

COMPTON SCATTERING CALIBRATION FOR CRYOGENIC SILICON
CALORIMETERS

by

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Abstract

The nature of dark matter remains unknown, with no experimental confirmation of existing theories. The upcoming SuperCDMS SNOLAB experiment seeks to probe dark matter particle models with masses below $10 \text{ GeV}/c^2$. To achieve this, the SuperCDMS collaboration has developed cryogenic sampling calorimeters with energy thresholds down to the sub-eV energy range.

The response of the SuperCDMS detectors is not fully characterized theoretically, requiring empirical calibration techniques down to their energy thresholds. A key challenge for an empirical calibration technique is to achieve a uniform distribution of energy depositions throughout the detector target, as expected from dark matter particles.

This thesis presents the development of a novel calibration technique for SuperCDMS silicon detectors utilizing energy signatures from the Compton scattering energy depositions. The simulations supporting this calibration method are discussed. Additionally, the inference model to identify the calibration signatures in the data, and the procedure to construct the calibration function is described. This thesis further demonstrates a successful calibration of experimental data from four SuperCDMS R&D detectors using this approach. Finally, a comparison is made between the new method and an alternative calibration technique using optical photons (2 eV).

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I am grateful to my colleagues Sudipta Das, Enze Zhang, and Stefan Zatchler for their contributions to the study presented in this thesis. Stefan led the Geant4 simulations described in Chapter 3, while I conducted the analysis of the simulated data. Enze spearheaded the processing of the experimental data detailed in Chapter 4, and I carried out additional validations and fine-tuning specific to the data in this study. Sudipta studied the triggering efficiency and analyzed the Compton K-step and copper K_α X-ray peak energy signatures presented in Chapter 5 using the Integral energy estimator. Sudipta also developed the core of the LED calibration described in Chapter 6. The comparison between the LED and Compton calibrations, including the uncertainty estimations discussed at the end of Chapter 6, was a collaborative work between Sudipta and me. Throughout this thesis, any plot or figure that is not my own work is credited in the caption.

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Glossary

BSM Beyond the Standard Model. [3](#)

CP Compton Profile. [x](#), [31–33](#), [174](#)

CT charge-trapping. [ix](#), [12](#), [19](#), [21](#), [39](#)

DCRC Detector Control and Readout Card. [49](#)

DDSCS double-differential scattering cross section. [170](#), [171](#)

DM Dark Matter. [1–9](#), [39](#), [43](#), [87](#), [90](#)

DSF Dynamical structure factor. [x](#), [32–34](#), [171](#), [175](#)

e⁻h⁺ electron-hole. [viii](#), [ix](#), [xiv](#), [16–21](#), [39](#), [41](#), [51](#), [64](#), [65](#), [68](#), [74](#), [110](#), [138](#), [142](#),
[144–149](#), [151](#), [153–155](#), [157](#), [159](#), [160](#), [165](#), [166](#)

ER electron recoil. [4](#)

GF Gaussian derivative filter. [49](#)

HDI highest density interval. [xii](#), [98–101](#), [104](#)

HV High-Voltage. [19](#), [42](#)

HVeV high-voltage eV-resolution. [viii–x](#), [xiii](#), [15](#), [27](#), [28](#), [38–40](#), [43](#), [48](#), [49](#), [51](#), [63](#),
[87](#), [94](#), [101](#), [103](#), [112](#), [113](#), [120](#), [140–142](#), [149](#), [165–167](#)

II impact-ionization. [ix](#), [12](#), [19](#), [21](#), [39](#)

KS Kolmogorov-Smirnov. [xiii](#), [26](#), [106–108](#), [117](#), [118](#)

LED light-emitting diode. [viii](#), [xiv](#), [xv](#), [142–147](#), [149](#), [150](#), [153](#), [154](#), [156–159](#), [161–164](#)

LEE low-energy excess events. [90](#), [106](#), [109](#), [111](#), [140](#), [141](#)

MAP maximum a posteriori. [xii](#), [98–101](#), [103](#)

MC Monte Carlo. [130](#), [136–139](#)

MCMC Markov chain Monte Carlo. [xv](#), [95](#), [177](#), [179](#)

MIDAS Maximum Integrated Data Acquisition System. [49](#)

MLE maximum likelihood estimation. [98](#)

NEXUS Northwestern EXperimental Underground Site. [43](#)

NR nuclear recoil. [4](#)

NRIXS Non-Resonant Inelastic X-ray Scattering. [170](#), [171](#), [174](#)

NTL Neganov-Trofimov-Luke. [17–19](#), [21](#), [43](#), [46](#), [88](#), [127](#), [138](#), [141–143](#), [146](#), [149](#), [155](#), [165–167](#)

OF optimal filter. [xiv](#), [49](#), [50](#), [52](#), [53](#), [58](#), [62](#), [71](#), [87](#), [111](#), [119](#), [144](#), [145](#), [149](#), [155](#), [157](#), [158](#)

PCB printed circuit board. [x](#), [41](#)

PDF probability distribution function. [xii](#), [20](#), [92–94](#), [100](#), [111](#), [113](#), [114](#), [120](#), [122](#), [130](#), [131](#)

PMT photomultiplier tube. [6](#)

PSD power spectral density. [48](#), [50–52](#), [67](#)

QET Quasiparticle-trap-assisted Electrothermal-feedback TransitionEdge Sensor. [ix](#), [x](#), [12–15](#), [43](#), [87](#), [140](#), [141](#), [166](#)

RIXS Resonant Inelastic X-ray Scattering. [170](#)

RQ reduced quantity. [49–52](#), [57](#), [70](#), [74](#), [84](#), [86](#)

SM Standard Model. 2–4, 6

SuperCDMS Super Cryogenic Dark Matter Search. 9, 10, 12–18, 20, 37

TES Transition Edge Sensor. ix, 12–16, 38, 41, 42, 55, 73, 90, 110, 119, 127, 131, 133, 135, 142, 143, 153, 166

WIMP Weakly Interacting Massive Particles. 2, 3, 7–10

Chapter 1

Introduction

Astrophysical observations at various scales provide overwhelming evidence for gravitational effects that cannot be explained by the observable mass in the universe. Measurements of these gravitational effects are many, including the formation of large-scale structures, properties of cosmic microwave background radiation, collisions of galaxy clusters, galactic rotation curves, and gravitational lensing [1, 2]. For instance, the most recent result from PLANCK [3] indicated that the known types of matter constitute less than 20% of the mass in the universe.

The observed and measured mass discrepancy can be explained in two ways. One possibility is changing the assumptions about the force of gravity, or with broader consensus, by introducing undetected type (or types) of matter called **Dark Matter (DM)**. Although the origin of the gravitational effects remain a mystery, we have strong historical motivations to continue the search. It echoes past efforts leading to the discovery of Neptune in 1846 and later Pluto in 1930. Similar to the gravitational effects attributed to **DM**, the pursuits of Neptune and Pluto were initiated due to unexplained gravitational forces distorting the orbit of Uranus [4, 5].

Assuming that new forms of matter are responsible for **DM**, astrophysical observations can provide hints about their general properties. A few common properties include:

- **DM** does not interact via the electric force at a leading order. Such interactions are strongly ruled out by the available measurements [6].
- **DM** is not composed of known forms of matter, typically referred to as baryonic matter in astrophysical literature. For instance, the abundance of light elements formed during Big Bang nucleosynthesis imposes strict limits on the amount of baryonic matter beyond what is currently understood [7].

- **DM** is expected to be cold, meaning it does not move at relativistic speeds. Cold **DM** can form gravitational halos in the early universe, which are essential for galaxy formation. Simulations of galaxy formation disfavor hot **DM** candidates, such as neutrinos, due to their inability to replicate the observed structures [8, 9].

The known types of matter are described by the **Standard Model (SM)**, which encompasses elementary particles (quarks, leptons, and bosons) and three of the four fundamental forces (electromagnetic, weak, and strong). Particle physicists have proposed various **DM** candidates to extend the **SM**. A common feature of these models is some level of interaction between **DM** and **SM** particles. Although such interactions are not strictly required, they are sometimes invoked to explain the origin and abundance of **DM** particles, such as the hypothetical **Weakly Interacting Massive Particles (WIMP)** that will be discussed shortly. Moreover, assuming **DM-SM** interactions narrows down the range of **DM** formulations, forming the foundation for many experimental efforts. For instance, using a new gauge symmetry to introduce **DM** and **SM** particles interactions through the kinetic mixing [10]. Among the various **DM** paradigms, some have garnered more attention because they feature simple production mechanisms in the early universe, are more accessible to be tested with current experiments, or address questions beyond just **DM**.

A prominent family of **DM** models that has been at the forefront of research for many years is that of **Weakly Interacting Massive Particles (WIMP)** [11, 12]. The **WIMP** family represent a broad category of non-relativistic (cold) hypothetical particles with masses ranging from the GeV/c^2 to TeV/c^2 scale. The interest in these models is partly due to their straightforward production mechanism in the early universe which is known as thermal freeze-out. According to the thermal freeze-out scenario, **WIMPs** were initially in thermal equilibrium with **SM** species. As the universe cooled below the **WIMP** mass, the production of **WIMPs** from **SM** particles became suppressed compared to their self-annihilation rate. This led to a decline in the **WIMP** number density. However, the expansion of the universe eventually halted the self-annihilation, leaving the **WIMP** number density stabilized at a constant value ever since.

Given the measurements for the expansion rate of the universe, and the observed density of **DM**, the self-annihilation probability for **WIMPs** with masses around the Fermi scale is found to be close to that of weak interactions. This seemingly coincidental alignment is often referred to as the "**WIMP** miracle" [12]. This serendipitous occurrence has been a key factor in shaping the design and scientific objectives of

previous generations of **DM** detection experiments. These experiments are either operational or nearing commissioning. Also, they have ruled out much of the originally favored **WIMP** parameter space [13, 14].

The waning of **WIMP** models has spurred interest in **DM** models across a broader mass range that are still theoretically justified. As shown in Fig. 1.1, the range of models with plausible **DM** mass values spans over 40 orders of magnitude. More information about the models can be found in many places including [15, 16].

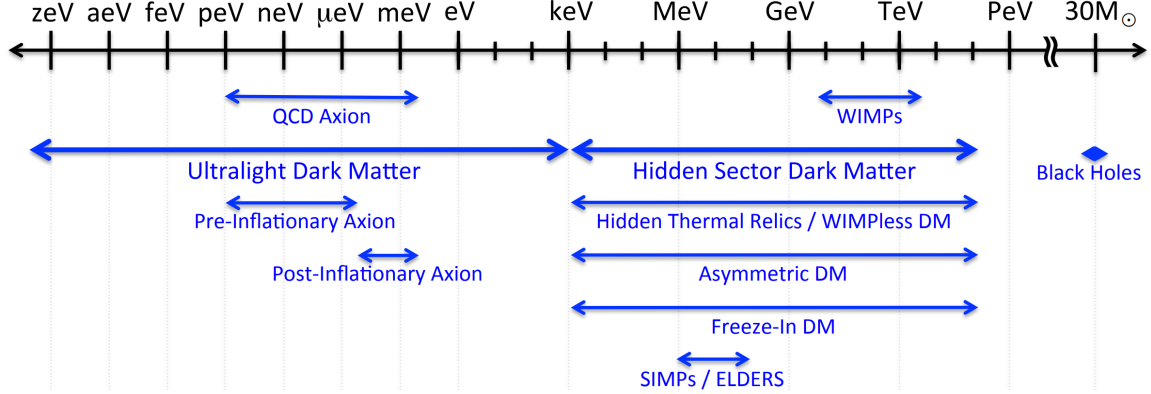


Figure 1.1: Approximate mass ranges associated with different **Dark Matter** candidates [16].

The experimental efforts dedicated to detecting signs of **DM** interactions with **SM** particles can be categorized as shown in Fig. 1.2. First, direct detection experiment that search for rare energy depositions from **DM** in detectors. Second, indirect detection experiments that scan the cosmos for any excess **SM** particles that could be attributed to **DM** self-annihilation. Finally, accelerator-based experiments that aim to create **DM** particles by colliding **SM** particles, and search for resulting signatures in the data, such as missing transverse momentum.

The strategies introduced may overlap or complement each other in the search for various **DM** models. A major difference among these strategies lies in their underlying assumptions. For instance, if we find a **BSM** particle in an accelerator search, do we know this is the cosmological **DM**? Clearly, approaches with fewer assumptions are preferred for a robust search. In this regard, some communities consider evidence from direct detection searches to be more indicative. This fact, coupled with the relatively lower operational costs of direct searches, has led to a surge in the variety and progress of experiments in this category.

Direct detection searches rely on measuring the recoil energy of nuclei or electrons

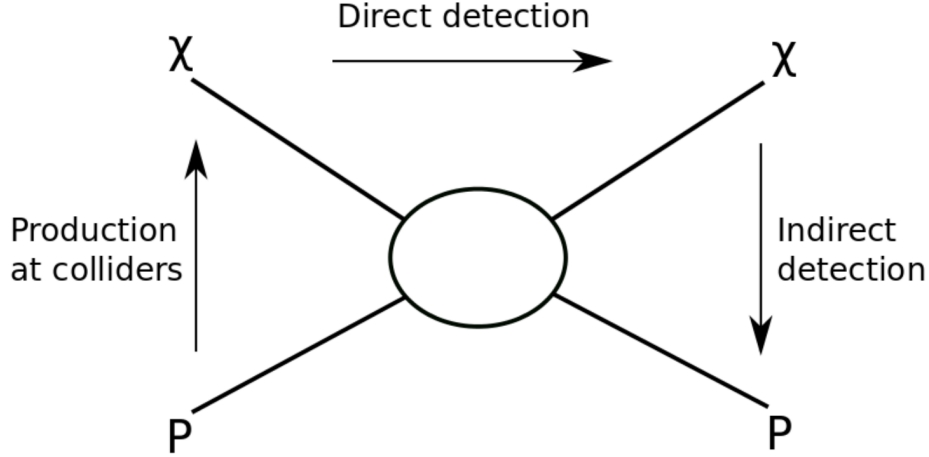


Figure 1.2: Schematic of **DM** detection mechanisms. Following the direction of the arrows: Right indicates direct detection, Downward represents indirect detection, and Upward corresponds to collider experiments. In the figure, “p” refers to **SM** particles, and χ represents **DM** particles [17]. The circle in the middle represents an unknown interaction.

when particles hit the detector. This strategy is illustrated in Fig. 1.3. The left panel shows the solar system rotating around the center of the galaxy through a halo of dark matter, while the right panel depicts **DM** particles entering the terrestrial detector.

Scatterings off the target material may produce light, cause ionization, or generate heat (phonons in crystals). Subsequently, experiments attempt to reconstruct the deposited energies through single or multiple signal channels, as depicted in Fig. 1.4.

A motivation to use multiple signal channels is to identify an **electron recoil (ER)** from a **nuclear recoil (NR)** through the parameters that quantify the features of an energy deposition in the detector. This enhancement arises from different responses of certain detector targets to **ERs** and **NRs**. More information about such differences in silicon and germanium is provided in subsection 2.2.1. An improved discrimination aids to preserve a high signal efficiency while rejecting the background events through the analysis of the data for various **DM** searches. For instance, some **DM** models only predict interactions with electrons (**ER**), whereas others primarily interact with nuclei through the weak force (**NR**). Additionally, energy depositions from **SM** particles, which are referred to as background for direct detection searches, mostly manifest as electron recoils. Common detector technologies, as depicted in Fig. 1.5, typically do not utilize more than two signal channels simultaneously.

In addition to the experiment data which provides a spectrum of energy deposi-

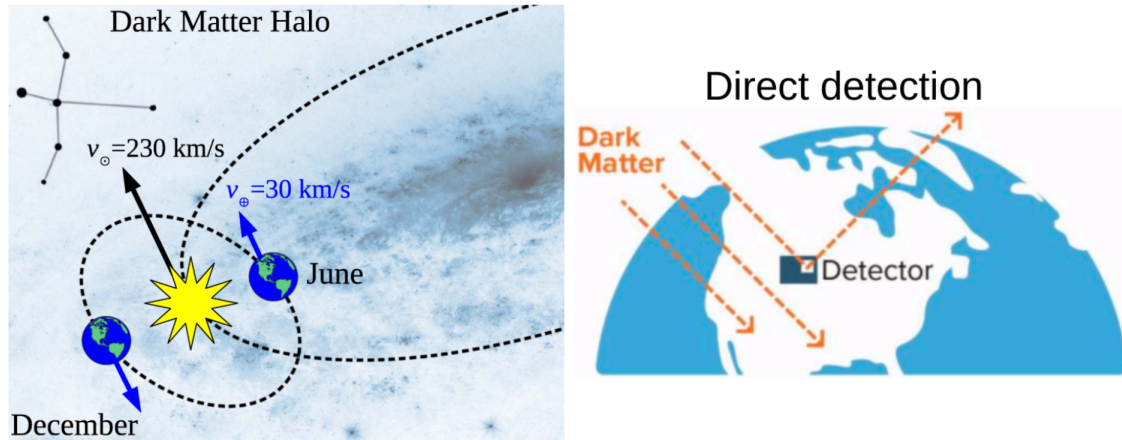


Figure 1.3: Schematic illustration of the direct detection strategy. The left panel shows the solar system rotating around the center of the galaxy through a dark matter halo, while the right panel depicts dark matter particles interacting with the detector in a direct detection experiment [18].

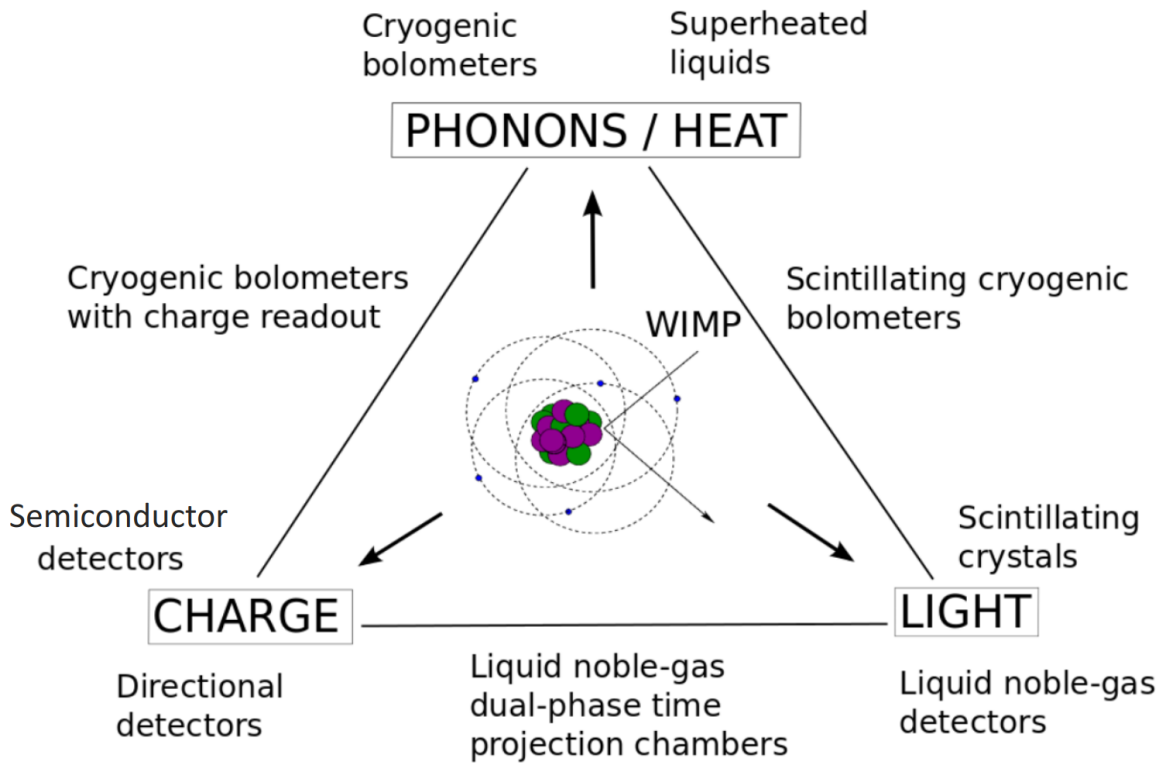


Figure 1.4: Schematic of the **DM** direct detection technologies and the signals they measure. Boxes on edges display the signal types, and names outside the triangle refer to detector technology [17].

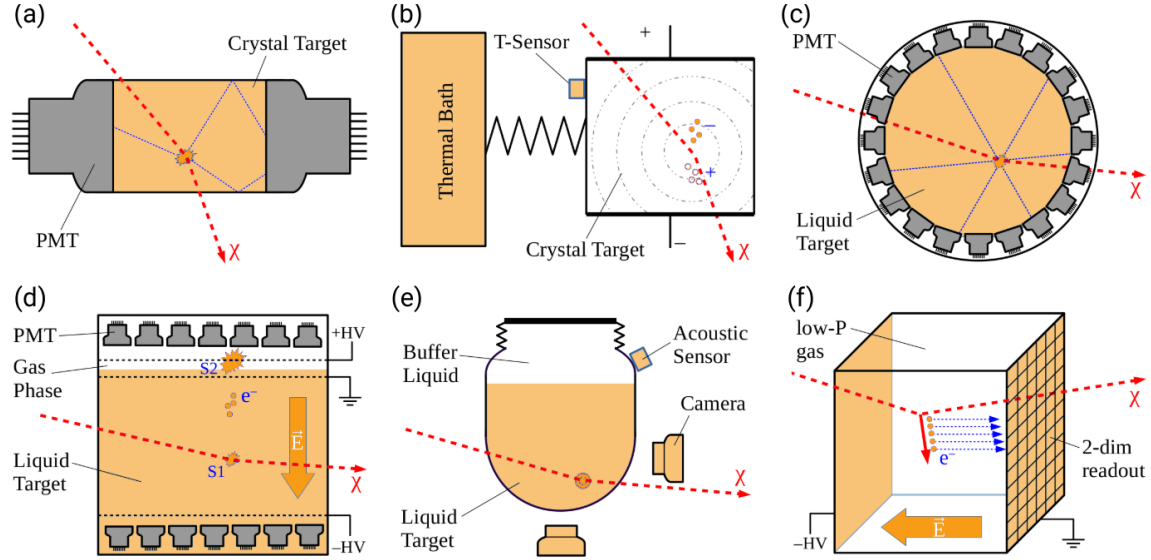


Figure 1.5: Common detectors for direct **DM** searches include: (a) scintillating crystals with **photomultiplier tube (PMT)** to measure light; (b) cryogenic crystal bolometers with phonon and ionization sensors; (c,d) one- and two-phase liquid noble-gas detectors with **PMT**; (e) superheated liquid detectors measuring heat; (f) directional time projection chambers with ionization sensors [19].

tions, a **DM** search requires an expected model for that spectrum. The model can then be compared with data through a statistical study to search for any **DM** indications. The model should account for the energy depositions from the **DM** particles under investigation, and preferably the background **SM** processes. Moreover, it should include the detector effects such as the energy resolution. The **DM** models typically depend on two key parameters: the mass of the individual **DM** particles and their interaction cross section with the detector target. Background processes are usually identified through extensive assays, and quantified using histogram templates created by intensive Monte Carlo simulations of **SM** energy depositions. Regardless of the precision of background modeling, a central objective of direct detection searches is to eliminate backgrounds. This is critical because any potential signal may be obscured by statistical fluctuations in the background. Background reduction involves using radiopure materials, operating the experiment underground to shield it from atmospheric **SM** particle flux, and implementing extensive neutron and gamma shielding to further protect the detectors.

Given the measured and expected spectra of energy depositions, direct searches employ various statistical methods to perform the comparison. From a high-level perspective, two motivations drive the statistical analysis. The primary motivation

is to identify and quantify an excess number of events above backgrounds, consistent with a **DM** spectrum. Alternatively, in the absence of sufficient evidence, studies quantify the confidence in the lack of evidence for a range of **DM** models. For instance, any study without a background model falls under the second category. In such scenarios, one assumes all data result exclusively from **DM** energy depositions in the detector, and subsequently claims a lack of evidence for **DM** cross sections and mass values that would produce a signal statistically inconsistent with the observed data. The statistical methods frequently used in direct detection searches include the Poisson counting, the optimum interval method, and the profile likelihood ratio tests, as illustrated in Fig. 1.6.

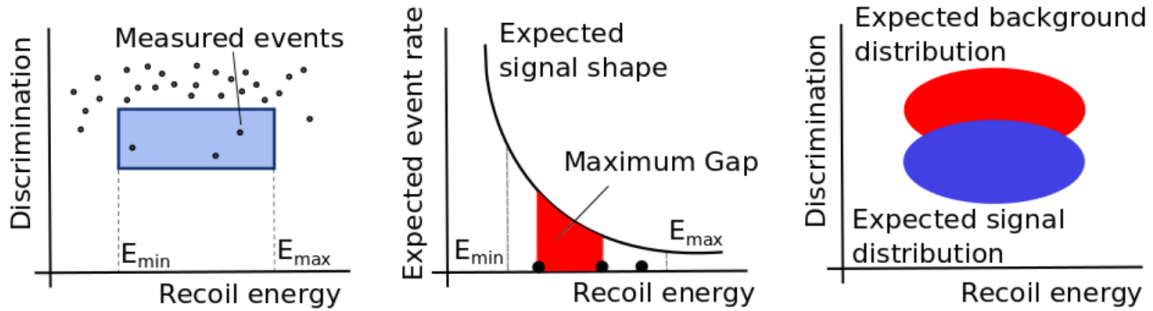


Figure 1.6: From left to right, the first plot represents a Poisson counting inference, where a small window with a high purity of signal-like events is chosen to quantify the detector’s sensitivity. The second plot illustrates the optimum interval method, in which the shape of the dark matter (**DM**) signal is used to establish a stringent upper limit without any knowledge of the background. The last plot represents the profile likelihood ratio tests, where information from both backgrounds and the **DM** model is incorporated to set limits [17].

Statistical comparisons are often presented in compact plots, where the x-axis represents the **DM** particle mass and the y-axis represents the cross section. These plots typically exhibit common features, as shown in Fig. 1.7 for **WIMPs**. The grey area enclosed by solid lines represents the region excluded by recent searches. Historically, some measurements reported evidence for **WIMPs**. Such claims correspond to colored contours inside the grey area, and are not supported by other measurements. The yellow region at the bottom, known as the neutrino fog, is where the flux of neutrinos begins to dominate, eliminating the ability to discriminate a **DM** signal. Finally, the green area on the left enclosed by the dashed line, shows the nominal sensitivity of a new experiment called SuperCDMS SNOLAB which is currently under construction. The statistical interpretation of the regions commonly follows: in a high fraction of

identical measurements, the true **DM** parameter values would fall within the contour; alternatively, they would not be above the exclusion curve.

