | 0.1688 | 0.0567 | 0.0859 | 0.0817 | 0.1238 |
| $^{177}\text{Hf}$   | 72  | 105 | 6.297 | 2.575    | 0.277   | 0.1388              | 2.275              | 6.81          | 0.1697 | 0.0568 | 0.0862 | 0.0829 | 0.1258 |
| $^{178}\text{Hf}$   | 72  | 106 | 6.317 | 2.607    | 0.296   | 0.1388              | 2.275              | 6.84          | 0.1663 | 0.0555 | 0.0845 | 0.0816 | 0.1242 |
| $^{179}\text{Hf}$   | 72  | 107 | 6.348 | 2.485    | 0.267   | 0.1388              | 2.276              | 6.824         | 0.1659 | 0.0551 | 0.0843 | 0.0819 | 0.1253 |
| $^{180}\text{Hf}$   | 72  | 108 | 6.318 | 2.57     | 0.286   | 0.1457              | 2.331              | 6.827         | 0.1673 | 0.0558 | 0.085  | 0.0837 | 0.1274 |
| $^{181}\text{Ta}$   | 73  | 108 | 6.367 | 2.446    | 0.255   | 0.1462              | 2.327              | 6.826         | 0.1678 | 0.0554 | 0.0855 | 0.082  | 0.1265 |
| $^{182}\text{W}$    | 74  | 108 | 6.334 | 2.594    | 0.273   | 0.1464              | 2.32               | 6.848         | 0.171  | 0.0567 | 0.0873 | 0.0826 | 0.1271 |
| $^{183}\text{W}^c$  | 74  | 109 | 6.343 | 2.536    | 0.243   | 0.147               | 2.33               | 6.837         | 0.1715 | 0.0567 | 0.0875 | 0.0835 | 0.1288 |
| $^{184}\text{W}$    | 74  | 110 | 6.36  | 2.569    | 0.26    | 0.1483              | 2.358              | 6.865         | 0.1684 | 0.0556 | 0.086  | 0.0824 | 0.1275 |
| $^{186}\text{W}$    | 74  | 112 | 6.384 | 2.559    | 0.254   | 0.1465              | 2.324              | 6.882         | 0.1656 | 0.0544 | 0.0845 | 0.0822 | 0.1277 |
| $^{185}\text{Re}^c$ | 75  | 110 | 6.36  | 2.498    | 0.221   | 0.1458 <sup>c</sup> | 2.311 <sup>c</sup> | 6.837         | 0.1737 | 0.0571 | 0.0888 | 0.0838 | 0.1302 |
| $^{187}\text{Re}^c$ | 75  | 112 | 6.374 | 2.498    | 0.221   | 0.1458 <sup>c</sup> | 2.311 <sup>c</sup> | 6.85          | 0.1718 | 0.0564 | 0.0878 | 0.0842 | 0.1311 |
| $^{186}\text{Os}^g$ | 76  | 110 | 6.414 | 2.572    | 0.261   | 0.1445              | 2.28               | 6.911         | 0.1676 | 0.0545 | 0.0859 | 0.0787 | 0.124  |
| $^{187}\text{Os}^c$ | 76  | 111 | 6.416 | 2.48     | 0.209   | 0.1445              | 2.285              | 6.88          | 0.17   | 0.0552 | 0.087  | 0.0806 | 0.1271 |
| $^{188}\text{Os}$   | 76  | 112 | 6.427 | 2.561    | 0.243   | 0.1445              | 2.289              | 6.92          | 0.1663 | 0.0539 | 0.0852 | 0.0793 | 0.1253 |
| $^{189}\text{Os}^c$ | 76  | 113 | 6.435 | 2.463    | 0.198   | 0.1445              | 2.29               | 6.892         | 0.168  | 0.0543 | 0.086  | 0.0808 | 0.1279 |
| $^{190}\text{Os}$   | 76  | 114 | 6.456 | 2.452    | 0.194   | 0.1445              | 2.292              | 6.907         | 0.1656 | 0.0534 | 0.0849 | 0.08   | 0.1271 |