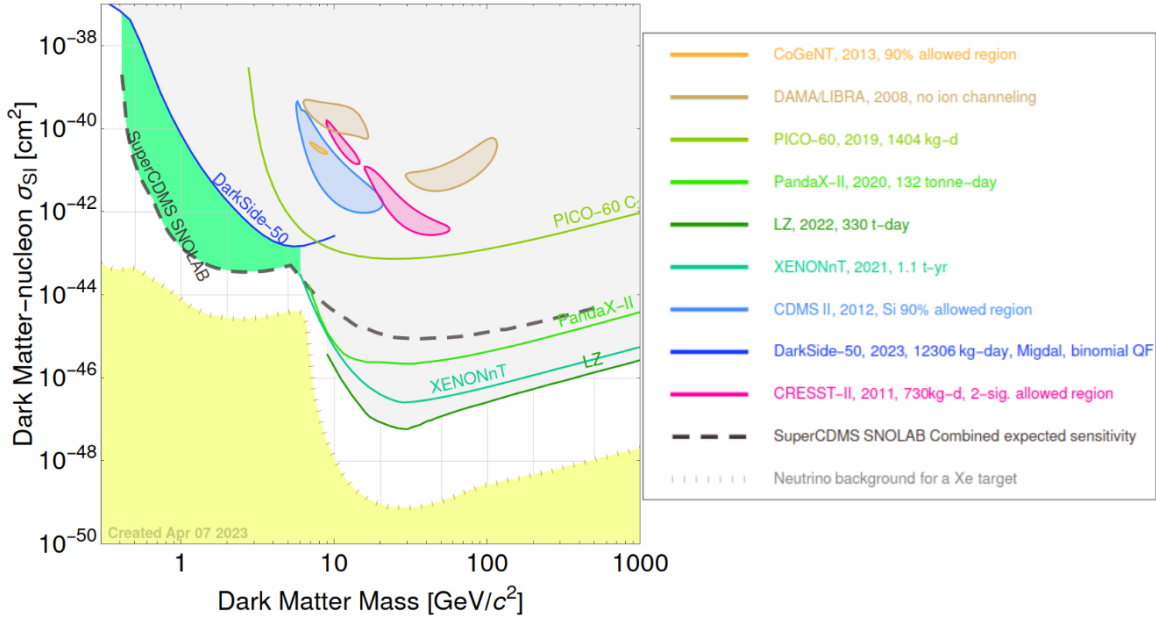


Figure 1.7: Parameter space of the spin-independent (SI) WIMP-nucleon scattering cross section σ_n^{SI} as a function of WIMP mass. The plot includes exclusion limits on σ_n^{SI} indicated by solid lines from various experiments. Additionally, the plot highlights discovery regions that have since been ruled out by subsequent measurements. The yellow shaded region represents the neutrino fog. This plot was generated using the SuperCDMS limit plotter [20].

The upward trend of the exclusion curve, either to the right or to the left in Fig. 1.7, is due to the reduction in the number of **WIMP** events for a fixed cross section value. On the right side, the detector remains sensitive to **DM**, but the flux of **WIMPs** decreases as the local **DM** density remains constant (the form factor for the dark matter interaction probability also has an energy dependence, which is beyond the scope of this summary). On the left side, the detector loses sensitivity due to kinematic suppression. This happens because **WIMP** particles become too light compared to the nuclei of the detector target material.

Following [18], the underlying **WIMP** model for any of the results in Fig. 1.7 is given by

$$\frac{dR}{dE_{\text{nr}}} = \frac{\rho_0 M}{m_N m_\chi} \int_{v_{\text{min}}}^{v_{\text{esc}}} v f(v) \frac{d\sigma}{dE_{\text{nr}}} dv, \quad (1.1)$$

where E_{nr} is the nuclear recoil energy, ρ_0 is the local density of **DM** in the solar system, M is the target mass of the detector, m_N is the mass of the nuclei in the

scattering target, m_χ is the **DM** particle mass, σ is the **WIMP** scattering cross section, $f(v)$ is the velocity distribution of **WIMPs** in the detector's reference frame, $v_{\min} = \sqrt{m_N E / (2\mu^2)}$ is the minimum **WIMP** velocity required to produce a detectable event at energy E , and v_{esc} is the escape velocity, i.e., the velocity at which **WIMPs** are no longer gravitationally bound to the Milky Way. The μ factor in $v_{\min}$ is the reduced mass of the **WIMP**-nucleus system that is given by $\mu = \frac{m_\chi m_N}{m_\chi + m_N}$. The differential cross section in Eqn. 1.1 is expressed as

$$\frac{d\sigma}{dE_{\text{nr}}} = \frac{m_N}{2v^2\mu^2} (\sigma_{\text{SI}} F_{\text{SI}}^2(q) + \sigma_{\text{SD}} F_{\text{SD}}^2(q)) \quad (1.2)$$

where $\sigma_{\text{SI}} F_{\text{SI}}^2(q)$ and $\sigma_{\text{SD}} F_{\text{SD}}^2(q)$ represent the spin-independent and spin-dependent form factors. A discussion of the spin-dependent term can be found in [18, 21]. The cross section for the spin-independent term can be written as

$$\sigma_{\text{SI}} = \frac{4\mu^2}{\pi} (Zf_p + (A - Z)f_n)^2 \quad (1.3)$$

where A is the number of nucleons, Z is the number of protons, and $f_{p,n}$ are the couplings of the **WIMP** to protons and neutrons. In most cases, the coupling to protons and neutrons are taken to be similar ($f_p \approx f_n = f$). Therefore, Eqn. 1.3 reduces to

$$\sigma_{\text{SI}} = \frac{4\mu^2}{\pi} A^2 f^2. \quad (1.4)$$

Finally, it is customary to rewrite the cross section per nucleon to facilitate the comparison of the **DM** search results across various experiments. The cross section per nucleon can be written as

$$\sigma_n^{\text{SI}} \equiv \frac{4\mu_n^2}{\pi} f^2, \quad (1.5)$$

where $\mu_n = \frac{m_\chi m_n}{m_\chi + m_n}$ is the **WIMP**-nucleon reduced mass. Consequently, the statistical test can be performed on the **WIMP**-nucleon cross section following

$$\sigma_n^{\text{SI}} = \sigma_{\text{SI}} \frac{\mu_n^2}{\mu^2} \frac{1}{A^2}, \quad (1.6)$$

which is the quantity shown on the y-axis in Fig. 1.7. For the interested reader, a more detailed discussion of dark matter scattering rate in condensed matter systems, which applies to detectors that are employed by the SuperCDMS experiment, is provided in [22].

The sensitivity curve of the **SuperCDMS** SNOLAB experiment for **WIMP** searches

is detailed in [23], with more recent information provided in [24]. The kink in the **WIMP** sensitivity curve, at approximately $6 \text{ GeV}/c^2$ in Fig. 1.7, results from using two different detector targets in the SNOLAB experiment (Si, Ge). Due to its lighter atomic mass, silicon is kinetically favored for low-mass **WIMP** searches which is indicated by $v_{\min}$ in Eqn. 1.1. Consequently, **SuperCDMS** SNOLAB silicon detectors have a higher sensitivity to low-mass **WIMP** particles. The higher sensitivity is evident by the green shaded area in Fig. 1.7, which belongs entirely to the silicon detectors. Therefore, the silicon detectors have the potential to probe new regions of the **WIMP** parameter space.

The sensitivity curve in Fig. 1.7 assumes a 100 eV energy threshold (total phonon Eqn. 2.12) for the silicon detectors. This threshold represents the optimal detector performance as predicted by theoretical models, and is governed by technologically-driven limitations. From the perspective of dark matter searches, sensitivity to even lower energy depositions would be desirable to expand the range of detectable dark matter models. However, achieving that will likely not be feasible with the **SuperCDMS** SNOLAB experiment.

The response modeling of **SuperCDMS** detectors depends on several factors, which will be briefly discussed in Chapter 2. The current understanding of the detector response is insufficient to fully simulate the detectors beyond a first-order approximation. Consequently, accurate detector response modeling requires data-driven studies. For example, data-driven methods are necessary to determine the energy calibration and resolution of the detectors.

This thesis focuses on developing a data-driven calibration scheme for **SuperCDMS** silicon detectors. The scheme, detailed in the following chapters, primarily relies on Compton step energy signatures resulting from Compton scatters. These signatures appear at approximately 0.1 keV, 0.15 keV, and 1.8 keV energies facilitating a sub-keV electron recoil calibration of the silicon calorimeters. We simulated these signatures to find their precise shape and energy values. A statistical framework based on likelihood fits was then developed to locate these signatures in the uncalibrated experimental data. The data calibration is performed by comparing the positions of the signatures in both the simulations and the data. We calibrated four **SuperCDMS** R&D silicon detectors to valid the workflow. Although these detectors differ from the **SuperCDMS** SNOLAB detectors, the Compton step simulations and the statistical model that are investigated in this thesis pave the way for future studies.

The chapters in this thesis are organized as follows: Chapter 2 reviews the key concepts behind **SuperCDMS** calorimeters. Chapter 3 discusses various simulations

with the theoretical background discussed in Appendix A. Chapter 4 describes the experimental setup and the data utilized in this research. Chapter 5 presents the analysis conducted for the calibration study. Since the statistical analysis in Chapter 5 partially depends on Markov Chain Monte Carlo sampling, a brief overview of this computational technique is provided in Appendix B. Finally, Chapter 6 presents further validations of the calibration and complementary studies, with supporting material provided in Appendix C.

Chapter 2

SuperCDMS phonon detectors

This chapter provides a brief overview of the **SuperCDMS** phonon detectors. These detectors are cryogenic calorimeters that measure a portion of the deposited energy by detecting athermal phonons, phonons with energies significantly higher than thermal phonons at tens of mK crystal temperatures ($E_{\text{thermal}} \approx 1 \mu\text{eV}$ [25]). The detectors consist of two components: a scattering target made of high-purity silicon or germanium crystals, and a group of sensing **Quasiparticle-trap-assisted Electrothermal-feedback TransitionEdge Sensor (QET)** modules instrumented on the surface of the crystal [26].

This chapter first discusses **QETs** including the phonon collection scheme, and key optimization requirements. Then it reviews the detector response to nuclear and electron recoils. Finally, it discusses the **charge-trapping (CT)** and **impact-ionization (II)** effects for charge carriers moving within the detector target both of which are crucial for modeling the detector response [27, 28].

2.1 SuperCDMS phonon sensing technology

The phonon sensors in **SuperCDMS** detectors consist of arrays of **QETs** distributed across the detector surfaces. The **QETs** within each array are connected in parallel, with each array providing a single readout signal.

A **QET** module (Fig. 2.1) consists of a wide aluminum (Al) fin that collects and traps athermal phonons from the scattering target, channeling their energy toward a relatively small volume of tungsten (W) **Transition Edge Sensor (TES)**. Athermal phonons in the detector with sufficient energy ($E > 0.3 \text{ meV}$) break Cooper pairs in the aluminum, producing quasiparticles. Subsequently, the quasiparticles diffuse into the **TES** before recombining. The lower gap energy in the W traps the Al

quasiparticles, leading to an energy transfer to the TES primarily through electron-electron interactions [26]. The trapping process is illustrated in the top left of Fig. 2.1.

The TES is voltage-biased to remain at its critical temperature, between the superconducting and normal states. The energy from a scattering particle raises the temperature of the TES, causing a sharp increase in its resistance. The increased resistance reduces the electric current through the TES, which in turn decreases the Joule heating, allowing the TES to cool down and reset. This thermal and electrical feedback cycle generates the signal in the SuperCDMS detector, and classifies these detectors as electrothermal feedback devices. While some SuperCDMS detectors also measure ionization in addition to phonons, this thesis focuses solely on phonon detectors.

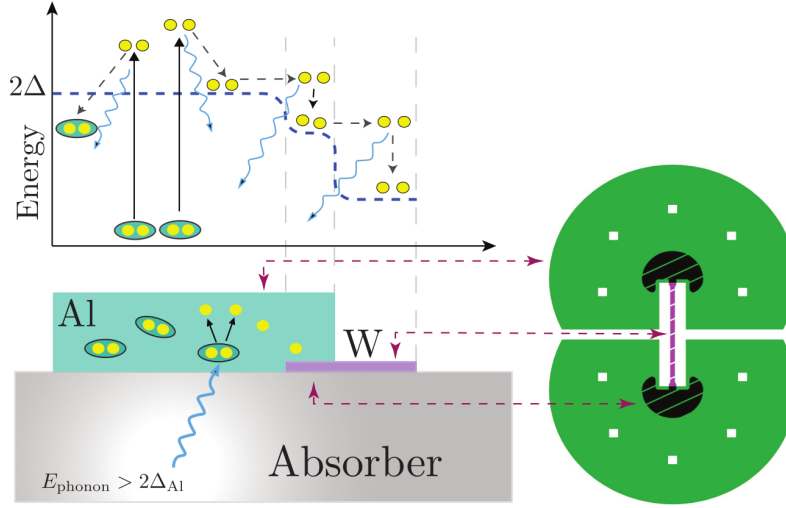


Figure 2.1: Illustration of the Quasiparticle-trap-assisted Electrothermal-feedback TransitionEdge Sensor (QET) design and operation. Phonons with sufficient energy break Cooper pairs in the aluminum, creating quasiparticles that diffuse into the tungsten. The lower gap energy in the tungsten traps the aluminum quasiparticles, transferring their energy to the Transition Edge Sensor (TES). The curvy lines represent sub-gap phonons emitted by the quasiparticles as they lose energy, while the energy levels (steps in the top-left plot) indicate the superconducting gap sizes. The intermediate steps corresponds to the interface of the Al and W [29].

The QET sensor design concentrates the energy from athermal phonons, initially dispersed throughout the detector bulk, into the small volume of the TES. This significant reduction in sensor volume, and consequently its heat capacity, enhances the electrothermal feedback, thereby lowering the energy threshold of the calorimeter. The SuperCDMS detectors are optimized to be sensitive to energy depositions as low as a few eV. Optimizing the detector performance involves tailoring the QET design

(the volume and shape of the Al and W, as shown in the right panel of Fig. 2.1), selecting the number of QETs connected in parallel to form a channel, and adjusting the coverage of channels across the detector surface.

The energy threshold of the detectors is primarily constrained by the noise level in the readout signal. This selection of the energy threshold value is data-driven, and is typically determined to have a negligible probability of triggering on random noise fluctuations. A major source of noise in SuperCDMS detectors is thermal fluctuation noise across the interface between the TES and the thermal bath. This contribution is characterized by white power noise, expressed as ([30, 31]),

$$N_G \approx 2Gk_bT_0^2, \quad (2.1)$$

where G is the thermal conductance between the TES and the thermal bath, k_b is the Boltzmann constant, and T_0 is the operating temperature of the TES. As an approximation, T_0 can be replaced by the critical temperature of the TES (T_c) when operating within a narrow transition width. The transition width refers to the small temperature range between the superconducting and normal states (≈ 0.5 mK in W [31]).

The thermal fluctuation noise leads a detector phonon energy resolution of the form ([25, 29, 32])

$$\sigma_{\text{ph}} \approx \frac{1}{\epsilon} \sqrt{2Gk_bT_c^2\tau_{\text{BW}}}, \quad (2.2)$$

where ϵ is the phonon energy collection efficiency, and τ_{BW} is the detector bandwidth. The bandwidth is determined by the sum of the phonon collection time and the effective time for the TES electrothermal response. Intuitively, a higher signal-to-noise ratio is expected when the detector signal is localized within a short time interval and when a greater fraction of the energy reaches the TES. These factors are captured in the detector bandwidth and the efficiency factor in Eqn. 2.2.

In Eqn. 2.2, $G \approx n\Sigma V_{\text{TES}}T_c^{n-1}$, where Σ is the electron-phonon coupling constant, and $n \approx 5$ according to the thermal conductance power-law exponent [25, 30]. Substituting G into Eqn. 2.2 gives

$$\sigma_{\text{ph}} \approx \frac{T_c^3}{\epsilon} \sqrt{2n\Sigma V_{\text{TES}}k_b\tau_{\text{BW}}}, \quad (2.3)$$

which shows that lowering the critical temperature of the TES can significantly improve the thermal fluctuation resolution.

As outlined in [31, 30, 25], the energy collection efficiency appearing in the de-

nominator of Eqn. 2.3 comprises of multiple components. These are

1. $\epsilon_{\text{ph Al}}$: The detector substrate is in contact with components other than the QETs. Athermal phonons can escape through these passive components without contributing to the signal. Additionally, athermal phonons may down-convert into multiple lower-energy phonons that lack sufficient energy to break Cooper pairs. This efficiency can be optimized by reducing the area of the passive components in contact with the detector substrate or by increasing the area of the aluminum fins.
2. $\epsilon_{\text{Al qp}}$: The energy of the athermal phonons arriving at the aluminum fin gets distributed between two populations: quasiparticles and aluminum sub-gap phonons. The fraction of energy converted into quasiparticles approaches an asymptotic value of approximately 55% for phonons with energies several times greater than the aluminum energy gap, but remains energy-dependent at lower energies.
3. $\epsilon_{\text{qp collection}}$ There are three possible outcomes for the aluminum quasiparticles: (a) they recombine into Cooper pairs, (b) they become trapped before reaching the tungsten, or (c) they successfully enter the tungsten. The first two reduce the energy collection efficiency. The size of the aluminum fin can be optimized to ensure that the recombination timescale is longer than the diffusion timescale required for the quasiparticles to reach the tungsten.
4. $\epsilon_{\text{W qp}}$: The efficiency of Al quasiparticles to transfer their energy to tungsten. This efficiency has a dependence on the interface between the Al/W. In one study this efficiency was measured to be approximately 62% [30].

The total energy collection efficiency is the product of the individual components listed above. Specifically, for the SuperCDMS high-voltage eV-resolution (HVeV) detectors with the NF-C mask design, used in the analysis presented in this thesis, the total efficiency has been measured to be approximately 27%. Further details about the HVeV detectors will be provided in Chapter 4.

Another important aspect of TES design is its dynamic range—the range of energy depositions over which the TES exhibits an approximately linear response. The thermal fluctuation resolution model, as described in Eqn. 2.3, is only applicable within this linear regime (sometimes referred to as the small-signal limit). When energy depositions exceed this range, the TES transitions into its normal state, resulting in a

saturated response. Figure 2.2 illustrates the schematic of a detector response, where saturation occurs when the temperature grows beyond the ΔT_c window.

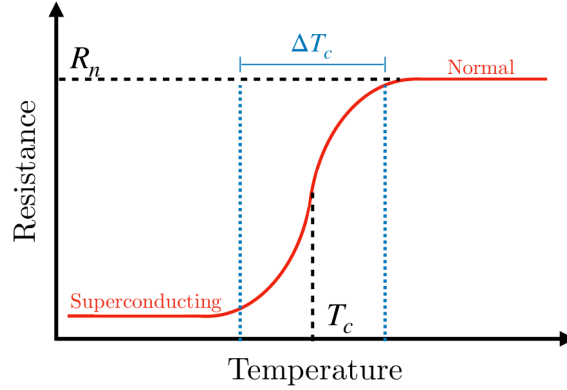


Figure 2.2: Schematic illustrating the change in TES resistance as a function of temperature. After each energy deposition the TES returns to its critical temperature (T_c) [32].

The energy required for a temperature shift of magnitude ΔT_c is estimated by

$$E_{\text{sat}} \approx \frac{1}{\epsilon} C(\Delta T_c) \approx \frac{1}{\epsilon} c_W V_{\text{TES}} T_c (\Delta T_c), \quad (2.4)$$

where c_W is the specific heat. Ideally, the energy resolution should be small compared to the saturation energy, ensuring that the measured energy is only affected by the inherent Gaussian detector resolution and not by non-linear effects. The ratio of E_{sat} to the energy resolution is thus a key parameter to optimize. This ratio, commonly referred to as the “dynamic range”, is given by

$$DR \sim \frac{E_{\text{sat}}}{\sigma_{\text{ph}}} \propto \frac{\sqrt{V_{\text{TES}}}}{T_c^2 \sqrt{\tau_{\text{BW}}}} (\Delta T_c). \quad (2.5)$$

This indicates that reducing the TES volume may improve the detector resolution; however, that also reduces the dynamic range which introduces non-linear effects at lower energies.

2.2 Detector response

Energy deposition in the detector target occurs through either nuclear or electron recoils. To model the detector response accurately, it is crucial to understand the ratio of energy that generates electron-hole (e^-h^+) pairs versus phonons. Additionally, SuperCDMS detectors can operate with a voltage bias applied across the crystal.

As the e^-h^+ pairs drift in the electric field, they quickly reach terminal velocity, releasing the excess energy as **Neganov-Trofimov-Luke (NTL)** phonons [33, 34]. Some **SuperCDMS** detectors utilize the **NTL** effect to amplify the phonon signal. A clear understanding of the **NTL** gain is also essential for accurate calibration and detector response modeling.

2.2.1 Ionization and phonon production

An incoming particle interacts with either an electron or a nucleus in the detector substrate. The recoiling electron or nucleus undergoes a scattering process, resulting in further ionization and phonon emission. By the end of this cascade, the deposited energy is partitioned as

$$E_r = E_{\text{ph}}^0 + N_{\text{eh}} E_{\text{gap}}, \quad (2.6)$$

where E_{ph}^0 represents the fraction of the energy that converts into phonons (often referred to as prompt phonons), N_{eh} is the number of created e^-h^+ pairs, and E_{gap} is the band gap energy of the detector crystal. Two possible outcomes can be considered for the e^-h^+ pairs: (a) they may eventually recombine, releasing their energy as phonons, or (b) they may become trapped or free other charges from impurity potential wells. In the first scenario, the recombination timescale must be taken into account. The second scenario is discussed in detail in [27, 28] and will be briefly summarized in the next subsection.

The number of e^-h^+ pairs (N_{eh}) is a function of energy and recoil type. For electron recoils the number is given by

$$\langle N_{\text{eh}} \rangle = \frac{E_r}{\epsilon(E_r)}, \quad (2.7)$$

where $\epsilon(E_r)$ is the average energy required to make an e^-h^+ (≈ 3.8 eV in Si) pair, which is greater than the band gap of the crystal (≈ 1.2 eV in Si). The $\epsilon(E_r)$ factor is studied in different works including [35, 36]. In [36] the $\epsilon(E_r)$ factor is modeled as a piece-wise function

$$\epsilon(E_r) = \begin{cases} \infty & E_r < E_{\text{gap}}, \\ E_r & E_{\text{gap}} < E_r < 2E_{\text{gap}}, \\ \epsilon_{\text{low}}(E_r) & 2E_{\text{gap}} < E_r, \\ \epsilon_{\infty} & E_r \rightarrow \infty, \end{cases} \quad (2.8)$$

where $\epsilon_{\text{low}}(E_r)$ is energy dependent. This model suggests that for energy depositions smaller than the band gap, no e^-h^+ pairs are created. At higher energies, up to twice the band gap energy, only one e^-h^+ pair can be produced. Subsequently, ionization follows an energy-dependent pattern at low to intermediate energies, and ultimately approaches an asymptotic value.

The uncertainty in N_{eh} is also energy dependent with an asymptotic behavior as quantified by the Fano factor following

$$F(E_r) = \frac{\sigma^2(E_r)}{N_{\text{eh}}(E_r)} = \frac{\sigma^2(E_r)\epsilon_{\text{eh}}(E_r)}{E_r}. \quad (2.9)$$

Similar to the ionization model in Eqn. 2.8, [36] also introduces a piece-wise model for the Fano factor given by

$$F(E_r) = \begin{cases} 0 & E_r < 2E_{\text{gap}}, \\ F_{\text{low}}(E_r) & E_r \geq 2E_{\text{gap}}, \\ F_{\infty} & E_r \rightarrow \infty. \end{cases} \quad (2.10)$$

For nuclear recoils, the fraction of energy that produces ionization is smaller than for electron recoils. In the literature, the ionizing energy from nuclear recoils is typically expressed relative to that of electron recoils. By convention, the number of e^-h^+ pairs generated in nuclear recoils is given by

$$\langle N_{\text{eh}} \rangle = \frac{Y(E_r) \cdot E_r}{\epsilon_{\infty}}, \quad (2.11)$$

where $Y(E_r)$, that is referred to as the quenching factor or ionization yield, is a function of the recoil energy and is less than 1. In the denominator of Eqn. 2.11, the asymptotic limit from Eqn. 2.8 is used. Determining the ionization yield for nuclear recoils in sub-GeV/ c^2 dark matter searches is critical, and has been an active area of research [37, 38]. For instance, one of the latest ionization yield measurements in silicon by **SuperCDMS** is shown in Fig. 2.3 by the red curve.

2.2.2 Neganov-Trofimov-Luke effect

According to Eqn. 2.6, a fraction of the primary deposited energy produces e^-h^+ pairs. A subset of **SuperCDMS** detector can apply an electric field across the detector crystal to accelerate the e^-h^+ pairs. The accelerated charges instantly (on the timescale of the detector) reach a terminal velocity and emit **Neganov-Trofimov-Luke (NTL)** phonons

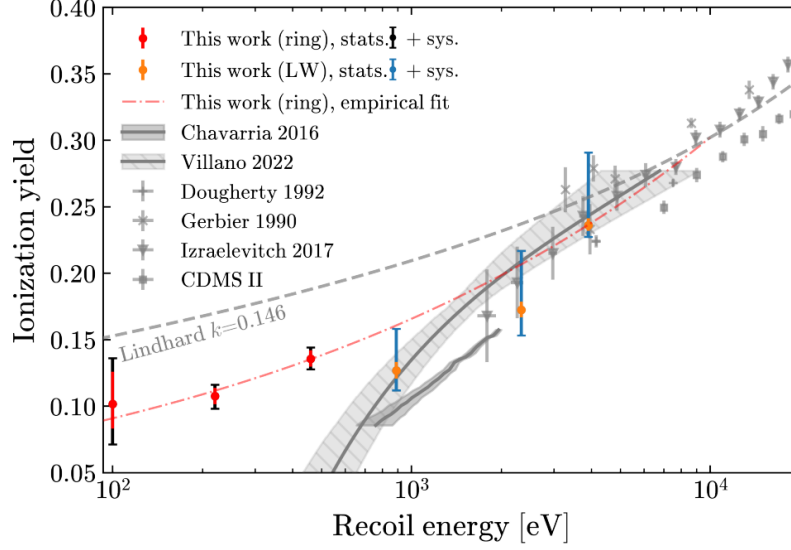


Figure 2.3: The ionization yield measurement that is reported in Ref. [37]. The paper provides more information regarding the other measurements.

[33, 34]. The total phonon energy including the contribution from **N****T****L** phonons is

$$\langle E_{ph} \rangle = E_r + \langle N_{eh} \rangle \cdot e \cdot V_{\text{external}}, \quad (2.12)$$

where e is the elementary electron charge, and V_{external} is the external voltage across the detector crystal. In the presence of a **H****V** applied across the crystal, the initial phonon energy E_r becomes negligible and can be ignored. For example, a 76 eV electron recoil produces $\langle N_{eh} \rangle = 20$, assuming $\epsilon(E_r) = 3.8$ eV. Thus, a 100 V bias would boost the total phonon signal to approximately $E_{ph} \approx 2$ keV.

A detector with a good phonon resolution operating in the **H****V** mode can count the number of **e**⁻**h**⁺ pairs as they form distinct peaks in the detector data. Figure 2.4 provides a schematic representation of how these quantized peaks appear in the data.

2.2.3 Charge trapping and impact ionization

The total phonon energy in Eqn. 2.12 represents a detector with an ideal crystal operating in the **H****V** mode. That assumes that the **e**⁻**h**⁺ pairs traverse the entire potential across the crystal. In a real crystal that is represented in Fig. 2.5, there are impurities which can trap charges (**C****T**); additionally, there is a chance that charges liberate other trapped charges **I****I**. The low probabilities of the **C****T** and **I****I** effects result in a small population of events with partial **N****T****L** gains. These events

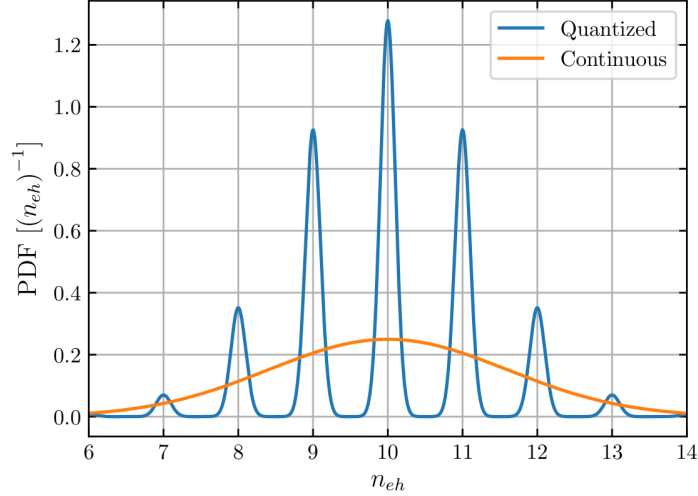


Figure 2.4: This plot illustrates the PDF for the number of e^-h^+ pairs, N_{eh} , observed by detectors with varying energy resolutions. The blue curve represents a detector capable of resolving individual e^-h^+ pairs. In contrast, the orange curve represents a detector with lower resolution, where individual electron-hole pairs are not resolved. Both distributions share the same underlying parameters, with $\langle n_{eh} \rangle = 10$ and a Fano factor of $F = 0.155$ [32].

populate the regions between the peaks in Fig. 2.4.

2.3 Summary

The discussion in this chapter provides a condensed summary of the detector physics and the response for SuperCDMS phonon detectors. Although brief, it should sufficiently set the stage for the analysis presented in this thesis. Further details about the detectors can be found in Refs. [30, 31].

Following Eqn 2.12, the Compton calibration data sets that are discussed in Chapters [4,5] were collected at 0 V bias, and the LED data sets in Chapter 6 were collected at 150 V bias.

This chapter concludes the review material for this thesis. The next chapter details the simulations we performed to model the expected spectrum of energy depositions for the Compton calibrations setup.

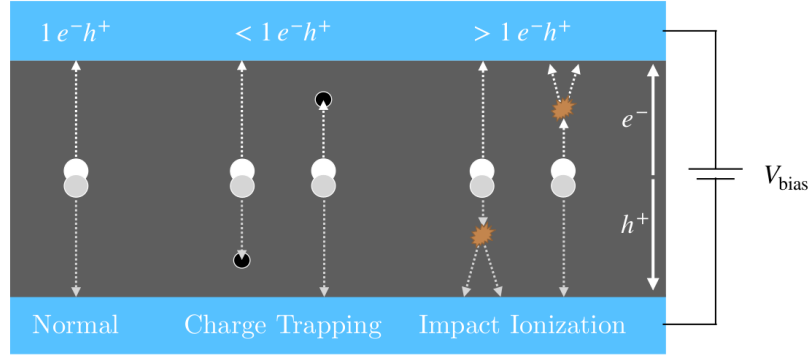


Figure 2.5: Illustration of the **charge-trapping (CT)** and **impact-ionization (II)** effects for a single electron-hole pair. The e^-h^+ pairs drift towards opposite sides of the detector crystal in the external voltage, emitting **NTL** phonons. Sometimes, an electron or hole may become trapped in a charge vacancy, or release an additional loosely bound charge. The figure illustrates a single occurrence of the **CT** and **II** effects. Charges may undergo multiple **CT** and **II** occurrences or a combination of both [32].

Chapter 3

Compton Scattering Simulations

The calibration result presented in Chapter 5 primarily depends on the position of energy signatures from Compton scatters in silicon. This chapter details the simulations that provide the expected spectrum of energy depositions in detectors. A comparison between the position of energy signatures in the detector data (uncalibrated) and the simulations (units of energy) provides a calibration function that transforms the x-axis of the data from the units of the measured signal to energy units.

Light interacts with matter through various channels, including Compton scattering. The scattering amplitude of light in matter is proportional to the attenuation length, as shown for silicon in Fig. 3.1. The study described in this thesis relies on energy signatures from Compton scattering. To maximize the probability of Compton scattering in silicon, the photon energy should be between 0.1 MeV and 1 MeV. Therefore, we used a ^{137}Cs gamma source, which has a prominent photopeak (approximately 85%) at 662 keV, for the calibration study. Additionally, we had a ^{133}Ba source with a photopeak at 356 keV; however, due to its lower activity, the ^{133}Ba source did not play a significant role.

We performed Geant4 [40] simulations at energies above 1 keV to obtain the expected spectrum of energy depositions. The geometry and results of the Geant4 simulations are discussed in Sec. 3.1. An overview of the approximations underlying Compton scattering simulations in Geant4 is provided in Appendix A. This overview motivates seeking more detailed simulations for scattering energies near the binding energies of the target's core electrons. Hence, Sec. 3.2 discusses an alternative simulation package called FEFF [41, 42, 43, 44, 45], which incorporates various condensed matter effects to provide a more accurate calculation of the cross section below 1 keV.

We primarily used simulations to investigate the Compton steps. These steps appear in the differential cross section as a function of energy when the energy deposited

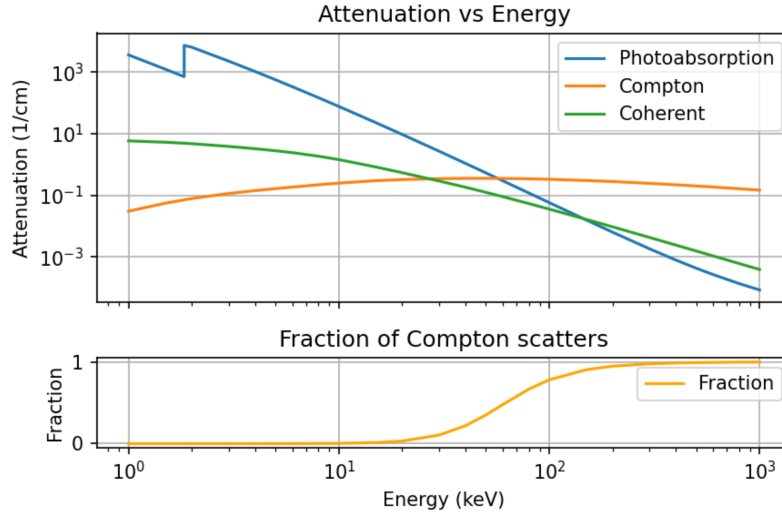


Figure 3.1: Top: The attenuation length of light in silicon as a function of incident energy. Bottom: The probability of Compton scattering [39].

in the scattering is below the binding energy of a subset of electrons. In such cases, these electrons do not contribute to the scattering process, as they lack available final states. This process is visualized in Fig. 3.2.

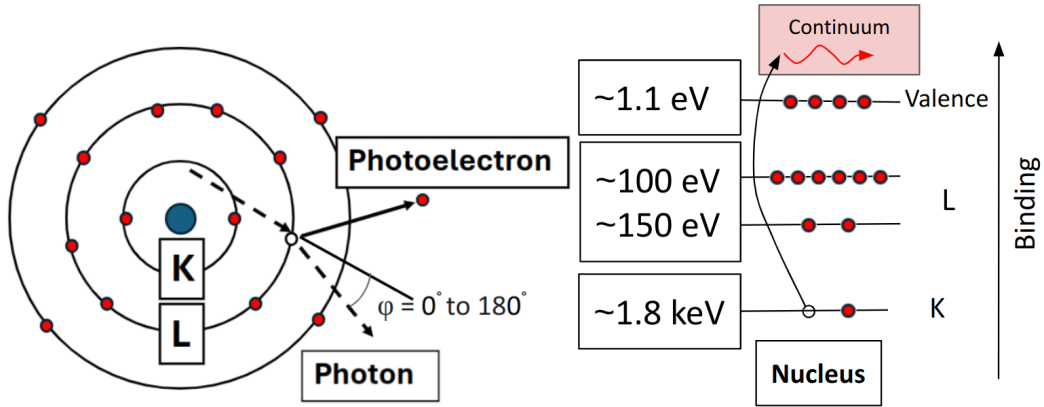


Figure 3.2: Demonstration of the Compton scattering. Left: A photon interacting with a core electron. A smaller scattering angle corresponds to a lower energy transfer. Right: The core electron contributed to the scattering cross section if the deposited energy is greater than the binding energy; otherwise, the transition is forbidden. The effects of forbidden electrons appear as step like features in the cross section.

3.1 Geant4 Simulations

The experimental setup for the calibration study comprises two radioactive sources, ^{137}Cs and ^{133}Ba , illuminating the detectors placed inside a tightly sealed copper housing. The detector housing was mounted inside a cryogenic refrigerator. A comprehensive description of the experimental setup is left for Chapter 4.

We conducted Geant4 simulations using the SuperSim package developed by the SuperCDMS collaboration. This package includes a detailed geometry of the laboratory and the experimental apparatus. These simulation were conducted with realistic and simplified geometries to gain a deeper understanding of the scattering spectrum in the presence of an experimental apparatus:

1. The simplified simulation includes a single HVeV detector inside a copper housing, surrounded by an isotropic gamma flux. In this version, we utilized the spectra of ^{137}Cs and ^{133}Ba with their respective activities, with the Cs source having orders of magnitude higher activity. We conducted simulations using different Geant4 low-energy electromagnetic physics lists including Monash [46], Livermore [47], and Penelope [48], to check for systematic changes in the spectrum, particularly at lower energies down to 100 eV. Such energies are far below typical energy ranges used in Geant4 simulations. Monash is the latest electromagnetic physics list for low-energy Compton scattering modeling. While Monash includes small improvements in modeling the kinematics of Compton scattering simulations, we did not observe significant effects in the energy window of interest. The Geant4 version number for these simulations is G4-10.06.p03.
2. The realistic simulation was conducted using the geometry described in Sec. 3.1.1, with a ^{137}Cs point source placed according to measurements. We opted not to model the ^{133}Ba spectrum as the dominance of ^{137}Cs had been demonstrated in the simplified simulations. We used the Monash [46] electromagnetic physics list (the latest and the default option) for this simulation. The Geant4 version number for this simulation is G4-10.07.p04.

3.1.1 Geometry

The detailed simulation included a lead wall with a gap holding the Cs source, a lead shield surrounding the cryogenic refrigerator, refrigerator parts, the detector housing, and detectors. The refrigerator consists of several nested vessels: an outer vacuum chamber (OVC) made of steel, and 50K, 4K, 1K, and mixing-chamber layers all from

copper. It also includes various copper stage plates. The main components of the fridge are shown in Fig. 3.3. The detector housing contains four HVeV detectors made from silicon wafers with aluminum fins and tungsten edge sensors instrumented on the surfaces.



Figure 3.3: Various components of the cryogenic refrigerator modeled in Geant4 simulations. From left to right: copper stages, the assembled fridge without nested vessels, with one of the internal vessels, and the full assembly including the OVC.

The geometry of Geant4 simulations is visualized in Fig. 3.4. The first and last columns depict the geometry from above, while the middle column provides a side view. In the first row, visualizations include the lead shield (left side of the images, in brown) and the lead wall (right side of the images, in blue) protecting the refrigerator in the center. Various layers of the refrigerator are also shown, with the outermost layer depicted in red. The ^{137}Cs source is placed in the lead wall, and the green lines represent the trajectory of gamma rays.

The second row represents the detectors and their housing. The first image on the left illustrates two out of four detectors, with red lines indicating the refrigerator layer. The second image shows the detector holder, with the detectors positioned on the middle two levels, and the grey area representing the detector mask. The final image displays an overhead view of the detectors within the copper housing.

3.1.2 Results

The full simulation was conducted for four detectors with similar scattering targets (silicon substrates). Initially, we compared the spectra across the detectors to ensure consistency. Subsequently, we combined these spectra into a single spectrum to re-

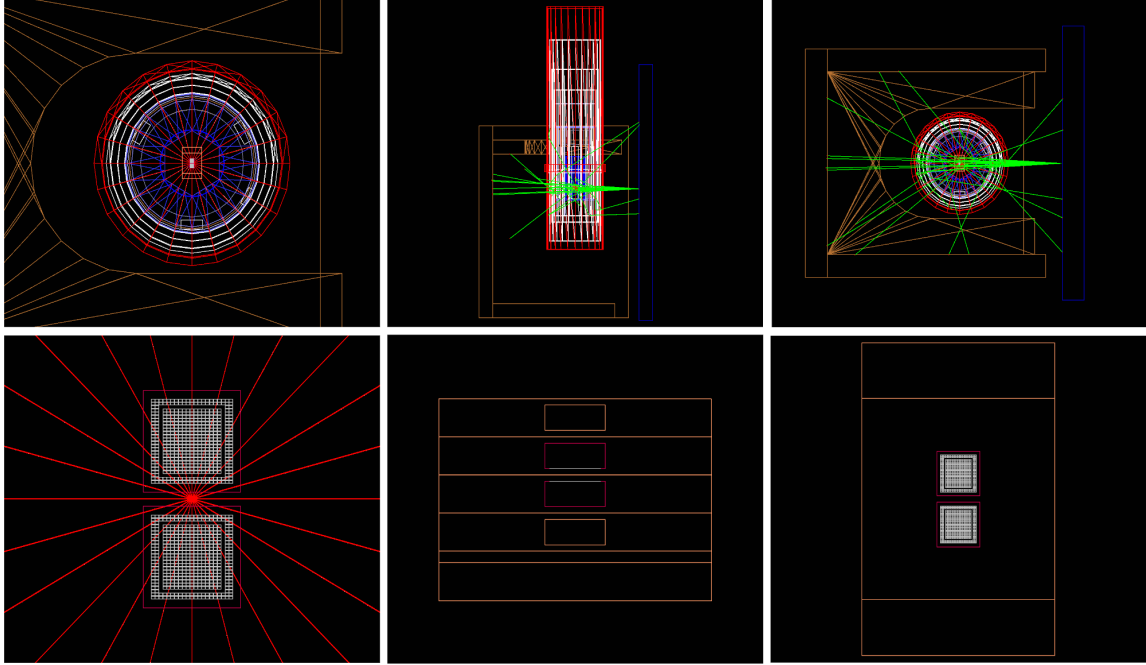


Figure 3.4: Geometry visualization of Geant4 simulations.

duce statistical uncertainty. Comparisons of spectra for various detectors is shown in Fig. [3.5,3.6,3.7]. These comparisons are based on **Kolmogorov-Smirnov (KS)** tests, with the respective p-values reported in the panel on the right. A small p-value indicates a low probability that the spectra from two detectors originate from the same underlying distribution. A p-value smaller than 0.05 is considered to be an indication of inconsistency.

The diagonal cells are expected to be equal to one, as they represent the comparison of each spectrum with itself. Moreover, none of the off-diagonal cells indicate a strong inconsistency between detectors when the comparison is performed within the limited energy windows shown in Fig. [3.5, 3.6]. However, they show inconsistency between detector pairs across the full energy range depicted in Fig. 3.7. This inconsistency is justifiable given the relative positions of the detector pairs with respect to the radioactive source. Based on these findings, we combined the spectra from all four detectors to reduce the statistical uncertainty of the simulation spectrum in the selected energy windows used in the calibration study.

Further investigation revealed that the lead shield in the full simulation was misplaced by approximately 15 cm relative to the stationary lead wall. Consequently, we chose to compare the comprehensive simulation with simplified ones to exam-

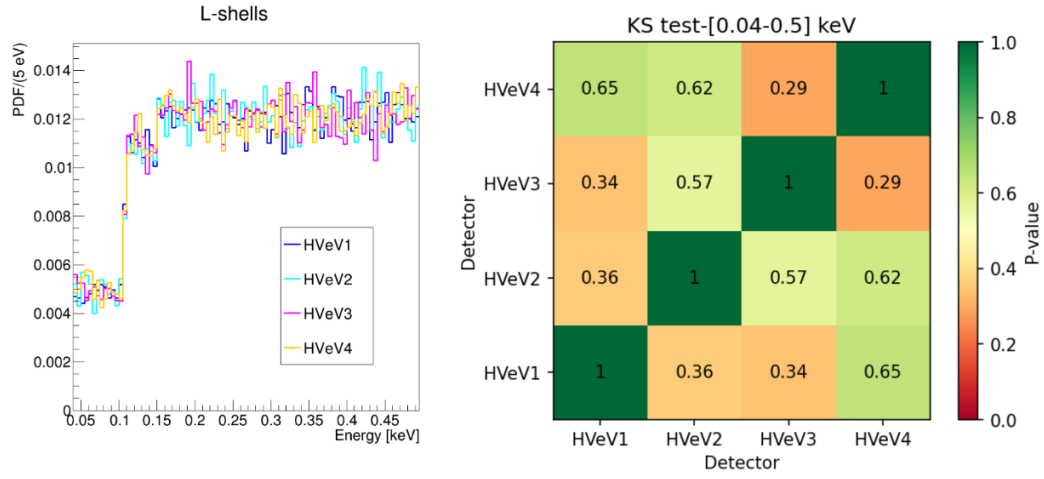


Figure 3.5: Comparison of Geant4 simulation spectra near the Compton L-steps between **HVeV** detectors. The table of p-values on the right indicates consistency between the spectra.

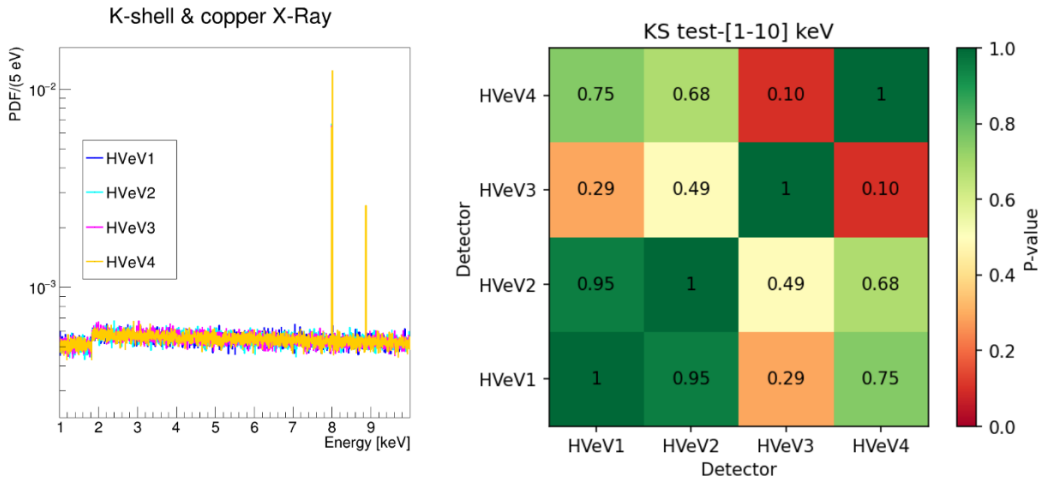


Figure 3.6: Comparison of Geant4 simulation spectra near the Compton k-step between **HVeV** detectors. The table of p-values on the right indicates consistency between the spectra.

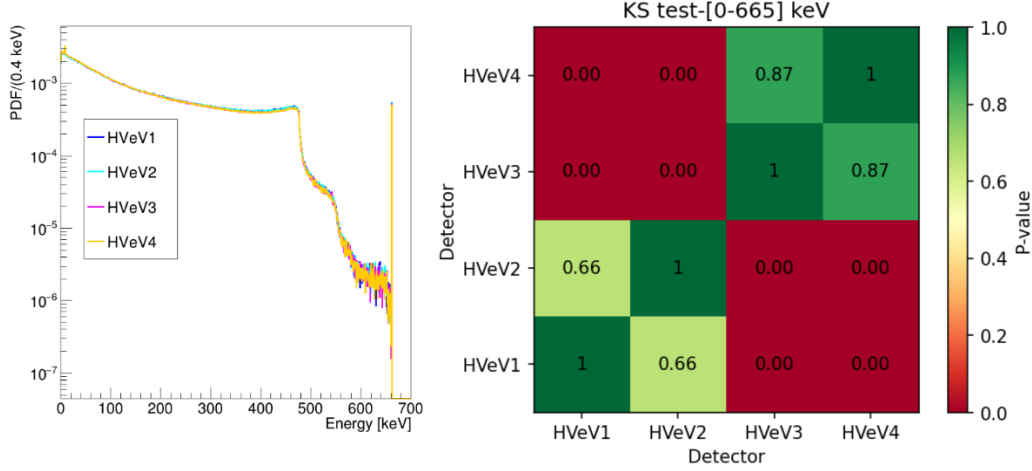


Figure 3.7: Comparison of Geant4 simulation spectra in the full energy range between **HVeV** detectors. The table of p-values on the right indicates consistency between two pairs of detectors.

ine the systematic uncertainty in the shape and position of energy signatures. The comparison in small energy windows is shown in Fig. 3.8.

We observed that the full simulation aligns well with the simplified Monash simulation within the L-shell energy window. At higher energies, the K-step consistency is maintained; however, the full simulation (indicated by the blue line) shows a significantly stronger copper X-ray peak. Additionally, the full simulation displays a slightly steeper slope in the 1 keV to 10 keV energy range. These differences can be attributed to the attenuation of gamma rays, or the reduction of the mean incident energy of photons, by various material layers in the full simulation.

The reduction in the mean energy is evident in the comparison shown in Fig. 3.9 for the complete energy range. According to Fig. 3.1, the interaction cross section increases rapidly at lower energies. Additionally, the scattering cross section in copper is naturally larger than in silicon. Therefore, we should expect an increase in the strength of the Compton peak for attenuated gamma rays. The differential cross section for Compton scattering depends on the ratio of deposited energy to the incident energy. The dependence on the incident energy in the denominator explains the steeper slope if the mean energy of incoming gammas decreases. More details about the differential cross section will be discussed in the next subsection.

The inconsistencies described do not affect the position of energy signatures and would introduce negligible systematic uncertainty in a calibration effort. Therefore, we concluded that a misplaced lead shield would not introduce a systematic uncer-

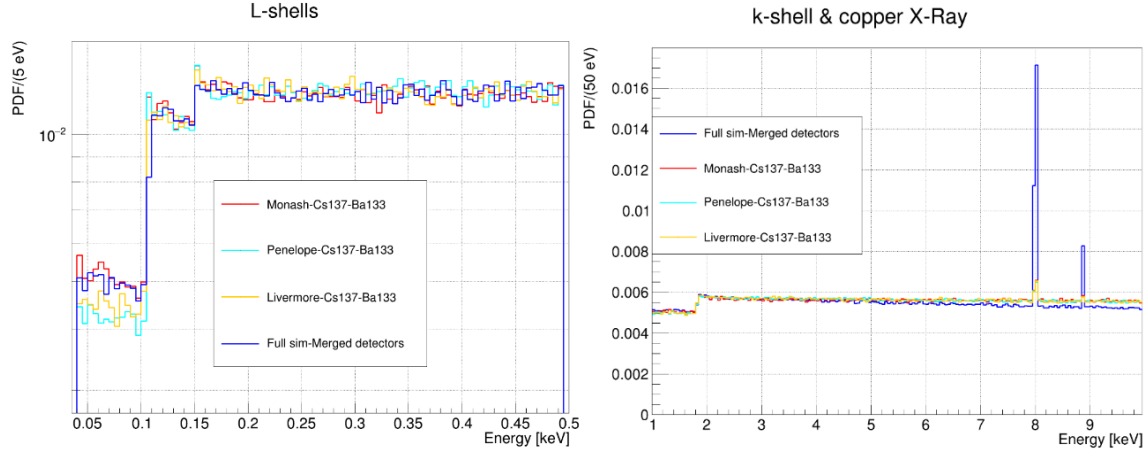


Figure 3.8: Comparison of spectra between the simplified and detailed Geant4 simulations up to 10 keV. The right panel shows the comparison at low energies relevant to L-steps. The left panel shows the comparison at higher energies that includes the K-step and the copper peak.

tainty greater than what is observed between the simple and full simulations. Consequently, we decided against running an enhanced full simulation due to the high computational cost.