| $^{192}\text{Os}$   | 76  | 116 | 6.483 | 2.37     | 0.169   | 0.1445              | 2.293              | 6.904         | 0.1642 | 0.0526 | 0.0841 | 0.0803 | 0.1283 |
| $^{191}\text{Ir}^c$ | 77  | 114 | 6.45  | 2.413    | 0.164   | 0.1455 <sup>c</sup> | 2.293 <sup>c</sup> | 6.888         | 0.1704 | 0.0548 | 0.0874 | 0.0812 | 0.1294 |
| $^{193}\text{Ir}^c$ | 77  | 116 | 6.472 | 2.384    | 0.141   | 0.1455 <sup>c</sup> | 2.293 <sup>c</sup> | 6.898         | 0.1683 | 0.0539 | 0.0864 | 0.0812 | 0.1301 |
| $^{194}\text{Pt}$   | 78  | 116 | 6.537 | 2.387    | -0.145  | 0.1465              | 2.298              | 6.959         | 0.1625 | 0.0513 | 0.0836 | 0.0761 | 0.1241 |
| $^{195}\text{Pt}$   | 78  | 117 | 6.541 | 2.373    | 0.13    | 0.1465              | 2.298              | 6.958         | 0.1624 | 0.0511 | 0.0835 | 0.0767 | 0.1252 |
| $^{196}\text{Pt}$   | 78  | 118 | 6.547 | 2.369    | -0.129  | 0.1464              | 2.298              | 6.963         | 0.1616 | 0.0508 | 0.0832 | 0.0768 | 0.1256 |
| $^{198}\text{Pt}$   | 78  | 120 | 6.56  | 2.349    | -0.108  | 0.1463              | 2.299              | 6.968         | 0.1605 | 0.0503 | 0.0825 | 0.0774 | 0.1269 |
| $^{197}\text{Au}$   | 79  | 118 | 6.554 | 2.365    | -0.125  | 0.1477              | 2.3                | 6.967         | 0.1637 | 0.0512 | 0.0843 | 0.0765 | 0.1259 |
| $^{198}\text{Hg}$   | 80  | 118 | 6.569 | 2.357    | -0.116  | 0.1488              | 2.303              | 6.978         | 0.1647 | 0.0513 | 0.0851 | 0.0755 | 0.1252 |
| $^{199}\text{Hg}$   | 80  | 119 | 6.571 | 2.356    | -0.115  | 0.1488              | 2.303              | 6.979         | 0.1645 | 0.0512 | 0.0849 | 0.0761 | 0.1262 |
| $^{200}\text{Hg}$   | 80  | 120 | 6.582 | 2.341    | -0.098  | 0.1487              | 2.303              | 6.985         | 0.1633 | 0.0507 | 0.0843 | 0.0759 | 0.1263 |
| $^{201}\text{Hg}^c$ | 80  | 121 | 6.583 | 2.33     | -0.084  | 0.1486              | 2.303              | 6.982         | 0.1635 | 0.0507 | 0.0844 | 0.0767 | 0.1276 |
| $^{202}\text{Hg}$   | 80  | 122 | 6.596 | 2.327    | -0.079  | 0.1486              | 2.303              | 6.992         | 0.1619 | 0.0501 | 0.0836 | 0.0763 | 0.1274 |
| $^{204}\text{Hg}$   | 80  | 124 | 6.611 | 2.319    | -0.066  | 0.1485              | 2.303              | 7.002         | 0.1601 | 0.0493 | 0.0826 | 0.0764 | 0.128  |
| $^{232}\text{Th}^h$ | 90  | 142 | 6.945 | 2.581    | 0.263   | 0.165 <sup>c</sup>  | 2.344 <sup>c</sup> | 7.387         | 0.1344 | 0.0363 | 0.0707 | 0.0572 | 0.1113 |
| $^{238}\text{U}^i$  | 92  | 146 | 7.011 | 2.627    | 0.288   | 0.1626 <sup>c</sup> | 2.35 <sup>c</sup>  | 7.467         | 0.129  | 0.0337 | 0.0681 | 0.0534 | 0.108  |