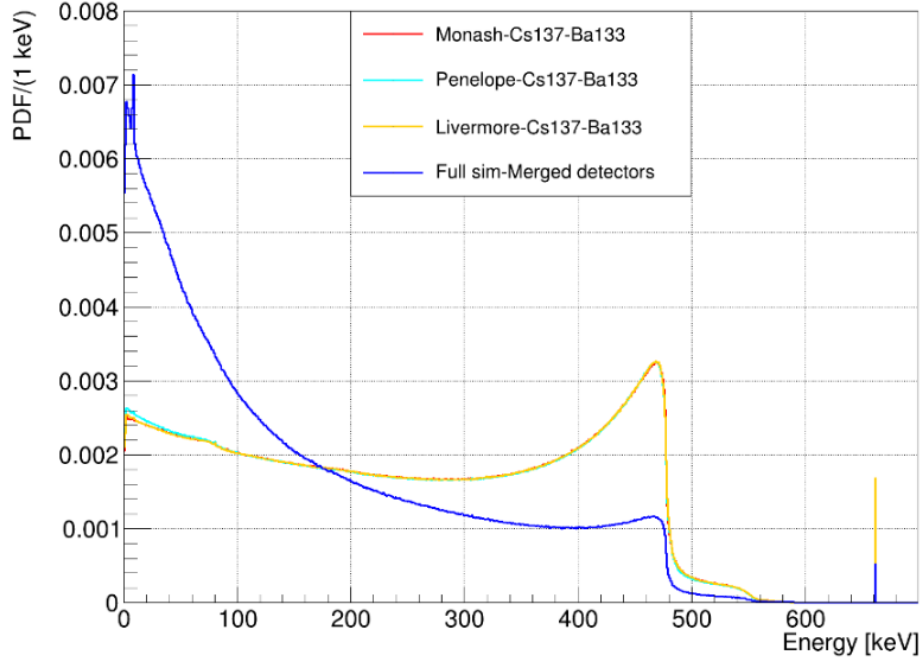


Figure 3.9: Comparison of spectra between the simplified and detailed Geant4 simulations in the full energy range. The blue curve is the latest simulation with the full geometry. The other curves show the the simplified simulations with different Geant4 physics lists.

3.2 FEFF Simulations

The low-energy electromagnetic physics lists in Geant4 utilize a theoretical approximation known, as the relativistic impulse approximation, to simplify modeling of Compton scattering. This approximation is not theoretically valid at low energies close to the binding energy of the core electrons. Therefore, we cannot expect the Geant4 simulations to model the Compton steps in silicon accurately. A previous measurement has shown a good agreement between Geant4 simulations and experimental data for K-steps, but not for the L-step [49]. The same study recommends modeling L-steps using FEFF simulations. Accordingly, we conducted FEFF simulations for silicon and incorporated the resulting Compton scattering cross sections into the calibration study presented in Chapter 5. This section first describes the setup for the FEFF simulations, and then presents the results.

The impulse approximation, along with the condensed matter background knowledge that is required to understand this subsection is reviewed in Appendix A.

3.2.1 Setup

FEFF simulations require an atomic arrangement (crystal) to calculate the inter-atomic Coulomb potentials. The code also requires selecting the absorbing atom to model the scattering process. The size of the crystal surrounding the absorbing atom is particularly important for modeling the cross section oscillations shown in Fig. 3.14. These oscillations arise from quantum mechanical interference in the photoelectron wave function when it is reflected by neighboring atoms. The photoelectron can be viewed as a spherical wave, with an amplitude that decreases as it moves farther from the scattering site; this amplitude also decays due to inelastic energy losses. The oscillation pattern is driven by the amplitude of the reflected wave function, making it a short-range effect, typically on the scale of tens of angstroms [42]. We selected the crystal size with this consideration in mind, opting for 71 atoms which is twice as large as the crystal used in a previous study by the DAMIC-M collaboration [49]. This crystal is constructed through an input shown partially in Table 3.1.

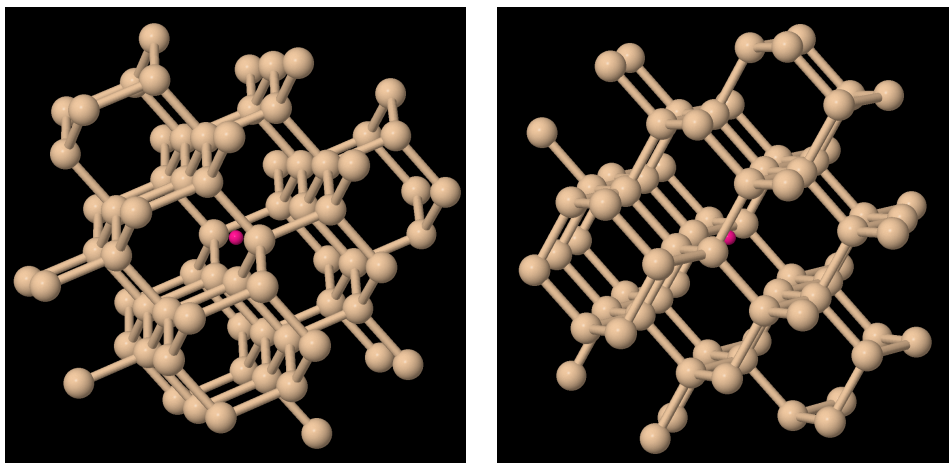


Figure 3.10: The silicon crystal for FEFF simulations from two angles. The pink atom in the center is the absorbing one.

This crystal is constructed through an input shown partially in Table 3.1.

In total, we ran FEFF simulations in 13 distinct modes. First, we conducted a CP calculation targeting the valence electrons. We then proceeded to calculate the directionally averaged structure factor, $s(q,w)$. Calculation for s included modeling the Near Edge region (up to approximately 40 eV above the absorption edge, known as XANES) and the Extended Energy Range (starting from 40 eV above the edge and beyond, referred to as EXAFS) individually. For each range, simulations were conducted with two options: either modeling the core-hole potential using the default setting or ignoring it by turning off the option in the simulations. Lastly, we carried

Count	x (Å)	y (Å)	z (Å)	Type	Atom	Radius (Å)
0	0.00000	0.00000	0.00000	0	Si	0.00000
1	-1.35750	1.35750	1.35750	1	Si	2.35126
2	1.35750	-1.35750	1.35750	1	Si	2.35126
3	1.35750	1.35750	-1.35750	1	Si	2.35126
4	-1.35750	-1.35750	-1.35750	1	Si	2.35126
5	2.71500	2.71500	0.00000	1	Si	3.83959
6	-2.71500	2.71500	0.00000	1	Si	3.83959
⋮						

Table 3.1: A subset of the coordinate points to construct the crystal in the FEFF simulation.

out calculations for each of the L edges – L1, L2, and L3 – individually. We also checked the status of the simulation for each iteration ensuring about the convergence and numerical stability through status output generated by the simulation code.

3.2.2 Results

We conducted simulations both with and without core-hole modeling due to the lack of evidence favoring one approach over the other. A measurement by the DAMIC-M collaboration [49] reports better consistency between data and simulations without core-hole modeling. However, other measurements support the inclusion of core-hole modeling [50]. Consequently, we decided to run simulations in both modes to investigate the differences between them, and assess the uncertainty introduced to subsequent studies.

A unit cell of silicon consists of 8 atoms on the corners, 6 atoms in faces, and 4 atoms within the cell. This leads up to 32 valence electrons per unit cell given that each atom has 4. Utilizing Eqn. A.12, the number of valence electrons resulted from the FEFF CP turned out to be slightly (less 5%) smaller than 32. We followed [51] and scaled the CP by a constant multiplicative factor to correct the deficiency. The corrected and the raw curves are shown in Fig. 3.11.

The CP was then turned into a DSF for valence electrons using Eqn. A.11. For core electrons FEFF gets a value for the momentum transfer, q , and outputs a spectrum of values for the DSF at various energy transfers. Based on preliminary estimations, we determined that the nominal momentum transfers corresponding to energy transfers between 50 and 500 eV would fall within the range of 0.1 to 20 atomic units (a.u.). Consequently, we chose to increment this range in steps of 0.02 a.u. to finely sample the DSF. The simulation results performed at a momentum transfer value of 5.1 (a.u.)

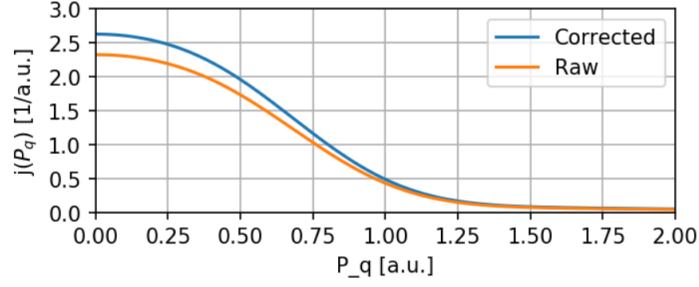


Figure 3.11: Simulated silicon **Compton Profile (CP)** for valence electrons. The orange curve shows the raw **Compton Profile (CP)** calculated using FEFF. The blue curve shows the corrected **CP** as described in the text.

is shown in Fig. 3.12 which can be cross-validated against a measurement reported in [52]. The plot illustrates the relative magnitudes of the **DSFs** computed for different electronic shells, each represented by a distinct color. The vertical lines indicate the transition point from calculations in XANES mode to those in EXAFS mode. Moreover, Fig. 3.13 illustrates the result of stacking up **DSFs** for the no-corehole

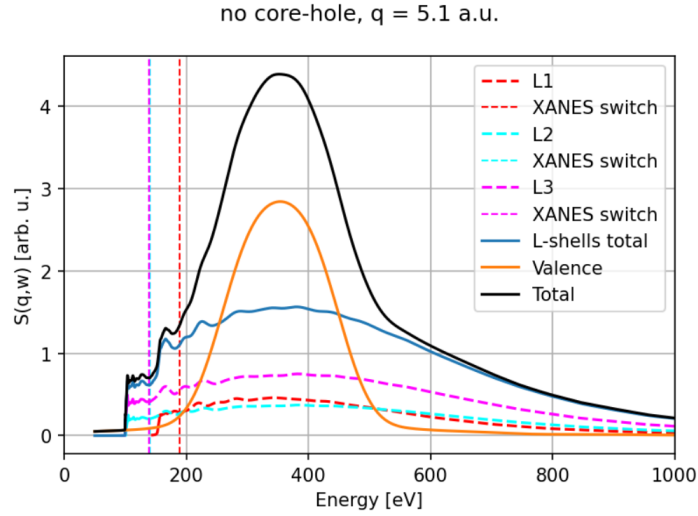


Figure 3.12: The **DSFs** for various electron shells are constructed using FEFF simulations without core-hole potential modeling. The edge energies of the L2 and L3 steps differ by less than half an eV [53, 54], making the XANES switch lines overlapping and indistinguishable.

FEFF simulations in two dimensional plots in natural units.

Given the **DSFs** spectra, we utilized Eqn. A.16 to extract the cross section. In this process, the integral over the scattering angle was replaced by the momentum transfer using the relation obtained from Eqn. A.17. A standard value of 662 keV was used for the primary energy of the scattered photons. The dependence of the

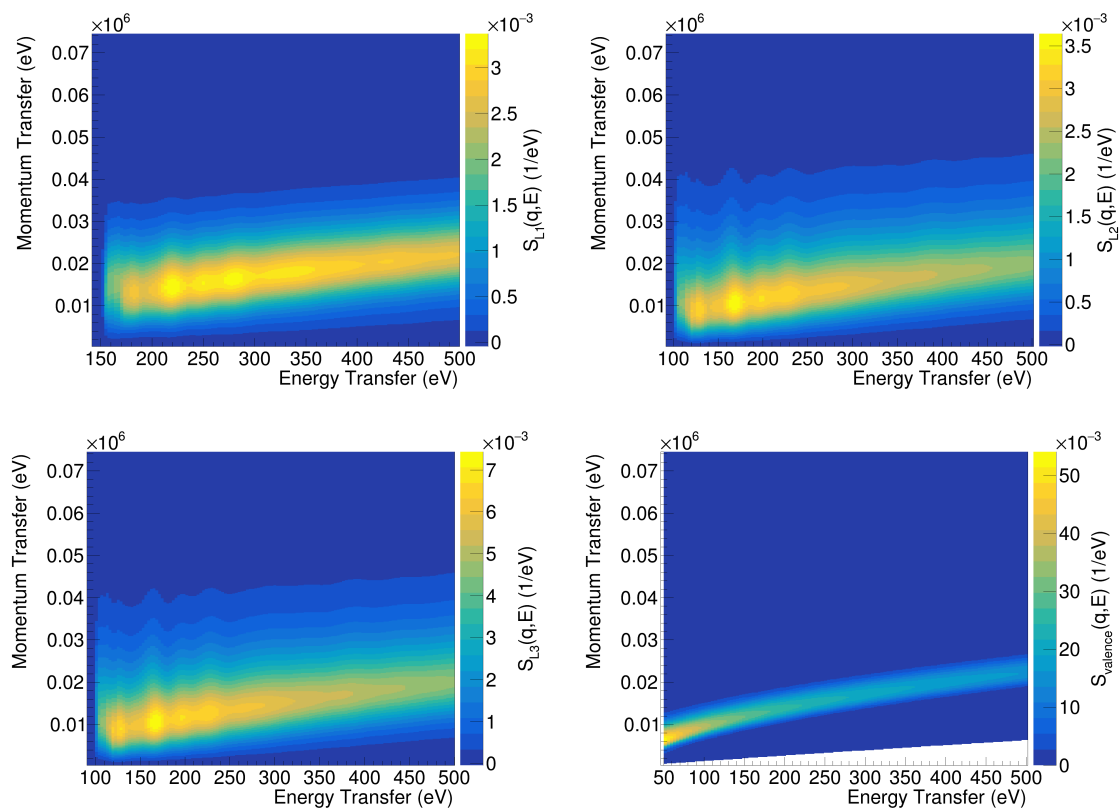


Figure 3.13: The **Dynamical structure factor (DSF)** functions constructed for various electron shells using FEFF simulations without modeling the core-hole potential.

cross section on the energy of the primary gamma rays is reflected in the coefficient $\left(1 - \frac{\text{Deposited energy}}{\text{Primary energy}}\right)$. This term can introduce a slope in the cross section spectrum as a function of energy, as illustrated in Fig. 3.8 for the "k-shell & copper X-Ray" plot. In the same figure, we observe no difference in the slope between full simulations and simple ones within the energy window for L-shells. This indicates that, despite the various layers of materials in the full simulation, the change in the mean energy of gamma rays hitting the detectors is not significant enough to affect the slope in the limited energy window for L-steps. Consequently, we used a nominal value of 662 keV for the primary energies of gamma rays to calculate the FEFF cross section. Additionally, we confirmed negligible changes to the cross section by reducing the initial energies to 100 keV and comparing the resulting cross section curves.

The resulting cross section with and without the core-hole potential, respectively on the right and on the left, is shown in Fig. 3.14.

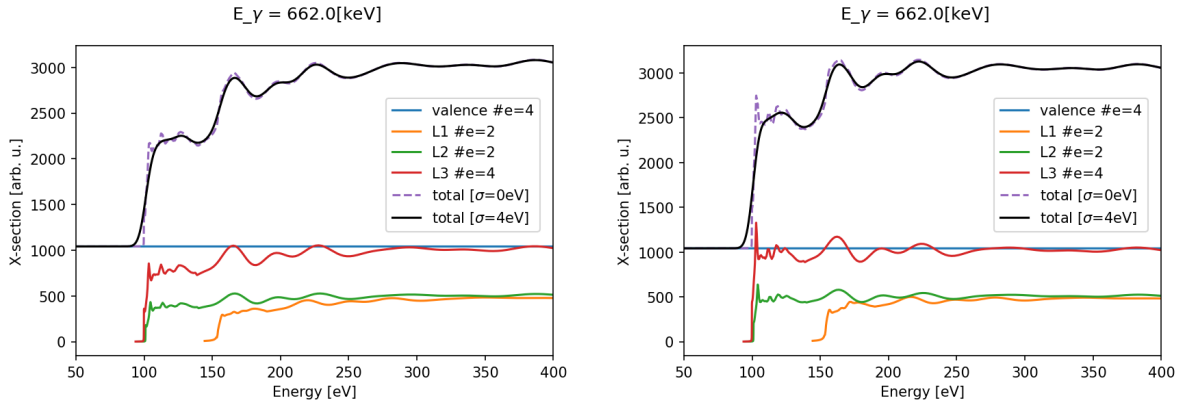


Figure 3.14: Compton scattering differential cross-section in silicon at low energies, computed using FEFF simulations. The left plot shows the result with modeling the core-hole potential, and the right plot shows the result without it.

Finally, we compare Geant4 simulations and FEFF simulations in Fig. 3.15. The simulations qualitatively agree at energies above 300 eV. The greatest deviation is observable in the vicinity of the L-steps at 100 eV and 150 eV. The cross section that is predicted by the FEFF simulation is smaller than Geant4. This observation is consistent with the previous observation by the DAMIC-M collaboration [49].

3.3 Summary

The work in this chapter provides the simulations that are used for the calibration study in subsequent chapters. I used the FEFF simulations at energies below 500 eV

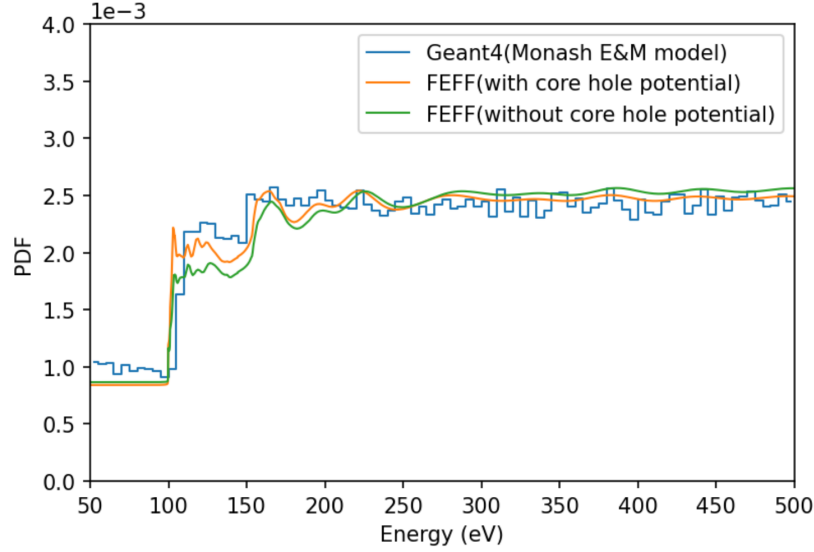


Figure 3.15: Comparison of Geant4 and FEFF simulations for the Compton scattering differential cross section in silicon. The Geant4 histogram and the FEFF cross section curves are weighted by their area to turn them into PDFs. The x-axis shows the energy.

to locate the Compton L-steps (≈ 100 eV, and ≈ 150 eV) in the data. At higher energies we used the Geant4 simulations to locate the Compton k-step (≈ 1.8 keV) and the copper K_α X-ray peak (≈ 8 keV) in the data. Note that we could not see the copper K_β peak due to the detector resolution as discussed in Chapter 5.

The FEFF simulations indicated a smaller number of Compton scatters between 100 eV and 150 eV compared to Geant4 simulations by approximately 20%. Further studies are required to validate FEFF simulations. Also, it might be interesting to adopt the FEFF cross section in the energy ranges close to the binding energies of core electrons in Geant4. This modification could be important for background modeling of rare-event searches.

The systematic uncertainty between the GEANT4 and FEFF simulations is unlikely to affect the background models for the SuperCDMS SNOLAB experiment. Based on the background budget, Compton scattering is not a dominant background in any of the detectors [23, 24] in the SNOLAB experiment. The main background sources for the SNOLAB detectors are due to tritium and ^{32}Si , respectively in germanium and silicon detectors. These backgrounds are inherent to the detector materials and produce beta decays. The SNOLAB shielding is designed to minimize other sources of background to levels below the irreducible detector contaminants.

The next chapter first provides a general overview of the science program with

SuperCDMS R&D detectors, which are the ones we used for the collection of the Compton calibration data. Then it discusses the experimental setup, the data sets, and the data preparation steps for the Compton calibration study.

Chapter 4

HVeV Run 4 and Compton Scattering Data

The data discussed in this chapter comes from the fourth generation (Run 4) of experiments using **high-voltage eV-resolution (HVeV)** detectors. These detectors have been previously utilized in various studies, including low-mass dark matter searches [55, 56, 57], ionization yield measurements in silicon [37], and investigations into the sources of low-energy background events in **HVeV** detectors [58]. We begin with a brief review of the **HVeV** science program that led to the design and planning of the Compton calibration effort¹. We then proceed to discuss the **HVeV** Run 4 and the Compton calibration data. In summary, this chapter presents the following:

1. A brief overview of the **HVeV** science program. It emphasizes a previous observation of a stronger **TES** response at high-voltage compared to a 0 V crystal bias, when the final phonon energy appears to be the same. This observation, along with the need for a calibration scheme for SNOLAB silicon detectors as discussed in Chapter 1, forms the basis for the Compton calibration study pursued in this thesis.
2. Detail of the experiment setup and data sets for the Compton calibration study.
3. Detail of the data cleaning procedure.
4. A processing bias correction for one of the energy estimators (pulse integral) used in the calibration study. This bias is a processing artifact caused by a high event rate and prolonged pulses.

¹For more information about the historical development up to **HVeV** Run 3 see [59].

4.1 HVeV science program

The first dark matter search using an HVeV detector, referred to as HVeV Run 1, was conducted at Stanford University. The detector demonstrated the ability to identify single electron-hole pairs with a resolution of approximately 0.1 electron-hole (e^-h^+), achieved by applying a high voltage across the detector target. This run investigated DM models depositing the energy through electron recoils for DM masses as low as 0.5 MeV. Additionally, it established an upper limit on the kinetic mixing of dark photons for mass values greater than 1.2 eV.

The second generation of dark matter searches with HVeV detectors, HVeV Run 2, saw multiple improvements. First, the detector design was enhanced, improving the resolution by approximately a factor of three to $\sim 0.03 e^-h^+$. Additionally, an anti-coincidence criteria for energy depositions between two HVeV detectors was implemented, assuming a negligible probability of simultaneous energy deposition from DM particles. Furthermore, the dark matter model was refined to incorporate charge-trapping (CT) and impact-ionization (II) effects as discussed in subsection 2.2.3 [27, 28]. Lastly, the statistical framework for setting exclusion limits was changed from the Optimum Interval (OI) method used in HVeV Run 1 to Poisson counting which was motivated due to a strong sensitivity of the OI method to systematic uncertainties. A comparison between the data from this run and the examined electron recoil dark matter model with a mass of 1 GeV is shown in Fig. 4.1. The excess number of events in the first e^-h^+ peak at 100 eV was a limiting factor for the exclusion curve set by HVeV Run 2. This observation, consistent with HVeV Run 1, raised questions regarding the source of low-energy depositions.

To identify the source of low-energy events, the HVeV group performed another measurement by collecting data at bias voltages of 0 V, 60 V, and 100 V. This measurement was performed with four detectors adjacent to each other to identify coincident energy depositions [58]. Across all data sets, the study identified events with slow decaying tails compared to the known calibration events. These long-tail events were followed by low-energy events, illustrated in Fig. 4.2, with energies of approximately 2 eV. Such low-energy events can produce only one e^-h^+ pair; hence, they would populate the first e^-h^+ peak when there is a bias across the crystal. The appearance of coincident long-tail pulses suggested that the source of these events is external to detectors. Furthermore, the comparison between 0 V and high-voltage data revealed that the long-tail events likely consist of multiple events occurring within time separations shorter than the detector's temporal resolution. Finally, the

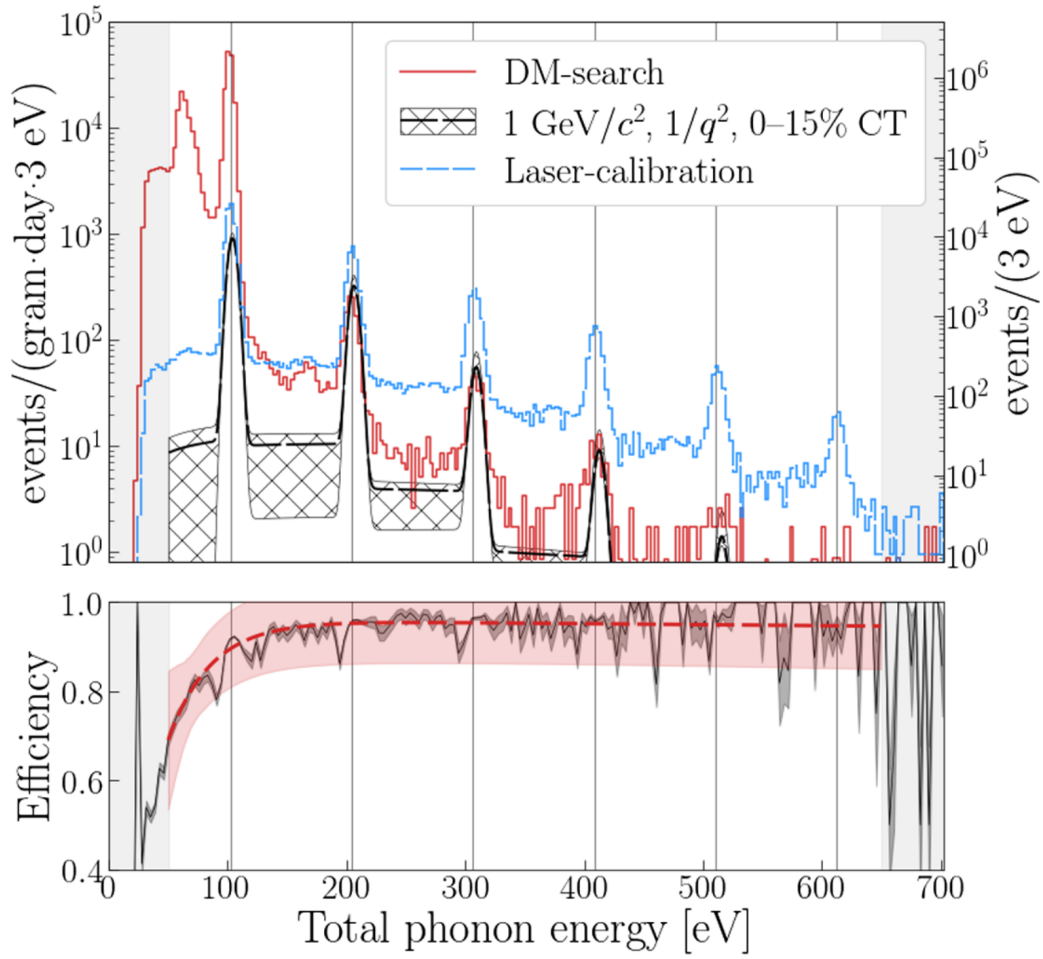


Figure 4.1: Dark matter search data from HVEV Run 2 [56]. The x-axis shows the energy, the y-axis in the upper panel shows the event rate, and the y-axis in the lower panel shows the efficiency of the data cleaning for the dark matter search data.

individual events on the tail were found to be consistent with the energy of a subset of luminescence photons from **printed circuit board (PCB)**. These observations led to the conclusion that the **PCB** board adjacent to detectors experiences luminescence and illuminates the detectors. Therefore, a decision was made to design a new detector housing without **PCB** components for HVEV Run 4.

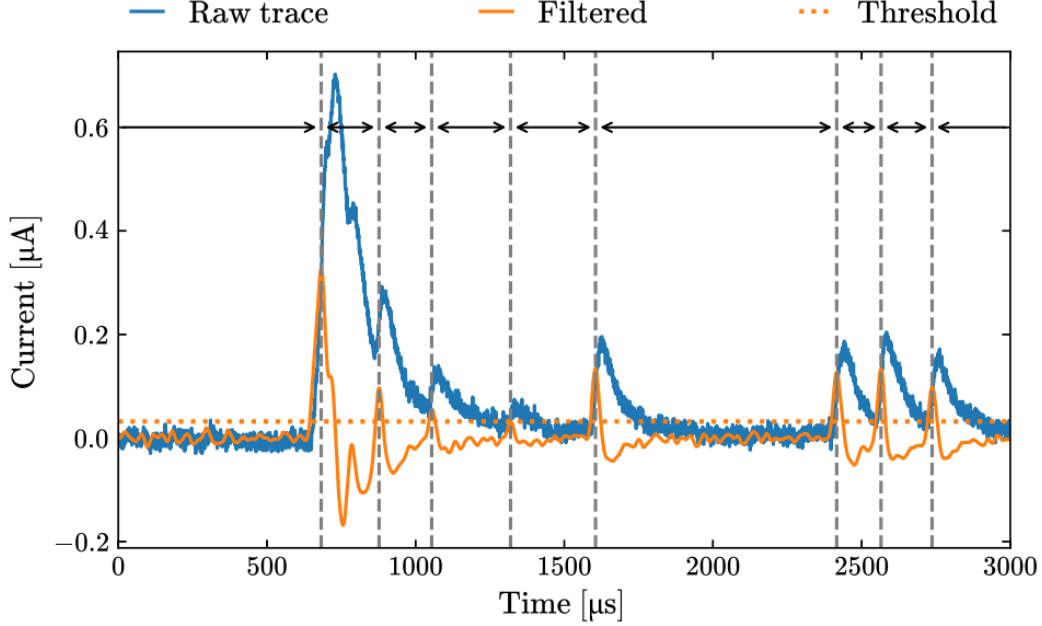


Figure 4.2: A long-tail event (burst event) followed by low-energy events on the tail. The blue trace represents the raw signal, while the orange trace shows the result after applying a Gaussian derivative filter. The dotted orange line indicates the threshold used for peak detection, with each peak above this threshold in the filtered trace corresponding to a pulse in the raw signal. Vertical dashed lines mark the rising edges of events detected above the threshold [58].

A key step in identifying the source of low-energy events is the calibration of the 0 V data sets. This calibration was first attempted in [25]. The results showed an approximately 11% stronger **TES** response when a high voltage was applied across the crystal for the same amount of energy deposition, as illustrated in Fig. 4.3. In the figure, the y-axis represents the energy estimator that quantifies the **TES** response, while the x-axis represents the energy. The number of e^-h^+ pairs created when a group of photons from the laser hits the detector determines the position of the blue and magenta points. The plot also includes the positions of X-ray energy signatures from a ^{55}Fe radioactive source, with the detector operated at eight different bias voltages to uniformly cover the energy range between 6 keV and 120 keV. A sixth-degree polynomial was fitted to the energy signatures with a bias greater than 40 V

(considered high voltage), as shown by the red curve. The same curve was then scaled with a single parameter to match the energy signatures at 0 V, including photopeaks and a Compton edge signature from a ^{57}Co source, as well as ^{55}Fe signatures at 0 V. The 0 V curve was not consistent with all 0 V energy signatures simultaneously. Moreover, the energy signatures from ^{57}Co are deep in the saturated energy range of the detector, as indicated by the non-linearity of the calibration function (saturation is defined in section 2.1). These observations motivated a more robust comparison between the calibration at 0 V and high-voltage operation modes. In particular, we were interested in repeating the comparison with 0 V energy signatures at values of a few keV and lower energy depositions to stay closer to the linear response region of the TES.

The discrepancy in the calibration between the 0 V and high-voltage operation, and the need for a low-energy calibration technique for SuperCDMS HV detectors, as described in Chapter 1, were the main motivations for the Compton calibration study that will be discussed.

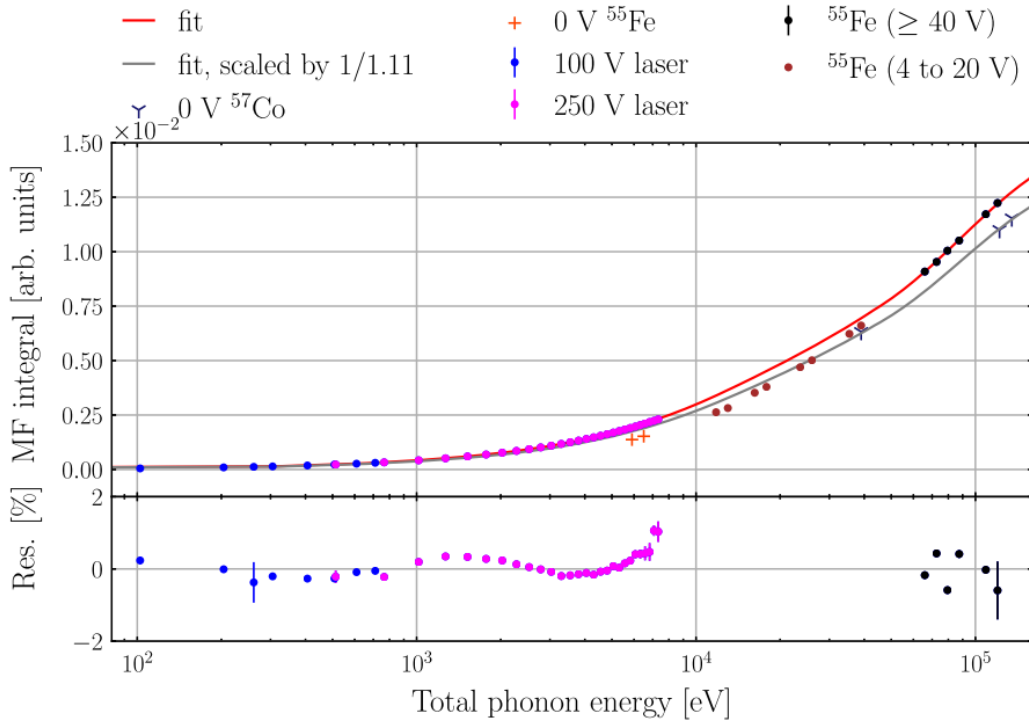


Figure 4.3: Calibration at 0 V and high-voltage [25].

4.2 HVeV Run 4 experiment setup

The data for the Compton step calibration study were collected during **HVeV** Run 4 at the **Northwestern EXperimental Underground Site (NEXUS)** facility at Fermilab between January and July 2022. The **NEXUS** facility is 107 m underground and has 225 m of water equivalent rock overburden [60] to mitigate the effects of cosmic rays.

Four **HVeV** detectors, each with a silicon scattering target measuring 10 mm x 10 mm x 4 mm (0.93 g), were employed. The **HVeV** detectors are named as follows: 2 x **NFC** (**NFC1**, **NFC2**), **NFH**, and **NFE**, where the last letter (C, H, and E) indicates the **QET** pattern, instrumented on one side of the silicon target. This side is maintained at 0 V and is equipped with two channels, each consisting of a series of **QETs** connected in parallel. The channels cover the inner and outer regions of the detector surface, distinguished by the red lines in Fig. 4.4. The opposite side of the silicon target is covered by an aluminum grid, which covers 5% of the total area and applies a voltage bias. This limited coverage is intentionally chosen to reduce the likelihood of phonon trapping in the grid. The bias across the crystal drifts charges and enhances the phonon signal through **Neganov-Trofimov-Luke (NTL)** amplification, as discussed in subsection 2.2.2.

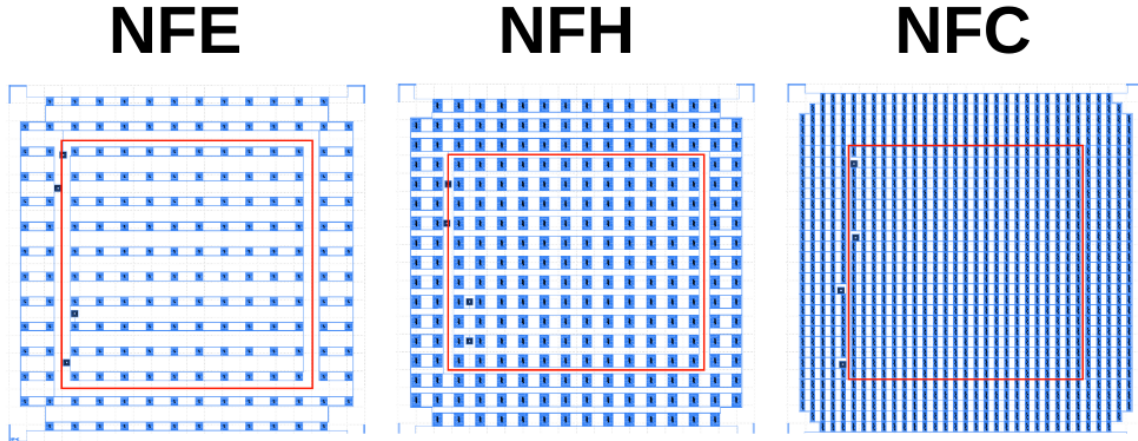


Figure 4.4: The **QET** configuration of detectors used in HVeV Run 4. Each detector consists of two channels, internal and external, that are identified by the red box. Each channel has an individual readout.

All detectors were installed adjacently inside a light-tight copper housing, as illustrated in Fig. 4.5. There is an opening between the detector floors providing a line of sight between the **QET** faces of detectors. The line of sight helps to remove coincidence events which increase the background rejection for a **DM** search. The detector

payload was placed in a copper cavity within the dilution refrigerator, which can reach a minimum temperature of approximately 10 mK. The exterior of the refrigerator was wrapped with a magnetic field shielding material. The shield reduces the external magnetic field, which could affect the readout electronics, such as the operation of the superconducting quantum interference device [32]. Additionally, the refrigerator was surrounded by a stationary lead wall on one side, and a lead shield mounted on a movable cart on the other sides. The refrigerator and shielding components are shown in Fig. 4.6.

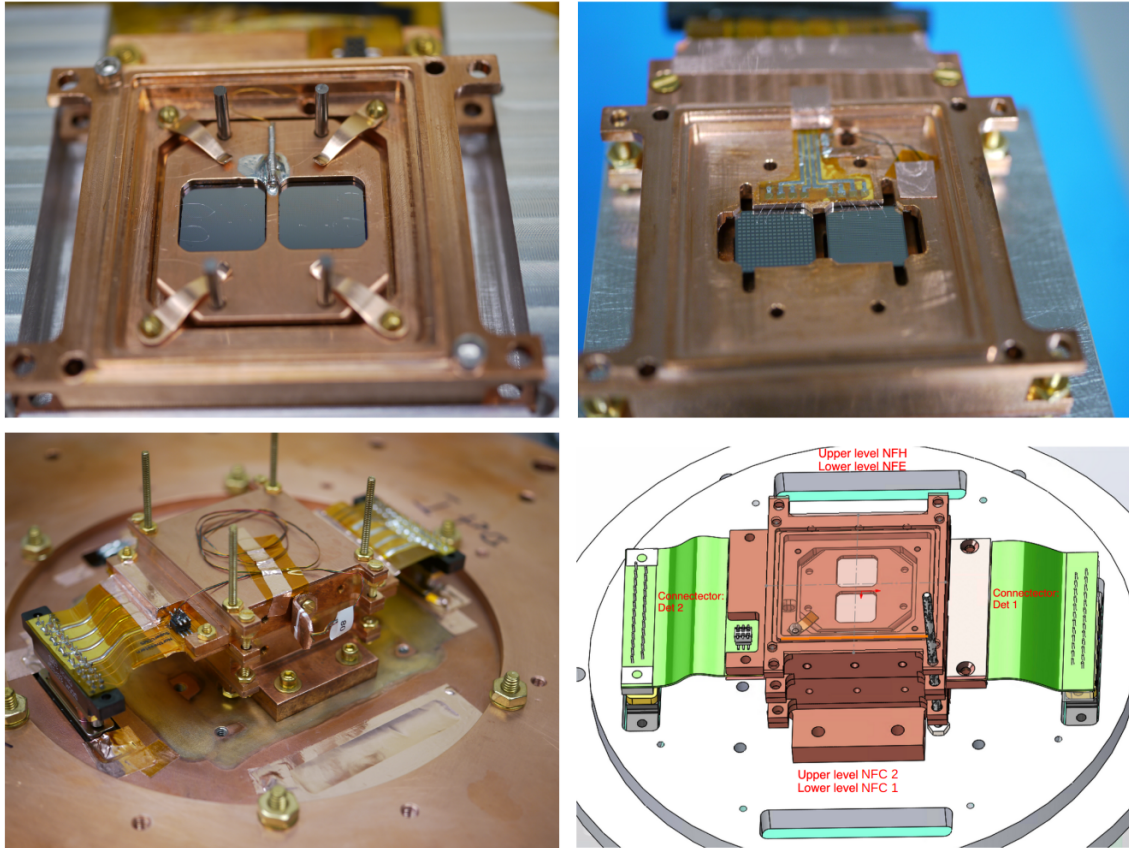


Figure 4.5: Top left: NFC1 on the left and NFE on the right. Top right: NFH on the left and NFC2 on the right. Bottom left: assembled detector housing. Bottom right: sketch of the assembly.

The detector housing shown in Fig. 4.5 was used to collect calibration data with radioactive sources placed next to the detectors. We also collected background data without the radioactive source to construct an empirical background model. Additionally, the housing was expanded with two extra levels to accommodate LEDs that emit low-energy photons at 2 eV. With this expansion, each detector was illuminated from the back (the side with the aluminum grid for voltage bias) by LEDs through a

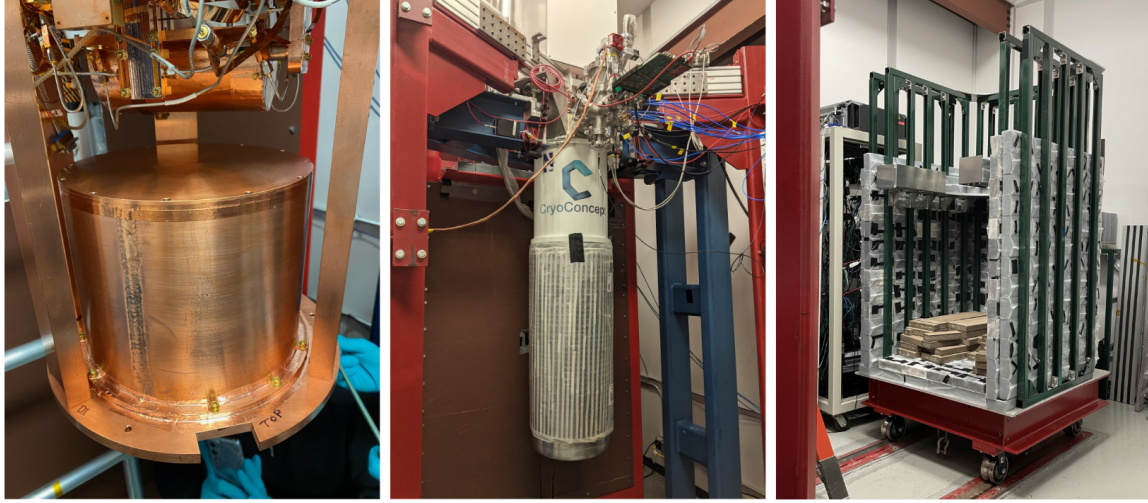


Figure 4.6: Left: Copper cavity. Middle: Assembled refrigerator wrapped in Metglas, positioned in front of a lead wall. Right: Movable lead shield.

pinhole covered by an IR filter. The primary purpose of the IR filter was to allow the LED photons to pass through while blocking any background light leakage through the pinholes. The expanded housing and the pinholes are shown in Fig. 4.7.

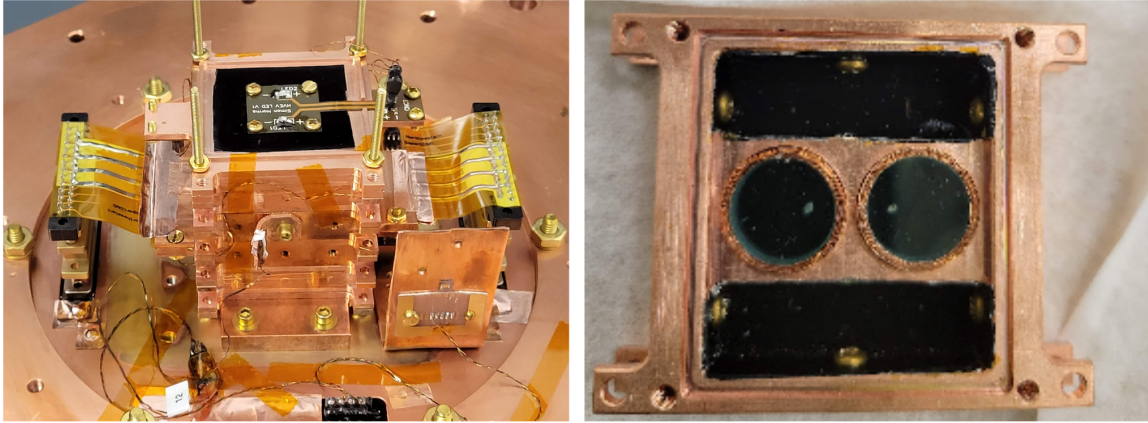


Figure 4.7: Left: Expanded detector housing with additional floors for LEDs. Right: LED pinholes covered with IR filter that face the back of HVeV detectors.

4.2.1 Radioactive source information

Two radioactive sources were employed: ^{133}Ba and ^{137}Cs . The primary gamma-ray energies from these sources exceed 100 keV, resulting in energy deposition in

the detectors primarily through Compton scattering, as discussed in Chapter 3. The collected data showed no identifiable energy signatures from ^{133}Ba , which is consistent with simulations (Fig. 3.9). This is likely due to the activity of ^{137}Cs being two orders of magnitude higher than that of ^{133}Ba . The characteristics of these sources are summarized in Table 4.1.

Source	FNAL ID	Activity Aug. 2020 [Bq]	Activity Mar. 2022 [Bq]	Significant Photo Peaks [keV]	Compton Edge [keV]
^{133}Ba	1330.13	22200	20002	81.00 (33%), 302.85 (18%), 356.01 (62%)	~ 19.5 , ~ 164 , ~ 207
^{137}Cs	1372.32	3265000	3139488	661.66 (85%)	~ 478

Table 4.1: Radioactive source information [61].

We collected multiple calibration data sets with varying configurations including different positions of the radioactive source relative to the detectors, different detector biases, and the presence or absence of the lead shield. The positions of the radioactive sources are detailed in Table 4.2. For the final analysis, only the calibration data collected at 0 V detector bias between February 25 and 28, 2022, were utilized. The exclusion of other data sets was based on several factors: fluctuations in refrigerator temperature causing instabilities in detector performance, the lack of suitable background data to construct an empirical background model, and a low data cleaning efficiency for the calibration data sets at 100 V bias. The low-efficiency is due to over-amplification of the phonon signals through the **N****T****L** gain, resulting in prolonged pulses that overlapped in time. As will be discussed, overlapping events cannot be processed with high accuracy and are therefore rejected during data cleaning. A schematic of the detector positions relative to the lead wall and a photograph of the radioactive source placement are shown in Fig. 4.8.

Source	Reference	Feb. 13-15	Feb. 25-28	Apr. 5-7	Apr. 7-10
^{137}Cs	Distance from the 300 K can	57-62 cm	21 cm	26 cm	57-62 cm
	Distance from the floor	150 ± 10 cm	138 cm	141 cm	130 ± 10 cm
^{133}Ba	Distance from the floor	134 ± 10 cm	135 ± 10 cm	N/A	N/A

Table 4.2: ^{137}Cs and ^{133}Ba source positions.

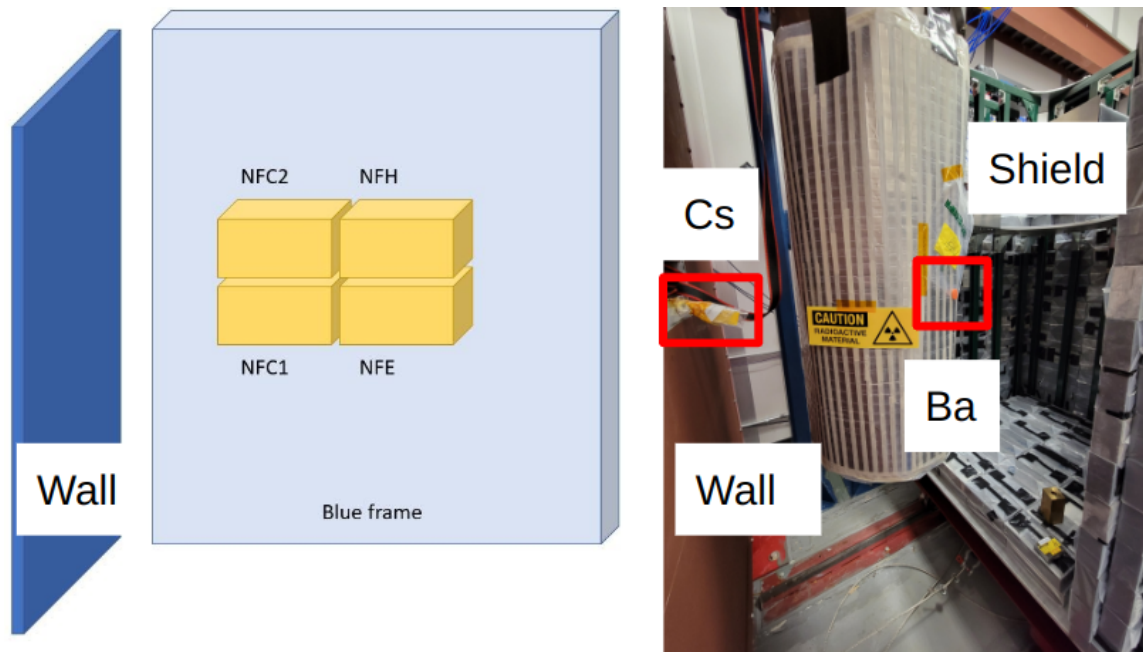


Figure 4.8: Left: Schematic of the detector positions with respect to the lead wall. Right: Placement of radioactive sources during the calibration data. The Cs source is positioned within a hole in the lead wall, while the Ba source is attached to the refrigerator.

4.3 Datasets

The collected data sets are summarized in Fig. 4.9. According to the legend, the black line represents the temperature of the mixing chamber, where the detector housing is mounted. Vertical dashed lines indicate the starting points of individual data sets under each configuration. The legend provides the information about the run configuration including the detector voltage bias, the radioactive source (or “bg” if none was in place), and the status of the lead shield which could be changed by moving the cart.

The “0V CsBa closed” data provided the Compton signatures used for the calibration. Additionally, the “0V bg closed” data were used to construct an empirical background model. The “100V Cs open” data were used to evaluate the performance of data cleaning cuts, and to investigate the efficiency of raw data reconstruction for prolonged pulses. The “0V CsBa open” and “0V Cs open” data sets were not used for the final analysis. The refrigerator temperature was unstable during the “0V CsBa open” run, and for the “0V Cs open” run, there was no background data with a similar detector configuration.

We also collected two additional data sets: a calibration data set at a 150 V bias while periodically illuminating the detectors with a LED, and background data sets at 100 V, which HVeV R4 used to perform a dark matter search. The dark matter search is not the focus of this thesis and is not documented here. However, we used the 100 V data sets to find the pulse templates and the noise **power spectral density (PSD)** for the detectors, which will be elaborated on in the processing subsection. The analysis of the 150 V LED data is standalone and will be discussed in the respective section.

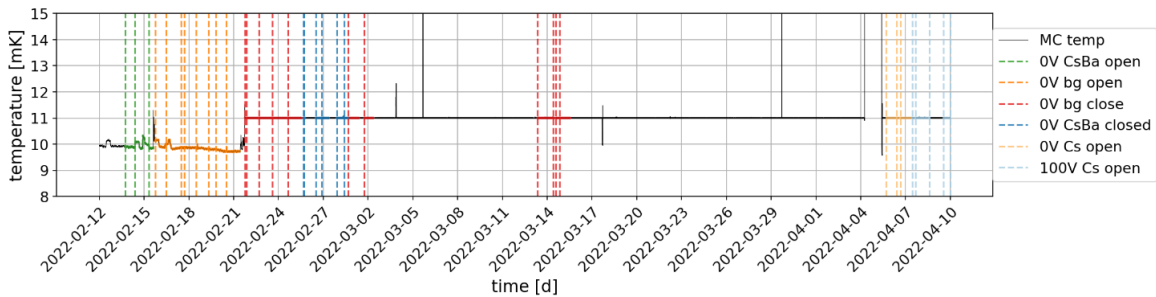


Figure 4.9: Summary of data sets collected for the calibration study. The final data sets for the calibration study are represented by the red (0 V bg close) and blue (0 V CsBa close) colors. The 0V bg close data is taken in three time intervals.

4.4 Readout and processing

The readout from the inner and outer channels of each HVeV detector were digitized by the SuperCDMS **Detector Control and Readout Card (DCRC)** card. Continuous data was recorded to disk in chunks of 0.5 s using the **Maximum Integrated Data Acquisition System (MIDAS)** package [62] at a sampling frequency of 156250 Hz. We then used “PyCRP”, a processing package developed by SuperCDMS (Runze (Tom) Ren), to perform an offline triggering and data processing.