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<sup>a</sup>Landolt-Börnstein (only rms radius) [88]

<sup>b</sup>deVries et al.[69]

<sup>c</sup>Angeli et al.[93]

<sup>d</sup>deWit et al. [89]

<sup>e</sup> $\alpha$  and  $k$  are interpolated using neighboring elements

<sup>f</sup>Landolt-Börnstein [88]

<sup>g</sup>Hoehn et al. [90]

<sup>h</sup>Zumbro et al. (1986) [91]

<sup>i</sup>Zumbro et al. (1984) [92]

### A.1 Comparison of overlap integral determinations

In three instances,  $^{13}_{27}\text{Al}$ ,  $^{142}_{58}\text{Ce}$  and  $^{208}_{82}\text{Pb}$ , we have been able to compare our calculation with earlier work and alternative experimental inputs [61, 64, 78, 122].

In calculating the CLFV matrix elements, Kitano *et al.* primarily used neutron distributions equal to proton distributions. In a few cases, they also compared the  $S(n)$  and  $V(n)$  values determined using direct measurements from pionic atoms and proton scattering. They also assigned an uncertainty in the pionic atom case based on the uncertainty of the  $C_n$  parameter. A recent measurement of the neutron radius of aluminum [122] provides a third example.

Figures A.1 – A.3 show comparisons of the overlap integrals for  $^{13}_{27}\text{Al}$ ,  $^{142}_{58}\text{Ce}$  and  $^{208}_{82}\text{Pb}$  from the different calculations. Ce and Pb are spherical nuclei and Al has a quadrupole moment  $\beta = -0.392$ . The overlap integrals for these nuclei are not surprisingly in excellent agreement. The uncertainties assigned to the pionic atom neutron distribution by Kitano *et al.* are shown. It is notable that the  $S(n)$  and  $V(n)$  values Kitano *et al.* that use the pionic atom measurements are in agreement with the values obtained using the Zhang *et al.* model for the neutron distribution. For aluminum, we use the recent measurement of the neutron radius via parity-violating electron scattering [122][123]. Since  $^{27}\text{Al}$  is an odd-even nucleus, there is no Zhang *et al.* result. We, therefore, use the neutron skin calculation of [124].

The results for aluminum are not particularly sensitive to the neutron model used, as there is only one more neutron than proton in the nucleus. For cerium and lead, the use of experimental measurements of the neutron distribution rather than proton distribution leads to better agreement with the Zhang *et al.* model results, providing support for our approach.

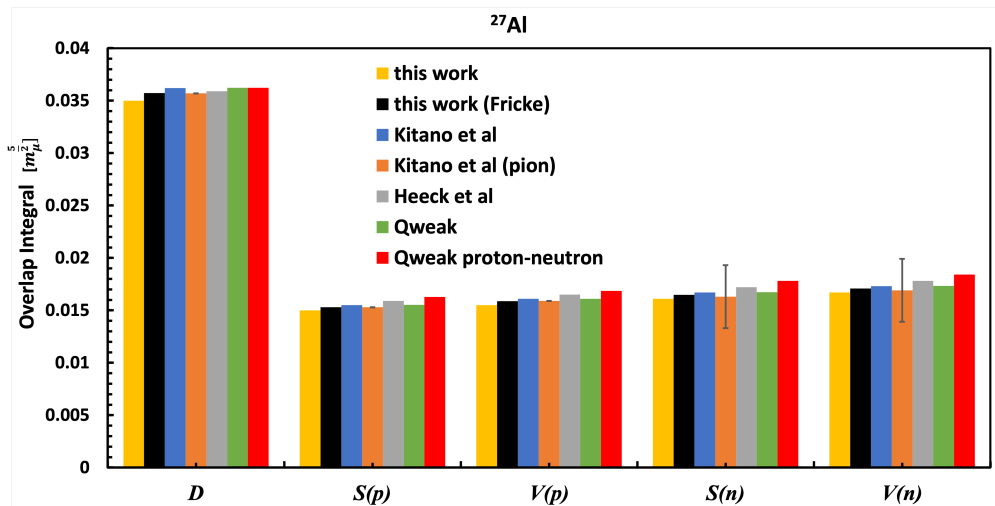


Figure A.1: Comparison of CLFV overlap integral values for aluminum using  $N/Z$  scaling for the neutron overlap integral with experimental measurements and the Zhang *et al.* model.