4.4.1 Triggering

Each half-second segment of raw data is filtered using the **Gaussian derivative filter (GF)**, followed by a constant threshold trigger to identify potential events. For each triggered event, a slice of 2048 samples ($13.1 \mu\text{s}$), centered around the maximum value of the filtered trace, is selected for further processing. In Fig. 4.10, the GF kernel is shown on the right, the raw data is shown in blue on the left, and the filtered trace using GF is in green. The orange curve is filtered with **OF** which will be explained later. The kernel is created by taking the first derivative of a Gaussian function with a standard deviation of 6 samples ($38.4 \mu\text{s}$), truncated at 4 times the kernel width, as recommended by previous HVeV studies [63].

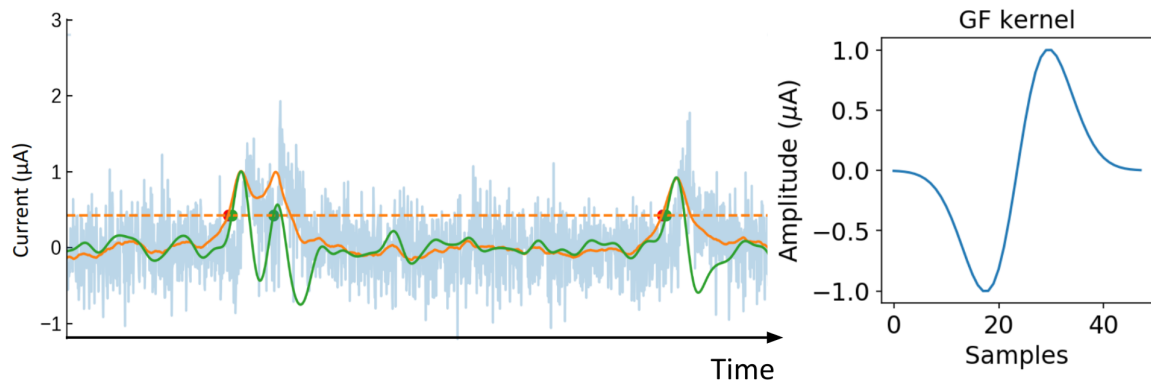


Figure 4.10: Left: Raw data and filtered traces according to **GF** in green, and **OF** in orange. Each time sample is approximately $38.4 \mu\text{s}$. Right: The kernel for the **GF**.

4.4.2 Data processing

We process the data across all detectors for a trigger issued in any of the detectors. Slices of raw data surrounding the trigger time are processed to extract **reduced**

quantity (RQ) values that summarize key information about the events. The list of **RQs** consists of two groups: those calculated directly from the raw trace, and those calculated using the **optimal filter (OF)** method [30, 64]. For instance, the mean value of the data slice before the pulse rise falls under the first group, while the pulse height and the χ^2 discriminator for the similarity of the event with an existing template belong to the second group (Fig. 4.2). The **OF** method requires a template (Fig. 4.11) for the expected pulse shape in the frequency domain, $T(f)$, and the underlying noise **power spectral density (PSD)** of the data, $J(f)$.

The **OF** method finds the best fit of the pulse template to raw data by minimizing a χ^2 value for the goodness of fit following

$$\chi^2(A) = \int_{-\infty}^{+\infty} \frac{|\nu(f) - AT(f)|^2}{J(f)} df, \quad (4.1)$$

where $T(f)$ is the template, $J(f)$ is the **PSD**, and $\nu(f)$ is the Fourier transform of the raw trace. In Eqn. 4.1, the assumption is that the template and the raw trace are aligned in time. It is possible to correct for a misalignment in time between the template and the triggered event by adding an extra degree of freedom following

$$\chi^2(A, t_0) = \int_{-\infty}^{+\infty} \frac{|\nu(f) - Ae^{-i2\pi ft_0}T(f)|^2}{J(f)} df, \quad (4.2)$$

where t_0 is the time shift that provides the best fit.

Minimizing Eqn. 4.1 with respect to A by setting the derivative to zero gives

$$A = \int_{-\infty}^{\infty} \phi'(f)\nu(f) df, \quad (4.3)$$

where

$$\begin{aligned} \phi'(f) &= \frac{\frac{T^*(f)}{J(f)}}{\int_{-\infty}^{\infty} \phi(f)T(f) df}, \\ \phi(f) &= \frac{T^*(f)}{J(f)}. \end{aligned} \quad (4.4)$$

Similarly, the minimization of Eqn. 4.2 with respect to A as a function of t_0 gives

$$A(t_0) = \int_{-\infty}^{\infty} e^{i\omega t_0} \phi'(f)\nu(f) df. \quad (4.5)$$

Consequently, $\chi^2(A(t_0), t_0) = \chi_{\max}^2(t_0)$ gives

$$\begin{aligned}\chi_{\max}^2(t_0) &= \chi_0^2 - A^2(t_0)N, \\ N &= \int_{-\infty}^{\infty} \phi(f)T(f) df \\ \chi_0^2 &= \int_{-\infty}^{+\infty} \frac{|\nu(f)|^2}{J(f)} df.\end{aligned}\tag{4.6}$$

Furthermore, one can minimize the $\chi_{\max}^2(t_0)$ numerically to find t_0 . The discrete version of Eqn. [4.4, 4.6] is reviewed in [30] and is implemented in the processing code. In our setup, the processing code used frequencies up to 78125 Hz.

To construct pulse templates for processing, we first applied the triggering scheme to background data collected at 100 V. Initial processing was then conducted using templates from previous HVeV studies. Subsequently, events near the first e^-h^+ pair, identified by their pulse height values, were selected. These events were filtered using their χ^2 RQ values to isolate high-quality events. The selected events were aligned according to the time offset provided by Eqn. 4.2 and averaged to produce refined templates. Through this procedure, we constructed three pulse templates for each HVeV detector: one for the inner channel, one for the outer channel, and one for the direct sum of traces from both channels (total template). The total template for detector NFC1 is shown in Fig. 4.11. Subsequently, the raw data were reprocessed with the fine-tuned templates.

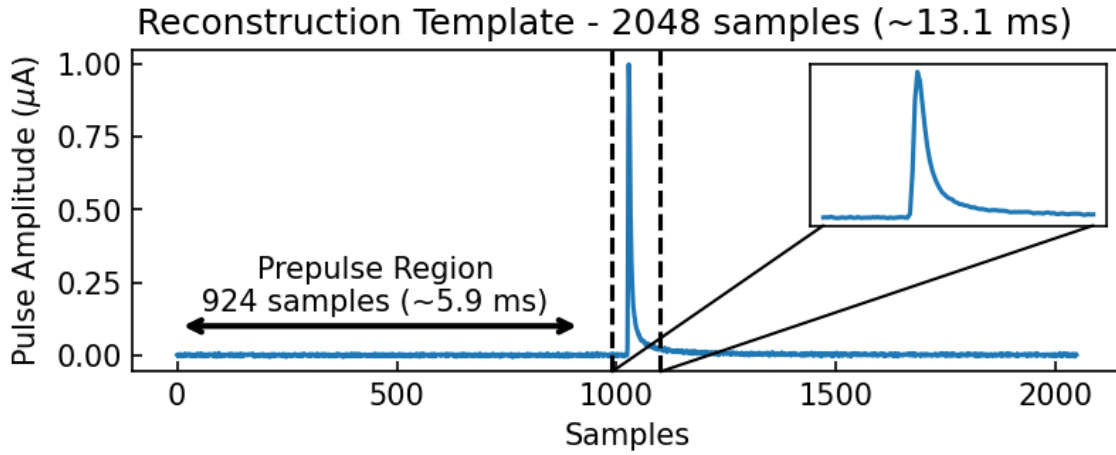


Figure 4.11: Pulse template for the sum of the inner and outer channels of NFC1 detector.

The noise PSD for various channels—inner, outer, or total—was constructed by

applying random triggering and rejecting traces that exhibited unusual mean, standard deviation, slope, or skewness. The remaining traces were Fourier transformed to calculate their respective **PSDs** and then averaged to obtain the final **PSDs** for each channel. Similar to the pulse templates, we used 100 V background data sets to construct the **PSDs**. This approach is justified because the signal from low-energy ionizing events gets amplified which improves the rejection of pulse-like features in random events. The square root of **PSD** (**ASD**) of various data sets across different detectors for the total channel is shown in Fig. 4.12.

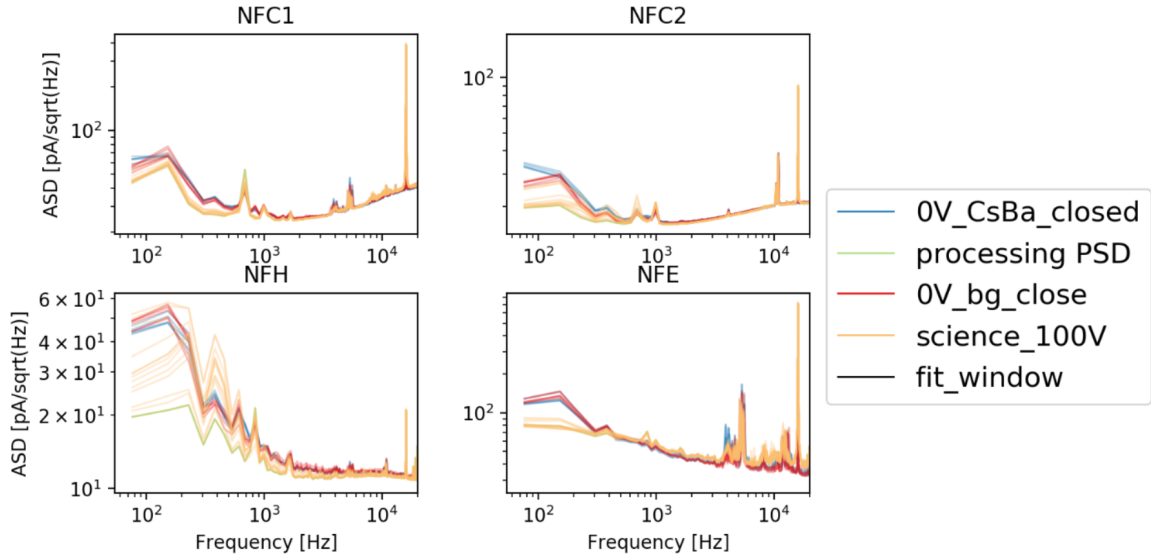


Figure 4.12: ASDs (square root of PSDs) for the total channel across different detectors and data sets in HVEV Run 4.

4.5 Data cleaning

This subsection outlines the steps taken to eliminate low-quality events from the study. These events include, but are not limited to, cross-talk triggers (caused by adjacent readout cables for different channels inducing current in neighboring cables, and causing triggers), electronic noise-induced triggers (referred to as the electronic glitches), and overlapping events that occur in close succession (referred to as the pileup events) leading to distorted **OF** results. To remove these problematic events, we defined a set of criteria (referred to as cuts) based on **RQs**. The main **RQs** used to define these cuts are summarized in Table 4.3.

We developed livetime and quality cuts for this study. The livetime cuts eliminate

Name of RQs	Description
trig_ch	The primary detector issuing the trigger.
trig_loc	The sample number for the the trigger point from 0 to 78125 (corresponding to 0 to 0.5 s) inside a trace of raw data.
filename_idx	The index of the MIDAS file.
trig_traceidx	The index of 0.5 s trace inside the MIDAS file.
timestamp_corr	Timestamp of the trigger point, corrected to prevent the 2^{32} rounding of MIDAS time.
OF0_*	Pulse amplitude from OF without a time shift freedom.
OFL_*	Pulse amplitude from OF with a time shift freedom.
OFL_chi2_*	The Frequency domain χ^2 (Eqn.4.2) which is a discriminator for the quality of the fit.
MeanBase_*	The mean of the prepulse region shown in 4.11.
Integral_*	The integral of the event (13.1 ms) after subtracting the MeanBase_* and applying a low-pass filter to retain frequencies below 20 kHz. Note that at low-energies the majority of the pulse template in the frequency domain is concentrated at frequencies below 20 kHz.
FallTime1_*	Fall time of filtered traces from 50% to 30%.
FallTime2_*	Fall time of filtered traces from 90% to 50%.
FallTime3_*	Fall time of filtered traces from 100% to 90%.

Table 4.3: List of RQs for Compton calibration analysis. The asterisk (*) represents the detector name and the channel—inner, outer, or total. For example, “OF0_NFC1_total” refers to the OF0 value for the NFC1 detector when the response of the total channel (inner + outer) is considered.

specific time intervals from the data, while the quality cuts filter out individual events. A summary of these cuts follows:

1. Trigger deadtime: Removes badly reconstructed events due to pileups that are adjacent to hidden events in the processing dead time intervals.
2. High-trigger rate: Removes triggers due to the external noise in some time intervals.
3. Temperature: The temperature is stable.
4. Coincidence: Removes cross-talk between NFC1 and NFE, and coincident glitch events in all detectors.
5. DT minimum: Removes pileup events.
6. Mean Base: Removes pileup events.
7. Frequency χ^2 : Removes elevated tail events at low-energy.
8. Pulse width: Removes elevated tail events at high-energy.

More information is available in Table 4.4, with detailed explanations presented in the following subsections.

Cut Name	Type	Domain	Low-energy OFL estimator (L-shells)	High-energy Integral estimator (K-shell and above)
Trigger deadtime	Time	N/A	Applied	Applied
High-trigger rate	Time	Series based	Applied	applied
Temperature	Time	N/A	Not applied	Not applied
Coincidence	Quality	N/A	Applied	Not applied
DT minimum	Quality	N/A	Applied	Applied
Mean Base	Quality	Series based	Applied	Applied
Frequency χ^2	Quality	All data	Applied	Not applied
Pulse width	Quality	All data	Not applied	Applied

Table 4.4: List of cuts used in this study.

The 'Domain' column in the Table 4.4 indicates whether a cut is designed for individual chunks of data collected over multiple days (referred to as series) or for the entire dataset. Cuts that are independent of the data are marked as N/A under the 'Domain' column. The decision to analyze individual series was motivated by the observation of time-dependent spikes in the trigger rate during certain series. Cuts

related to energy estimators, such as Pulse Width and Frequency χ^2 , were developed after combining data from multiple days.

Finally, we used the OFL energy estimator for low-energy calibration (linear TES response) and the Integral energy estimator at higher energies. we also tailored the cuts to the low- and high-energy intervals of the data. Minor differences between the sets of cuts will be discussed in the respective subsections.

4.5.1 Trigger deadtime

This cut removes the first and the last 13 ms of time from a 0.5 s trace of data. It is designed to eliminate events that deviate from the main cluster shown in Fig. 4.13 to arrive at Fig. 4.14.

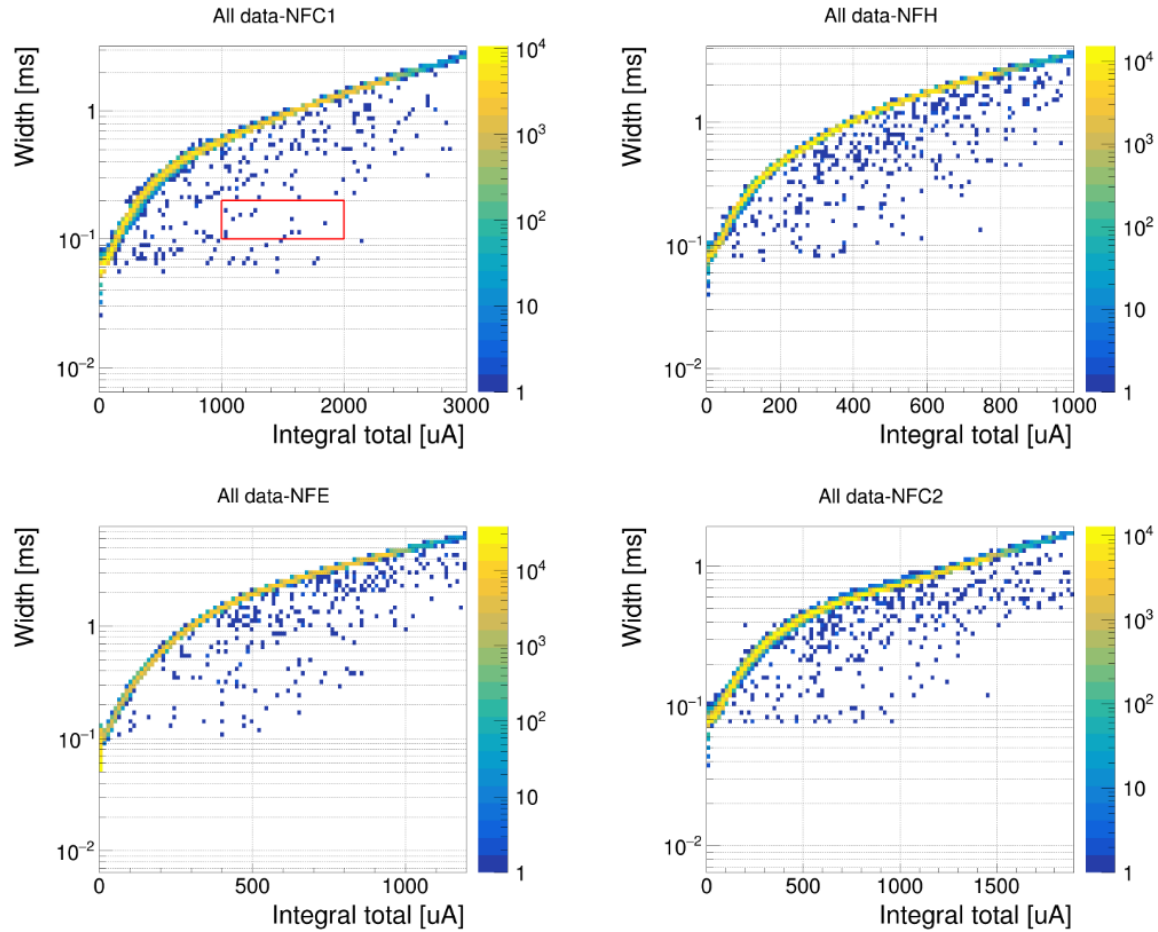


Figure 4.13: Pulse Width versus Integral before the cut. For each detector, the energy estimator values for the events under the main cluster is off due to pileups. The red box point to a few events which the raw data for one of them is shown in Fig. 4.15.

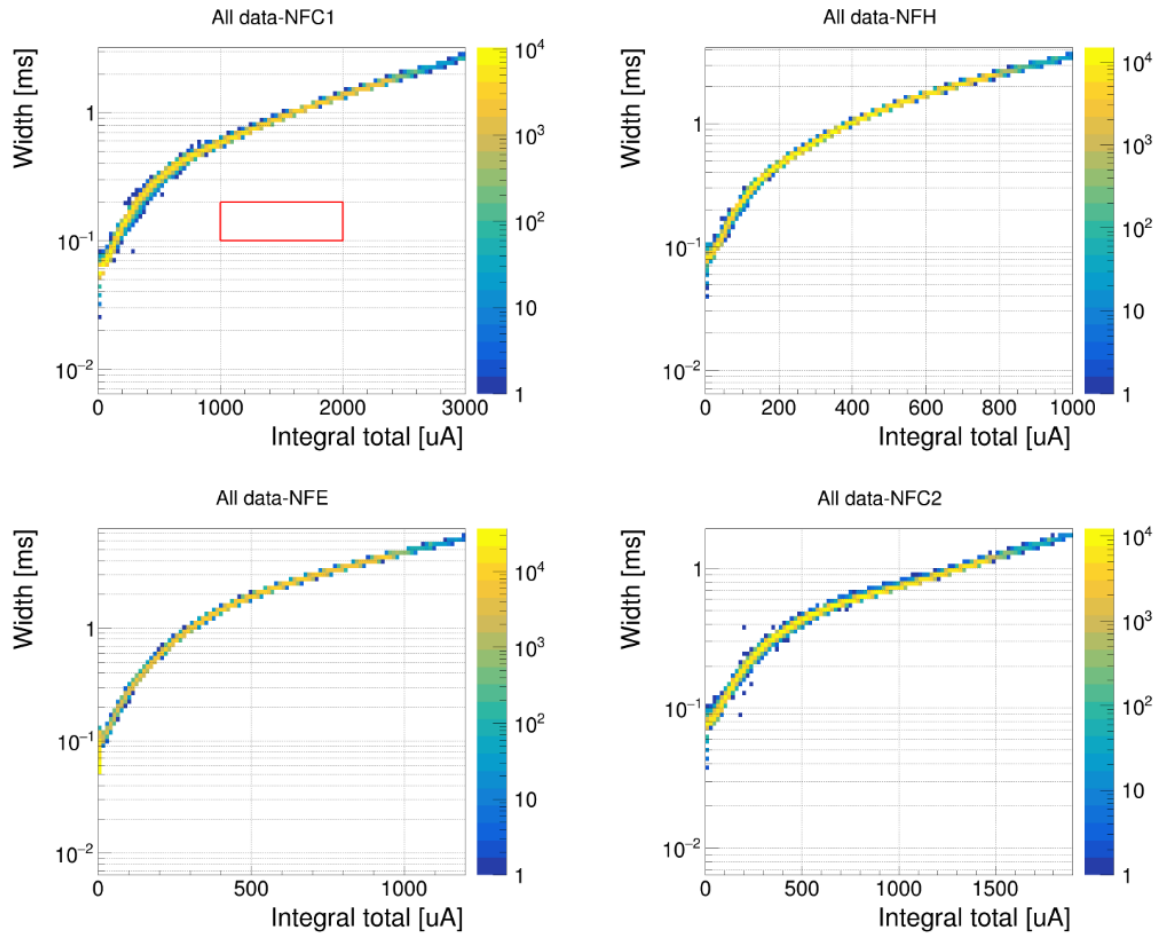


Figure 4.14: Pulse Width versus Integral after the trigger deadtime cut.

The readout data is continuously written to disk in chunks of 0.5 seconds (78125 samples), known as traces. The reconstruction algorithm uses an analysis window of 2048 samples centred around triggers to extract RQs. To ensure sufficient sample points within the analysis window, the processing code does not trigger in the first and last 1024 samples of each trace. Consequently, there is a chance of having an event not triggered close to the edges of the trace. For instance, if there are two pulses that are 1100 and 900 samples away from trace edges, the code would trigger on the first one, but not on the second one. Hence, the second pulse causes a pileup without being identified as a triggered event.

This problem is illustrated in Fig. 4.13. It shows the pulse Integral versus the pulse Width distribution for the data with the radioactive source in place. The outliers below the main cluster are due to pileups. The untriggered events misleadingly elevate the Integral of the triggered event as they fall inside their reconstruction window. The raw trace plot in Fig. 4.15 shows a triggered events, indicated by the dashed black line that is removed by this cut. This event is from the red box in Fig. 4.13 for detector NFC1.

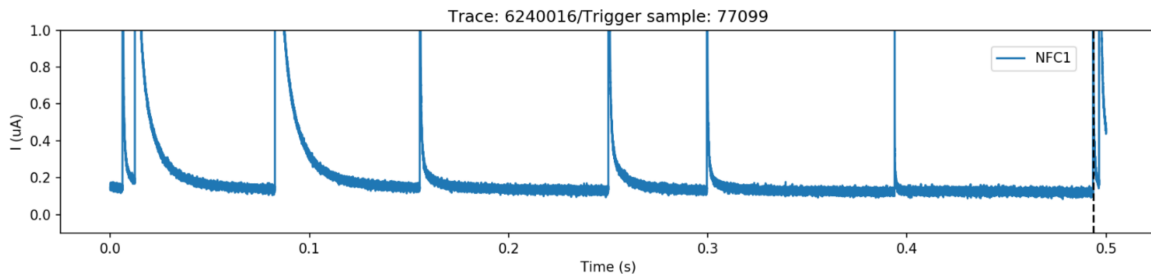


Figure 4.15: A raw trace selected from the red box in Fig. 4.13 for detector NFC1. The pulse is cut-off at the top because of the plot range. The second event in this trace also overlaps with a preceding event. The baseline cut that will be explained rejects such events.

4.5.2 High trigger rate

Some series include time intervals with spikes in the trigger rate. These intervals are characterized by trains of square-shaped pulses shown in Fig. 4.16.

The trigger rate spikes are due to radio-frequency noise from activities of other experiments operating in the same refrigerator. To remove these high trigger rate intervals, a trigger rate cut has been developed. The cut works as follows:

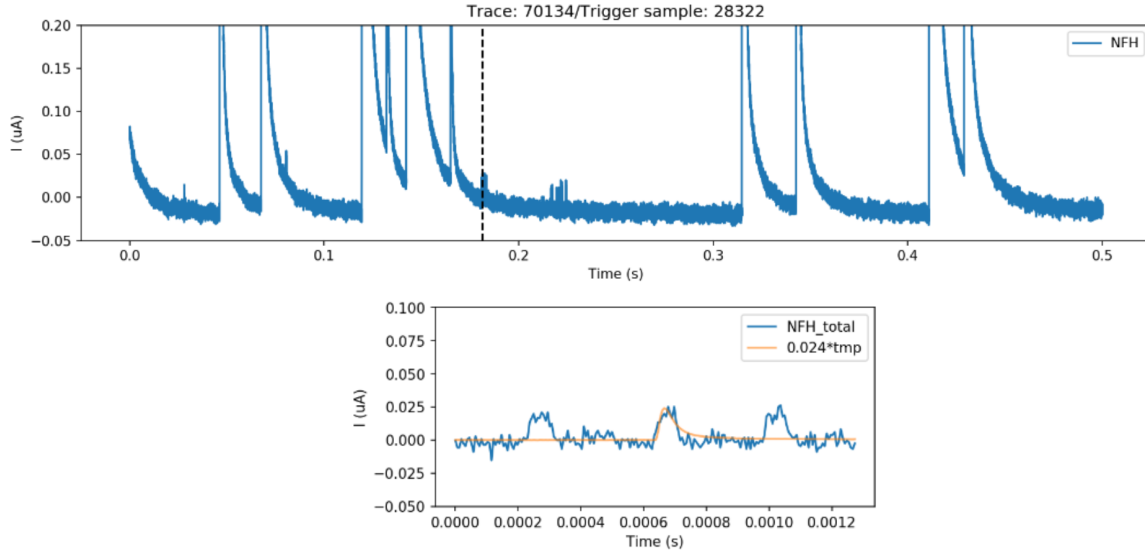


Figure 4.16: Raw data during the time interval with elevated rate in the NFH detector. We chose NFH as an example. The smaller plot at the bottom shows the vicinity of the trigger point shown by the dashed line. The solid line shows the best template fit according to the **OF** algorithm.

1. Divide the data into smaller time bins for each detector. We used 10 s bins for calibration data and 100 s bins for background data.
2. Create a histogram of the bin counts for each detector individually.
3. Fit the histograms with Poisson distributions to determine the mean values. An example is shown in Fig. 4.17.
4. Set a threshold at 5σ above the mean values. The red lines in Fig. 4.18 represent these thresholds which are specific to each detector.
5. Identify high-rate time intervals that exceed the threshold for each detector.
6. Merge the high-rate intervals across all detectors.
7. Remove these high-rate intervals from all detectors.
8. Finally, exclude two additional time bins, one at the beginning and one at the end of the removed time intervals.

Bad time intervals are merged and removed across all detectors to be conservative. That is based on the understanding that the noise originates from an external source.

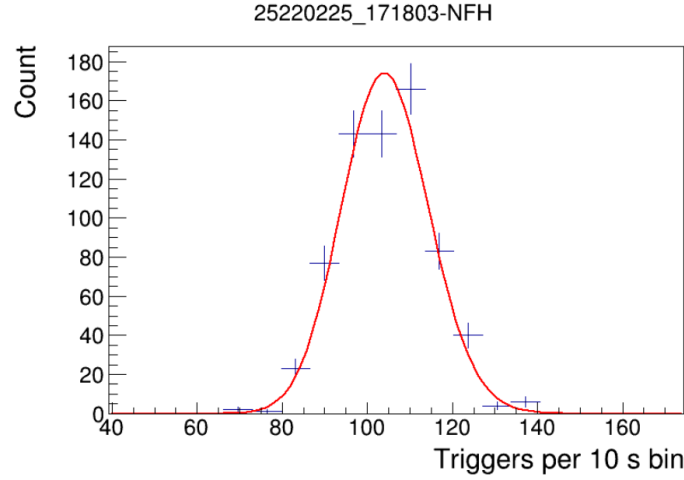


Figure 4.17: Histogram for the number of triggers per time intervals of 10 s in the NFH detector during one of the series.

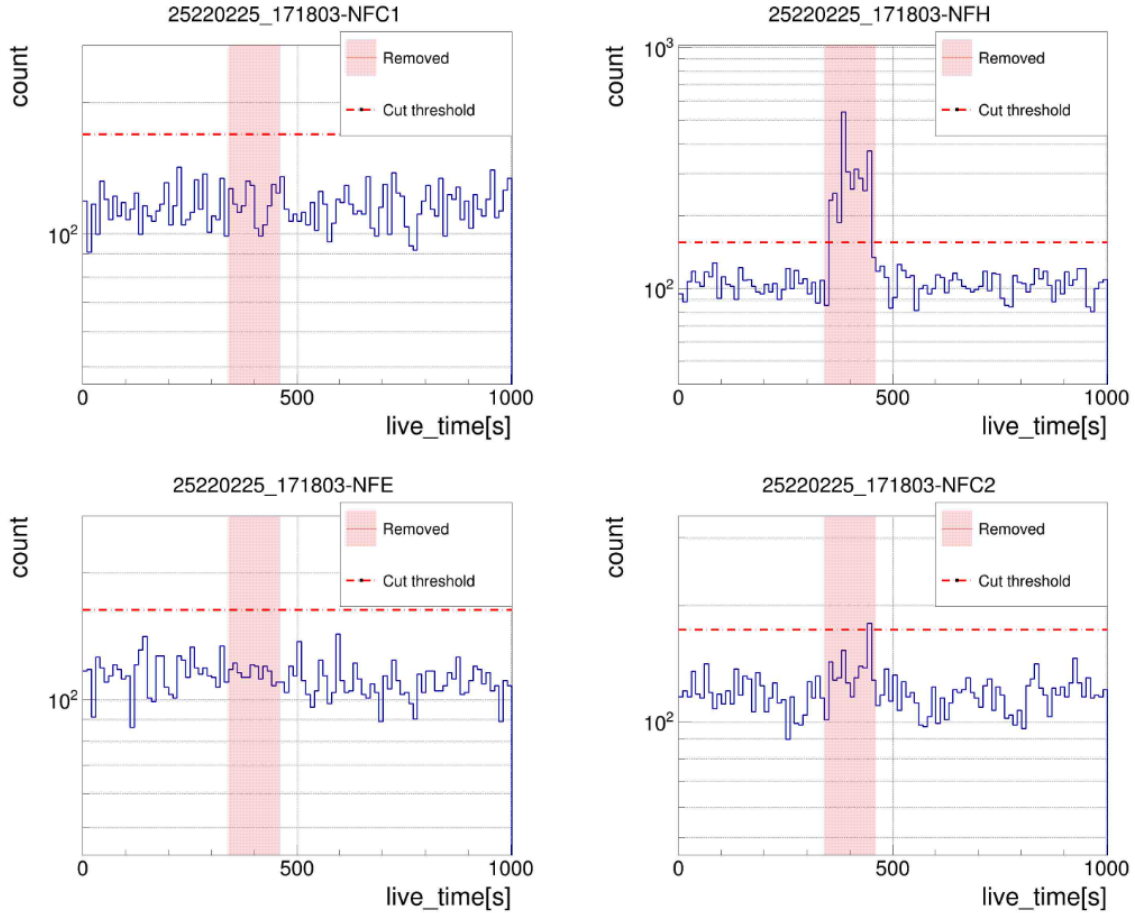


Figure 4.18: The time histogram shows an elevated event rate, with the interval highlighted in red representing the time range excluded from all detectors. These bad time intervals, caused by external noise, are conservatively removed from all detectors, even though the noise impact may vary in intensity across different detectors.

4.5.3 Fridge temperature

The temperature of the refrigerator was stable as indicated by Fig. 4.9 during the “0V CsBa closed” and “0V bg closed” data sets. We ignored other series for this study.

4.5.4 Coincidence and DT-min

DT-min and Coincidence cuts remove events that are too close to their immediate events in a single detector (DT-min), or across multiple detectors (Coincidence).

- Coincidence: Removes events with a time gap smaller than 15 samples (96 us) to consecutive events triggered by any of the detectors.
- DT-min: Removes events with time gaps smaller than 1039 samples (6.6 ms) to their consecutive events triggered by the same detector.

DT-min

Each triggered event is accompanied by both a preceding and a subsequent triggers; DT-min selects the smaller time gap between these two triggers. If this smaller time gap exceeds half the size of the analysis window (2048 samples or 13.1 ms), it indicates that no other trigger is present within the window. This criteria prevents pulse pileup at the front of the analysis window but may not fully eliminate prior pileups as shown in Fig. 4.19.

Events that follow a Poisson distribution produce an exponential distribution for DT-min. However, temporally correlated events, such as periodic noise triggers, can distort this distribution, leading to peaks in the DT-min data. The DT-min distributions for the calibration and background datasets in this study are qualitatively consistent with an exponential distribution, as shown in Fig. 4.20. Based on this observation, we conclude that time-correlated events are statistically insignificant, if they exist at all. Therefore, we have implemented a DT-min cut of 1024+15 samples, slightly longer than half the pulse reconstruction window, with the primary goal of eliminating pileups.

Coincidence

There are two main motivations to implement the coincidence cut:

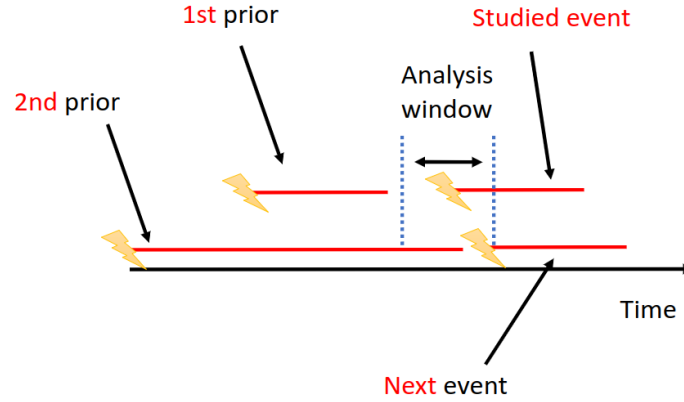


Figure 4.19: Schematic of consecutive events on a timeline. Sparks indicate the triggering points of the events. Red lines represent the duration of each pulse. Blue dashed lines show the analysis window centered around the trigger. This illustration demonstrates that pileups in the reconstruction window can show up after or before the trigger. The time gap to the immediate preceding event is not enough to check for pre-trigger pileups. The diagram illustrates that such pre-trigger pileups may be due to the second, third, ... prior events.

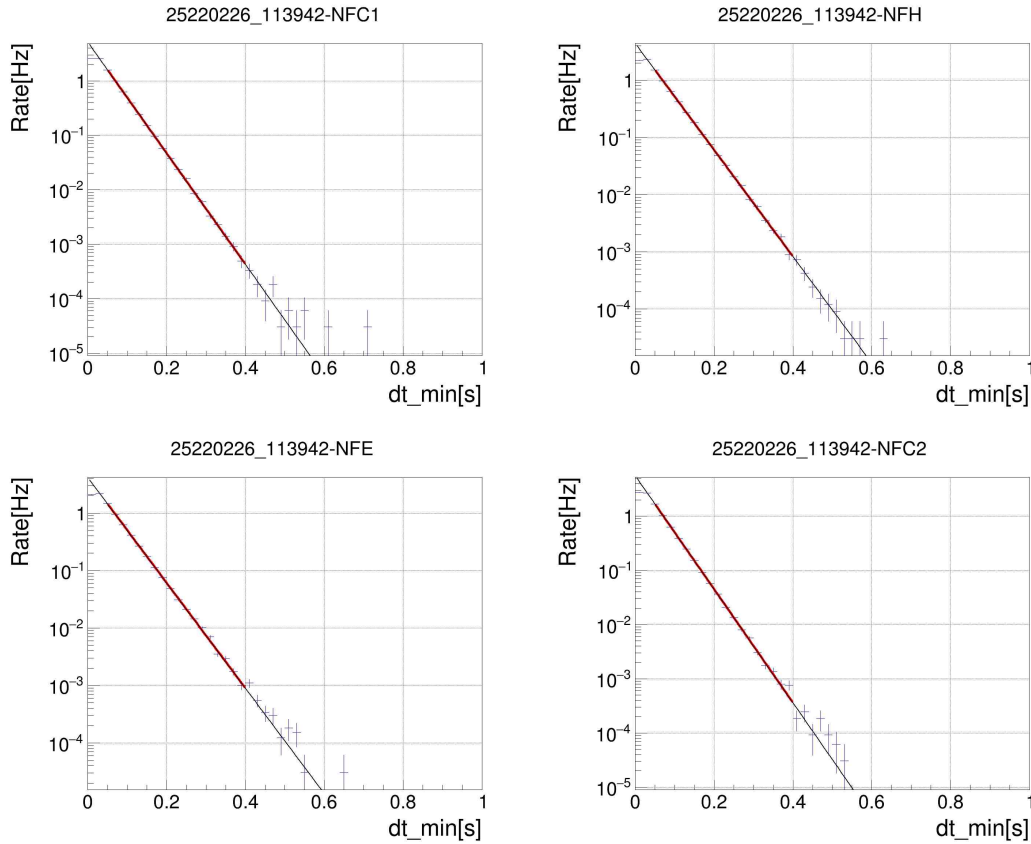


Figure 4.20: DT-min histograms with exponential fits (red lines), and an extension to the tails of the fitted functions (back lines).

1. To remove low-energy cross-talk triggers in NFE caused by high-energy events in NFC1 as shown in Fig. 4.21. We identified that these low-energy events fall within the energy range of interest for L-step calibration. The readout cables for the NFC1 and NFE detectors were placed adjacently. Consequently, high-energy events in NFC1 generated a strong electric current, leading to triggers in the outer channel of the NFE detector, as shown in Fig. 4.22.

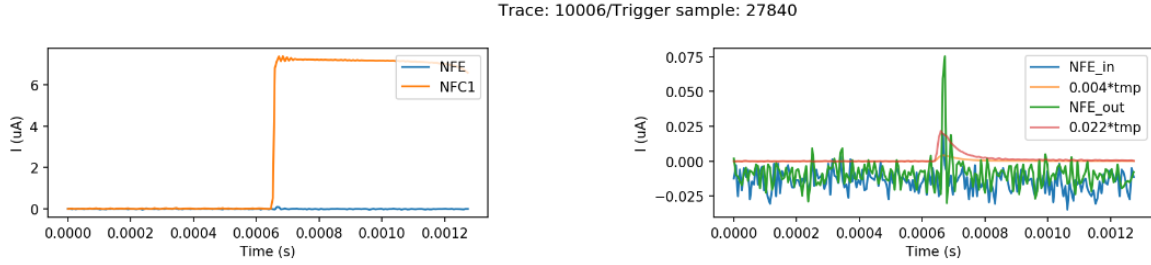


Figure 4.21: A high-energy event in the NFC1 detector (left-orange) causes a spike in NFE (left-blue) which is above the triggering threshold. The pulse in NFC1 exhibits a flat-top shape due to energy deposition beyond the device’s linear response. Left: The total signal from the sum of the inner and outer channels for the selected event in the NFC1 and NFE detectors. For each detector, we use the total signal to determine the energy estimators for all events. Right: Individual signals in the inner and outer channels of the NFE detector. The solid lines represent the best template fits according to the OF algorithm.

2. To eliminate simultaneous low-energy triggers across all detectors, which are most likely due to electronic glitches. We observed similar events in the HVEV R4 datasets used for a dark matter search. For a comprehensive discussion about these events see [65]. Two examples of these events are shown in Fig. 4.23.

4.5.5 MeanBase

The MeanBase RQ is calculated by averaging 924 samples from the beginning of the reconstruction window to 100 samples before the trigger point, as illustrated in Fig. 4.11. This average serves as a real-time measure of the detector condition, providing a reference to evaluate the nominal detector response. In the absence of pileups or changes in the run conditions, we expect the MeanBase histogram to exhibit a symmetric Gaussian distribution due to the baseline noise. However, the presence of a radioactive source increases the pileup rate between adjacent pulses, leading to a noticeable distortion in the symmetric distribution.

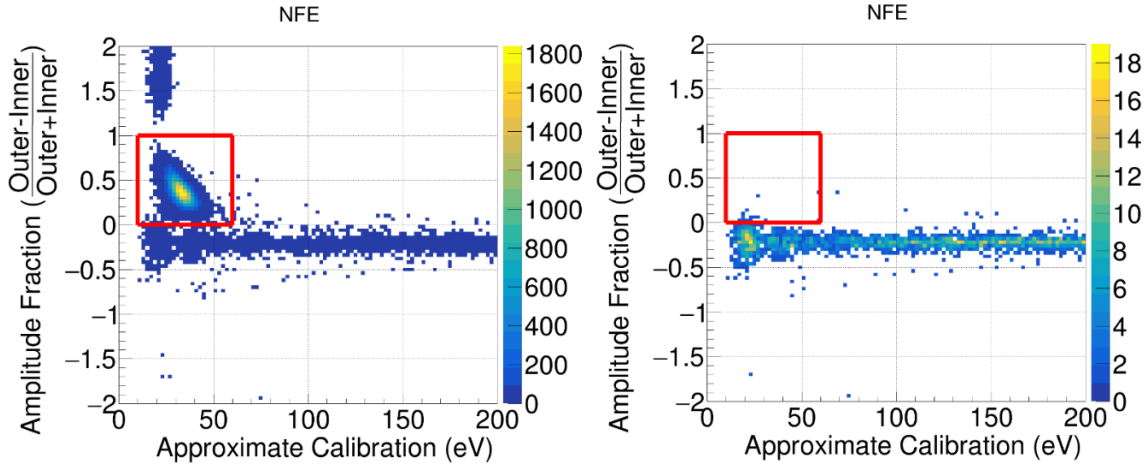


Figure 4.22: The left and right plots show the distribution of events before and after the coincidence cut. The y-axis represents the normalized amplitude difference between the inner and outer channels of the **HVeV** detector. A value closer to 1 indicates that the pulse is predominantly captured by the outer channel. Events with values beyond +1 or -1 are either noise or cross-talk triggers that exhibit a negative reconstructed amplitude in one of the channels. The rejected events by this cut are very localized. Their relative fraction to all energy depositions is small as indicated by Fig. [4.32, 4.33].

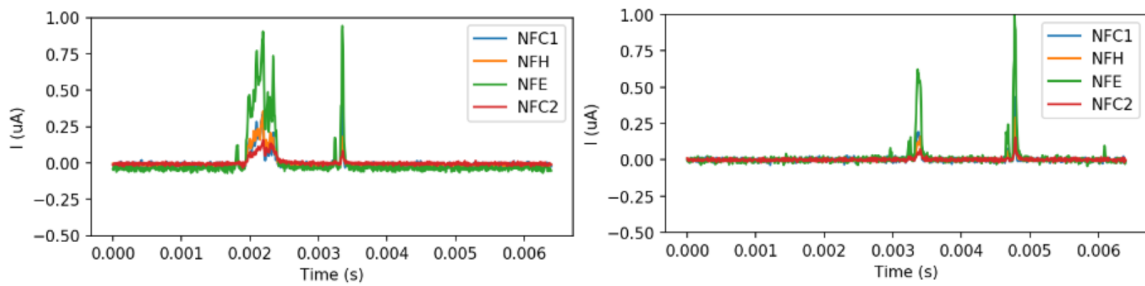


Figure 4.23: Electronic glitch triggers appearing in all detectors.

The MeanBase cut is defined using random triggers instead of real triggers, as the MeanBase distribution does not depend on the type of event. This choice increases the statistics in the distribution of the MeanBase, particularly in background datasets with a limited number of real triggers. We assume that baseline noise causes a Gaussian shape in the pre-peak region of the MeanBase distribution, while pileups distort the post-peak region. With this assumption, we fit the pre-peak region with a Gaussian distribution and exclude events that fall outside of 3 standard deviations from the peak on both sides. The cut for one dataset is illustrated in Fig. 4.24.

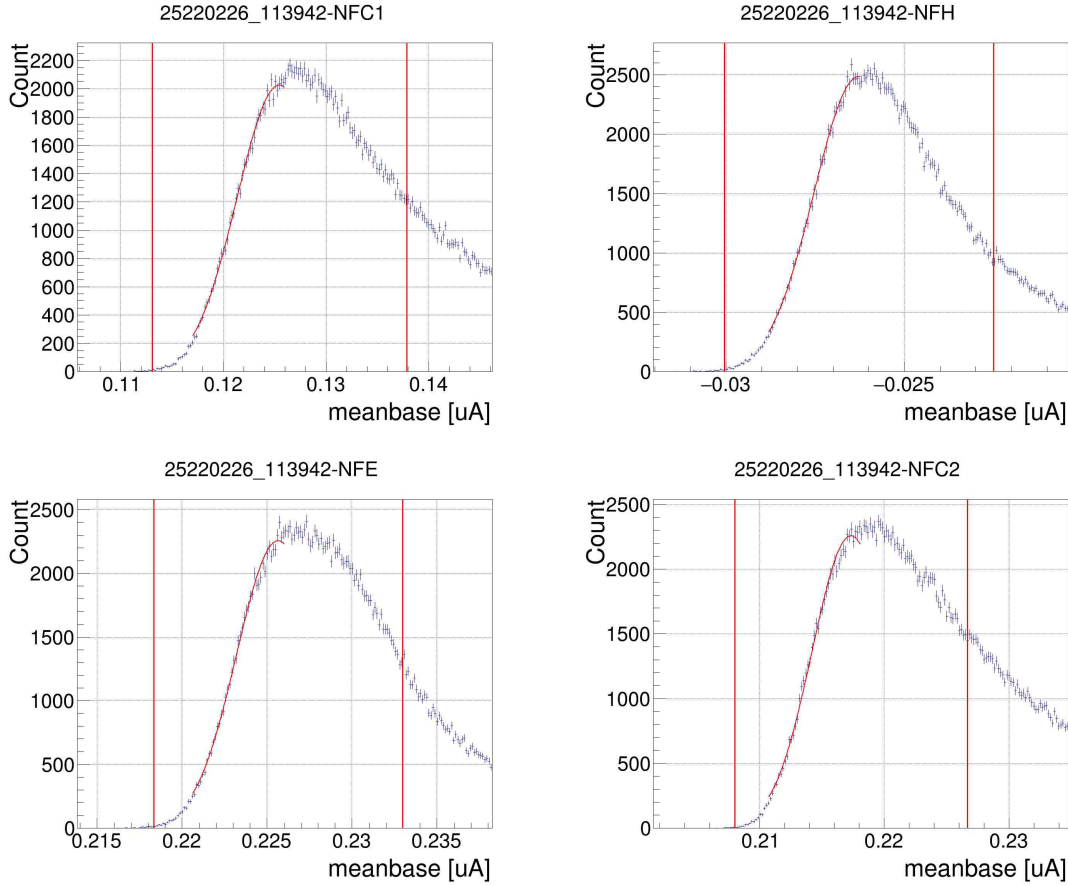


Figure 4.24: Gaussian fits to the pre-peak region of MeanBase and resulting 3σ cuts around the peak.

The threshold for the MeanBase cut on the right (see Fig. 4.24) affects the amount of pileup retained in the data. We used the available 100 V Cs data from April 2022 (refer to Fig. 4.9) to study the impact of this cut on the first e^-h^+ peak with a known energy of 100 eV. Comparisons showed that the systematic effects introduced by events with elevated MeanBase values are not significant compared to the baseline

resolution, as shown in Fig. 4.25. The x-axis represents the MeanBase, shifted so that the peak of the distribution is centered at zero. The y-axis shows the ratio of the first peak position at a given MeanBase with respect to the peak position at $x=0$. Across all detectors, these ratios were found to be between approximately 0.99 and 1.01, indicating a peak position offset of about 1%. At 100 eV, this corresponds to a shift of 1 eV, much smaller than the baseline resolution expected from these detectors which is on the order of a few eV.

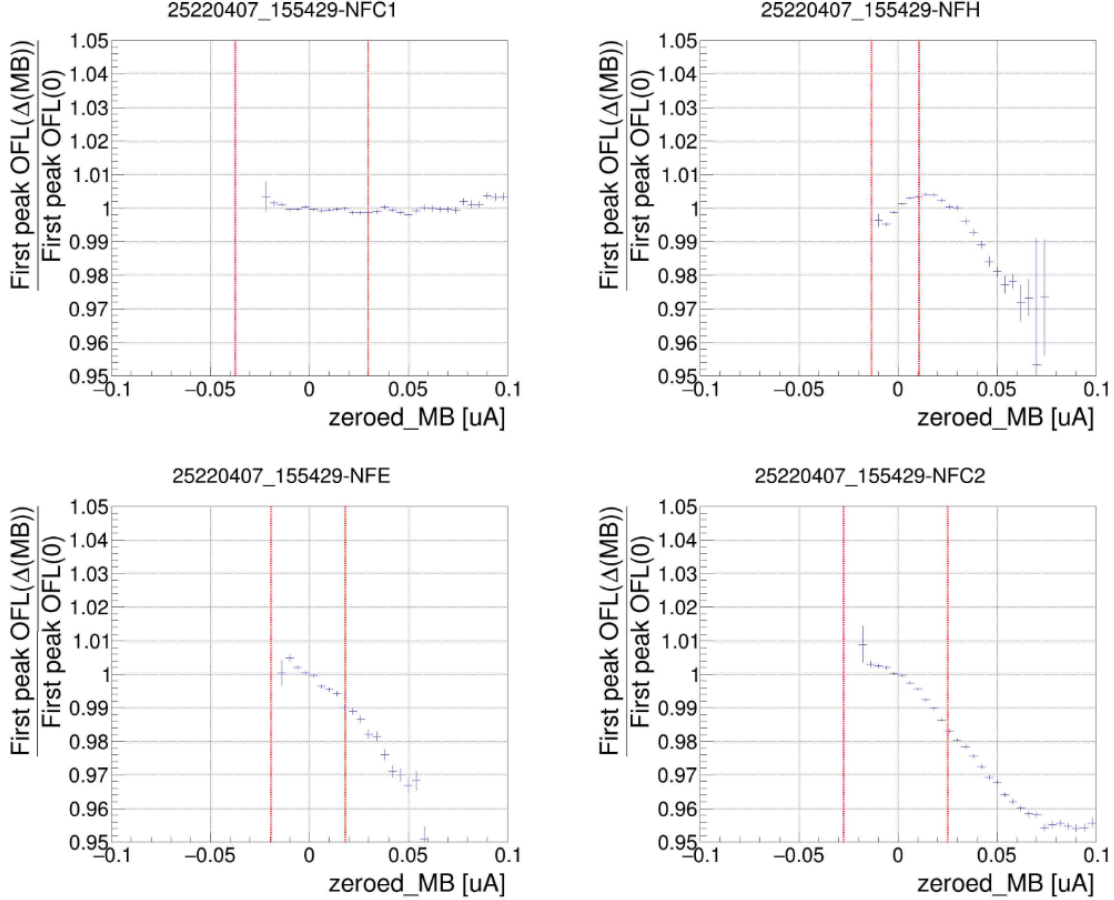


Figure 4.25: Systematic changes in the positions of the first e^-h^+ peak as a function of MeanBase.

Additionally, we compared the baseline resolution with the resolution of the first e^-h^+ peak. The baseline resolution was determined from the width of the energy estimator distribution for random triggers that was modeled by a Gaussian function. Similarly, the resolution of the first e^-h^+ peak was measured by fitting a Gaussian to the distribution of the events after applying a MeanBase cut. The comparison is shown in Fig. 4.26. Consistently across various datasets and detectors, baseline reso-

lution remains the dominant—or at least a significant—contributor to the resolution observed at 100 eV. Therefore, any additional impact on resolution due to MeanBase variations is considered minimal. We also compared the OFL and OF0 resolutions at 100 eV, and found the differences between these energy estimators to be negligible.

The OFL algorithm permits a time shift of up to 6 samples around the trigger point to find the best template match. However, this added time-shift flexibility introduces a double-peak structure in the baseline OFL distribution for randomly triggered events as demonstrated in Fig. 4.27. For this reason, we used OF0 to measure the baseline resolution.