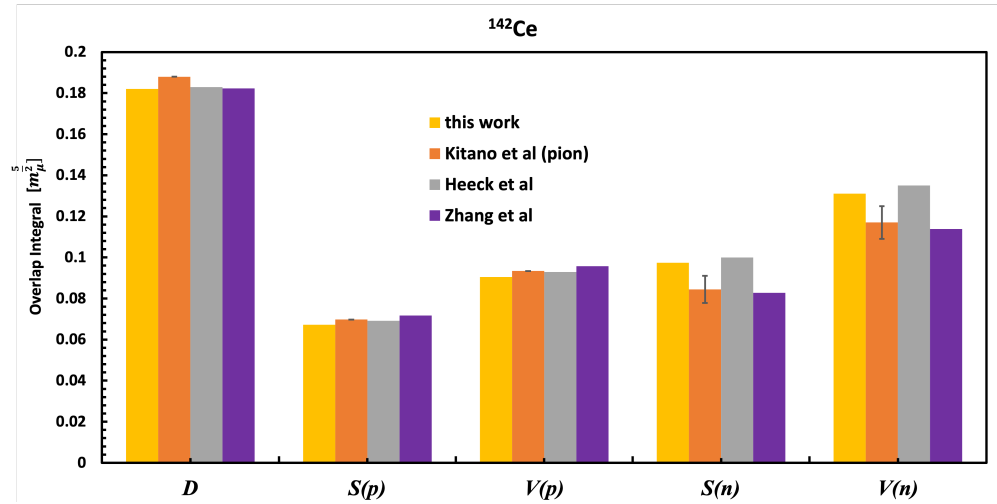


Figure A.2: Comparison of CLFV overlap integral values for cerium using  $N/Z$  scaling for the neutron overlap integral with experimental measurements and the Zhang *et al.* model.

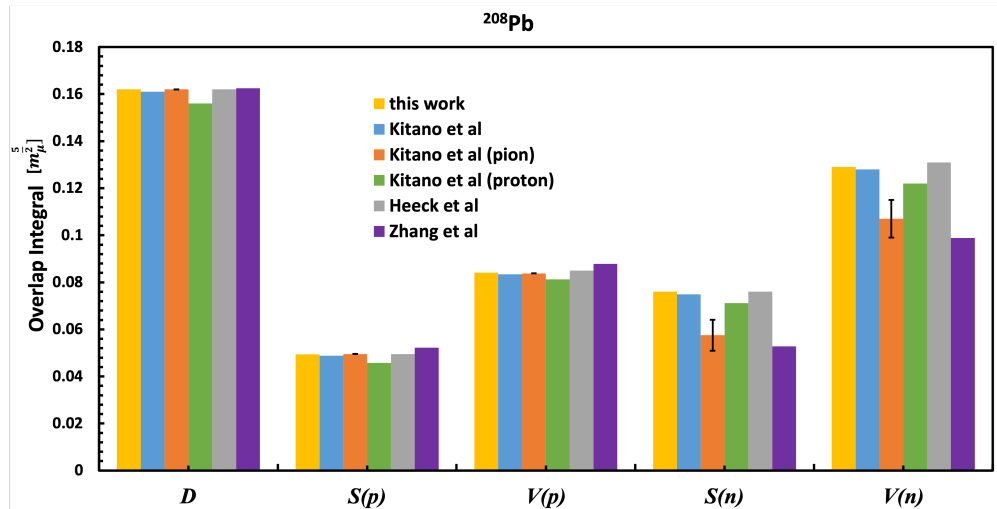


Figure A.3: Comparison of CLFV overlap integral values for lead using  $N/Z$  scaling for the neutron overlap integral with experimental measurements and the Zhang *et al.* model.