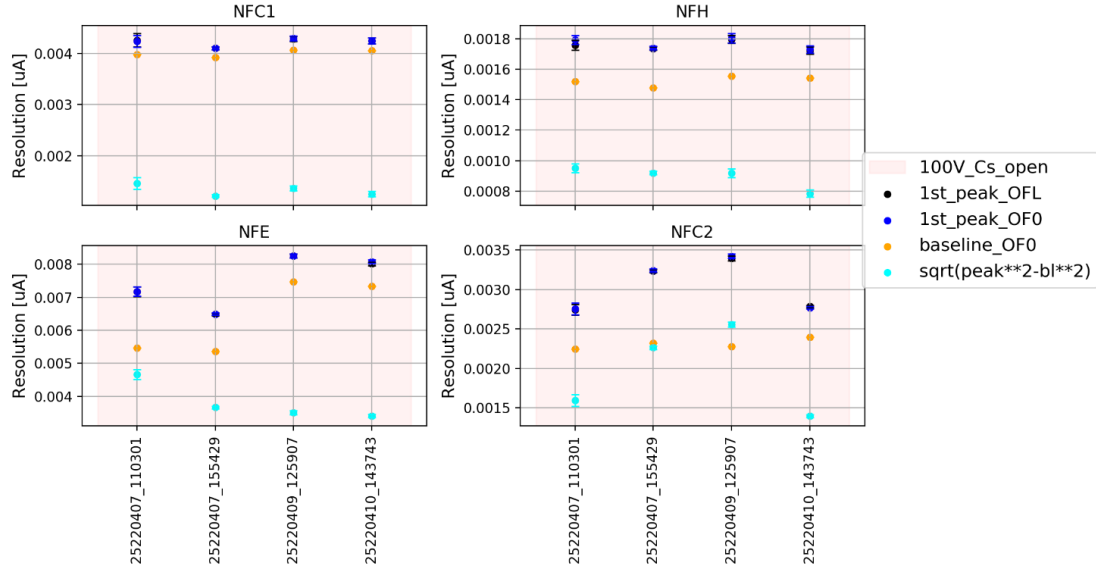


Figure 4.26: Comparison of resolutions at 100 eV and 0 eV (baseline).

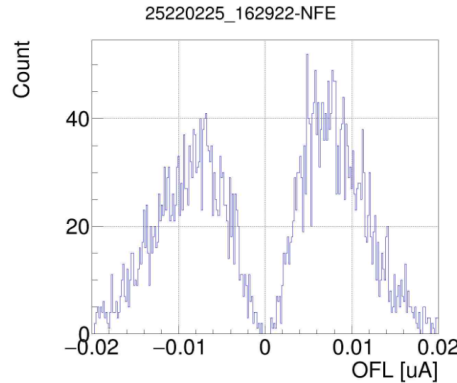


Figure 4.27: The OFL values for randomly triggered events (no energy deposition). The time-shift freedom in the reconstruction algorithm causes a double-peak structure which prevents the measurement of the baseline resolution.

4.5.6 Frequency space χ^2

The χ^2 value quantifies the discrepancy between the **PSD** of the raw data and the noise in the reconstruction window after subtracting a fitted pulse template. If the template differs significantly from the pulse in the reconstruction window, the fit will be poor, resulting in an increased χ^2 . We implemented a uniform χ^2 cut at low energies to eliminate events that deviate significantly from the main clusters. First, we apply a preliminary calibration to the 0 V data using the 100 V LED calibration. Then, we identify a low-energy interval with subtle step-like features due to Compton scattering, as shown in Fig. 4.28 (notice the drop in the NFH or NFE). Subsequently, we fit a Gaussian function to the χ^2 distribution of events within this low-energy window, as illustrated in Fig. 4.29. Finally, we exclude any events above the upper 3σ threshold of this distribution. This cut primarily removes high-tail events. The next cut also removes high-tail events but at higher energies.

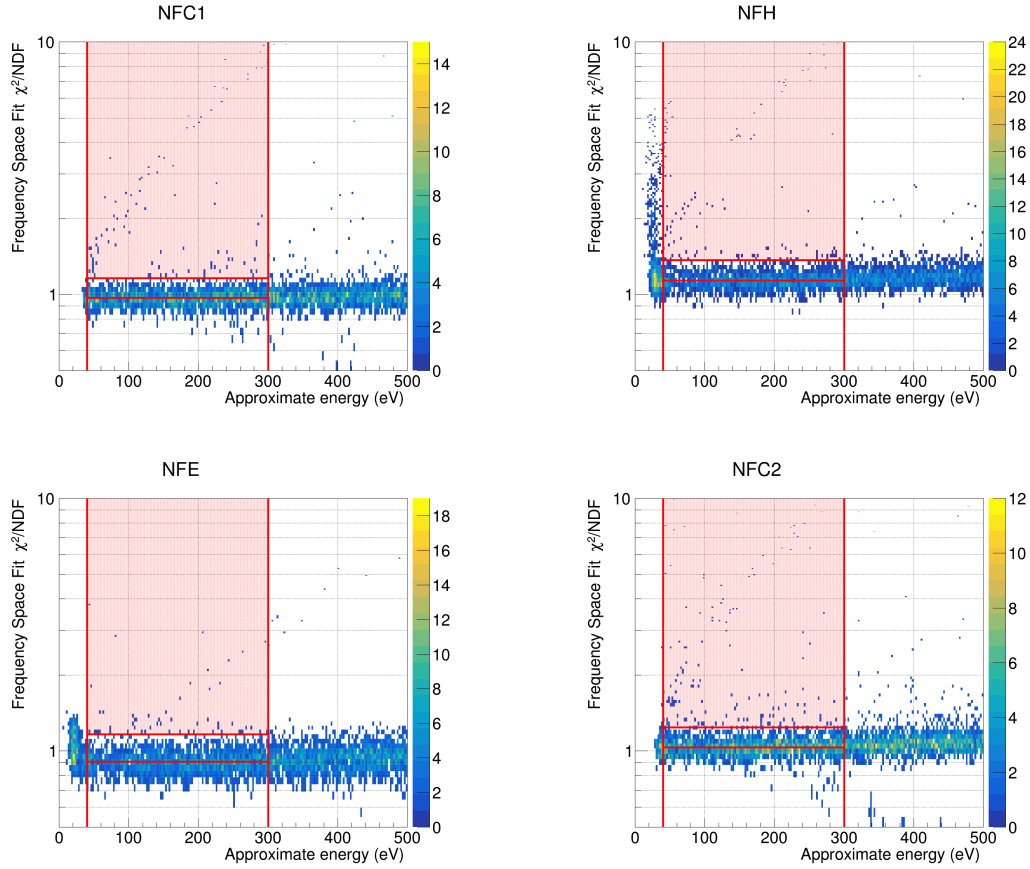


Figure 4.28: Histogram as a function of the χ^2 frequency and energy values. Vertical lines indicate the energy window selected for the cut, while horizontal lines represent the 3σ boundaries around the mean. The x-axis is calibrated using the position of the first e^-h^+ peak when the detector is biased at 100 V, although the data shown was acquired at 0 V.

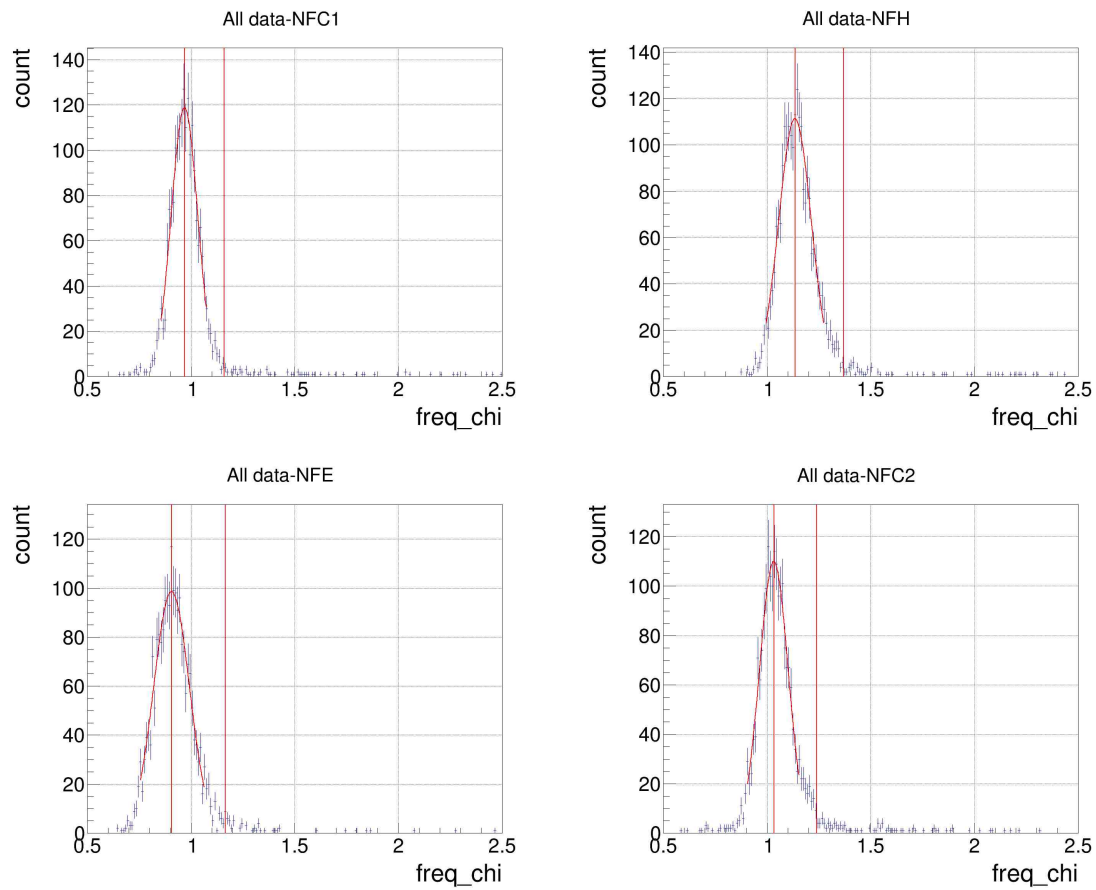


Figure 4.29: The Gaussian fits to the projected events along the χ^2 axis within the 40–300 eV energy window.

4.5.7 Pulse width

The detector response shows nonlinear effects at energies above approximately 500 eV. This leads to systematic differences between the pulse template, constructed from low-energy events, and the actual pulse shape observed in the trace. Consequently, the χ^2 RQ may not be the best quantity to define for a cut at higher energies. To address this, the χ^2 was replaced with a pulse width cut, measured from the rise to the fall of the pulse at 30% of its maximum height.

To implement this cut, Gaussian functions were fitted to the projected distribution of events along the y-axis for each bin on the x-axis in Fig. 4.30. The center of each Gaussian fit is represented by red horizontal lines at the midpoint of the distributions, while the 7σ upper threshold is marked by black dots. These black dots were then fitted with a fourth-degree polynomial, and all events above the curve were rejected. The choice of the 7σ threshold ensures that the rejected events are well separated from the main cluster, helping to avoid an energy-dependent efficiency.

The Width RQ is measured relative to the maximum height of each pulse and should therefore remain constant as a function of energy, provided the pulse shape remains unchanged (though the pulse amplitudes may vary). In the data, the pulse width distribution at low energies (below approximately 200 eV) remains relatively flat, ranging from 10 to 12 samples. However, at energies below approximately 80 eV, the width distribution begins to increase. At such low energies, the width measurement becomes more sensitive to noise. That increases the probability that the Width cut could remove events in an energy-dependent manner. For this reason, we did not apply this cut at low energies. Also, the χ^2 cut clearly shows a superior performance at low energies. It is evident since the distribution of the Pulse Width in NFC1 and NFC2 does not show a separation between high-tail events, and the main cluster.

Similar to the χ^2 cut, the pulse width cut removes elevated tail events, as shown in Fig. 4.31. These events may result from direct energy depositions in the aluminum fins. The surface coverage of the detectors, from highest to lowest, is as follows: NFC, NFH, and NFE. A qualitative similarity in the density of rejected events across these detectors is evident in Fig. 4.30.

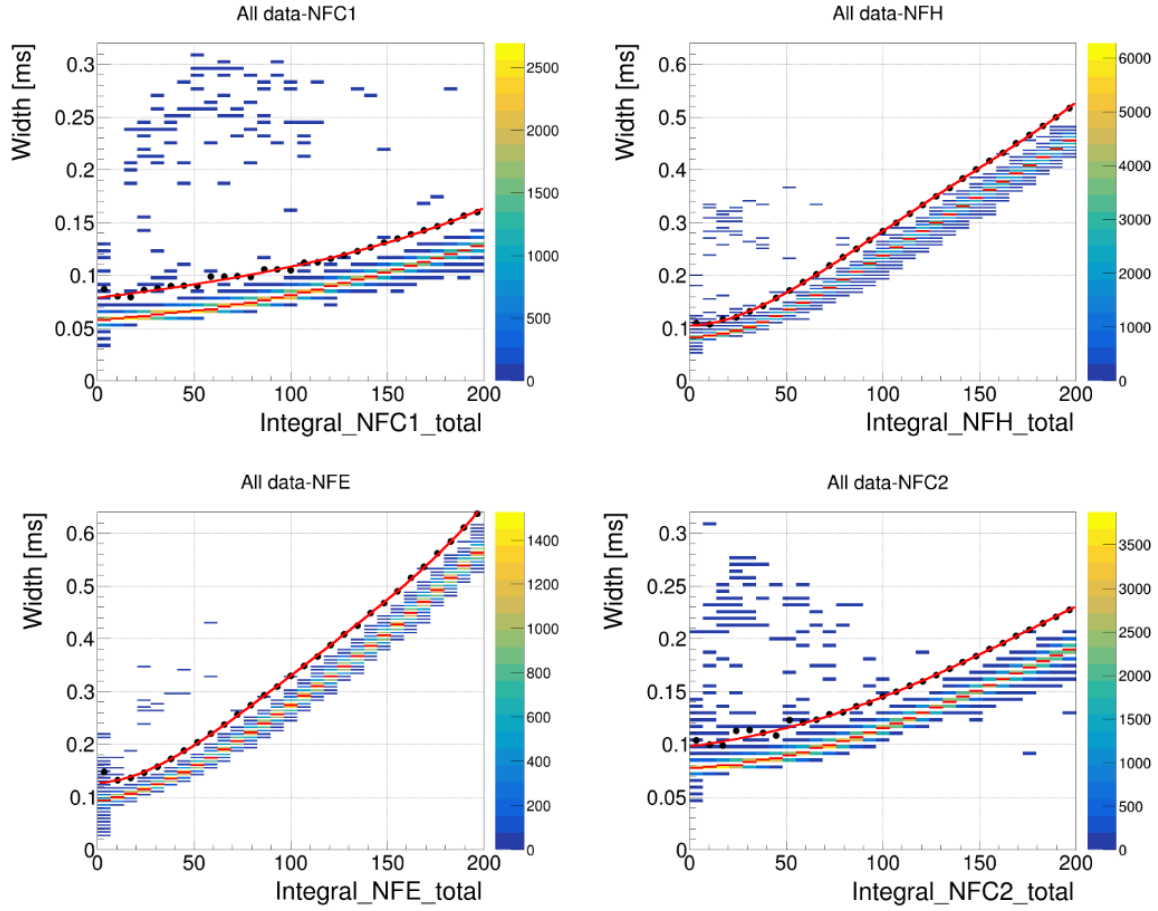


Figure 4.30: Distribution of the pulse width as a function Integral energy estimator. The red curve shows the 7σ band above which we reject events.

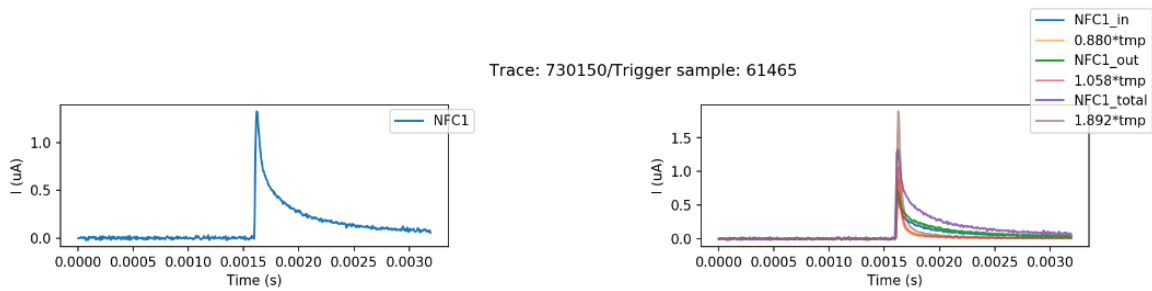


Figure 4.31: An elevated tail event selected from detector NFC1. Right: The total signal from the sum of the inner and the outer channels for the selected event. We used the total signal to find the energy estimator corresponding to this event. Left: Individual signals across all channels. The solid lines show the best template fits according to the **OF** algorithm.

4.6 Passage fraction

The spectra of passing events after sequentially applying the cuts is shown in Fig. [4.32, 4.33]. Each color represents the population of the events after applying the preceding cuts, including the corresponding cut named in the legend.

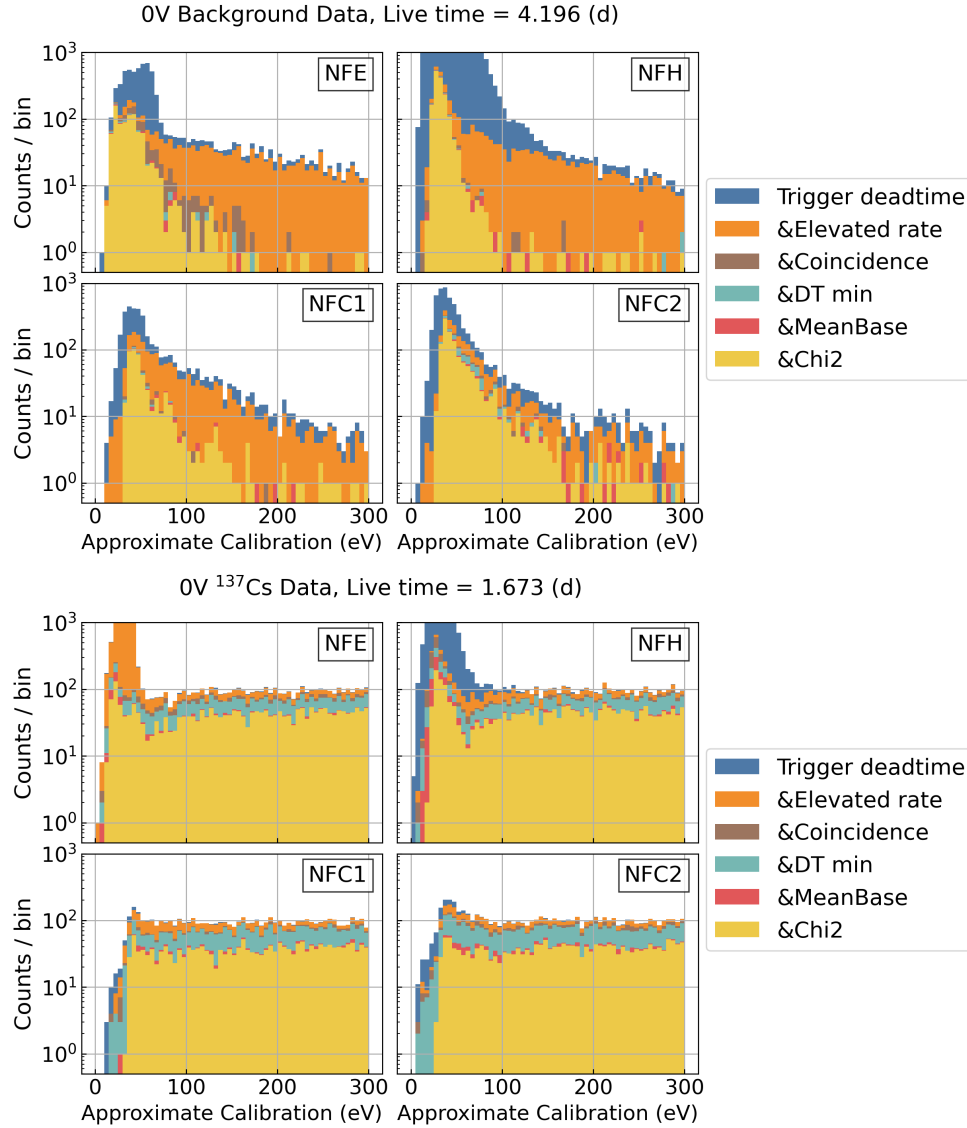


Figure 4.32: The plots illustrate the effect of sequentially applied cuts on the **low-energy** interval of data sets. Each color shows the remaining spectrum of events after applying all the cuts up to the one names in the legend.

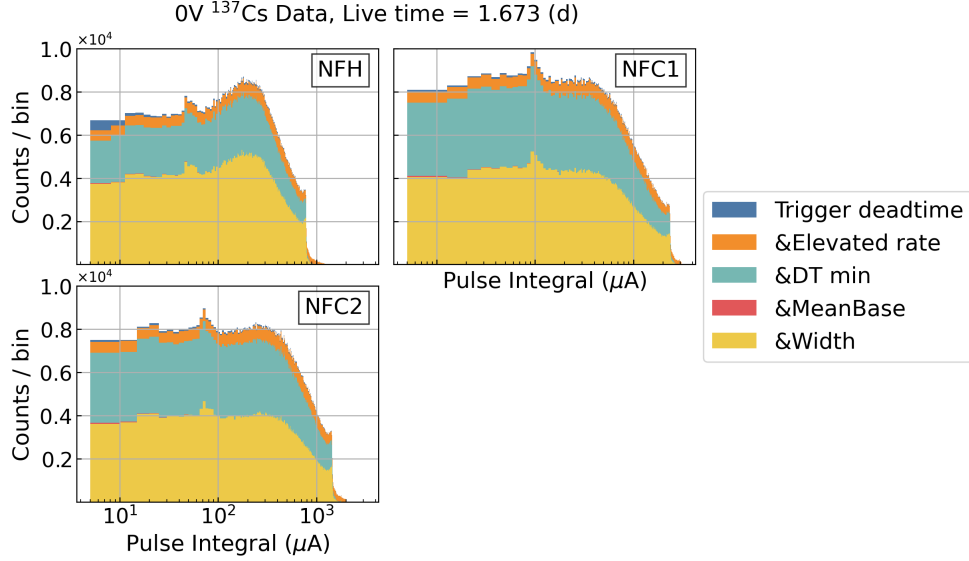


Figure 4.33: The plots illustrate the effect of sequentially applied cuts on the **high-energy** interval of the datasets. The overall **TES** volume of the NFE detector is significantly smaller than that of the other detectors. That makes the detector response significantly non-linear at high-energy depositions. Consequently, we did not study this detector at such energies.

We do not expect any of the previously discussed cuts to introduce an energy-dependent efficiency. The livetime cuts only remove time intervals. The strongest quality cuts, MeanBase and DT-min, primarily remove pileup events. In the next chapter, we present an analysis showing that the MeanBase and DT-min cuts should exhibit a flat efficiency as a function of energy. The other cuts are designed to target specific events that are inconsistent with regular pulse shapes, thus removing background events.

The calibration effort described in the next chapter focuses only on the shape of energy signatures in the spectrum of the calibration datasets. Since the calibration does not rely on the number of events, determining explicit efficiency values is unnecessary.

4.7 Integral energy estimator correction

The MeanBase and DT-min cuts remove strong pileups. However, weak pileups, caused by the long tails of energetic events extending into the reconstruction window of other events cannot be entirely rejected. We observed a bias in the Integral energy estimator associated with these weak pileups and applied a correction to remove it.

In contrast, the OFL energy estimator exhibited negligible effects and did not require any correction.

The study of bias requires a set of events associated with an energy signature (known energies). By profiling the energy estimator values of these events as a function of pileup strength, measured by the MeanBase **RQ**, we can identify systematic changes in the energy estimator. We decided to use random triggers to study the reconstruction bias. Random triggers have some benefits:

1. Their true energy should be 0 eV. Therefore, they provide an energy signature.
2. We have a large population of random events which reduces the statistical uncertainty of the measurement. It is important to note that e^-h^+ peaks from the LED data cannot be used to identify the energy estimator bias when processing calibration data with a radioactive source. The reconstruction bias depends on both the population and the shape of the pileups. Since the frequency and strength of pileups in the 150 V LED data differ from those in the 0 V Compton calibration data, the findings from one dataset cannot be applied to the other.
3. We do not expect the reconstruction bias to be energy-dependent if it arises solely due to preceding pileups. Therefore, once the bias is quantified using random triggers, it can be corrected across all events. Two sanity checks that confirm the dominance of preceding pileups as the primary source of the observed bias will be explained.
4. Random triggers should not exhibit any effects related to changes in the TES response. Therefore, random events naturally isolate the reconstruction bias from other potential variations in the energy estimator.

4.7.1 Bias of the Integral energy estimator

As a reminder, the Integral energy estimator is defined as

$$\text{Integral} = \text{Area}(\text{Trace}) - \text{mean}(\text{Prepulse region}), \quad (4.7)$$

where for convenience “mean(Prepulse region)” will be called MeanBase. Without pileups, the distribution of MeanBase is expected to be Gaussian because of the baseline noise. In the presence of pileups, the MeanBase acquires a positive value, biasing the reconstructed Integral to negative values. This bias is expected to remain independent of the deposited energy if it results from preceding pileups. In other

words, any event has the same chance of being preceded by a pileup, as long as energy depositions occur independently over time (consistent with Fig. 4.20). The distributions of Integral for random triggers of the Compton and background data sets are shown in Fig. [4.34, 4.35].

The histogram of Integral distribution for the Compton data shows a strong offset (Fig. 4.34), whereas for the background data the distribution is centered around $0 \mu A$ (Fig. 4.35). Based on a preliminary calibration, the Integral offset in the Compton data is between 20 eV and 100 eV depending on the detector. We performed two sanity checks to ensure that the offset in random triggers of the Compton data is due to pileups:

1. Checked the relation between the strength of the DT-min cut, and the strength of the offset. Making the DT-min cut stronger increases the time gap between accepted events which is expected to reduce the probability of preceding pileups. We observed that a stronger DT-min cut reduces the offset as shown in Fig. 4.36. The top plot displays the spectra of passing random events as we increased the time gap between random events and adjacent energy deposition triggers. The bottom plot shows the center of the Gaussian fit to the spectra of passing random triggers as a function of the DT-min cut criteria. As the cut becomes stronger, the center of the Gaussian fits moves closer to zero [μA] (equivalent to zero [eV]).
2. Checked the relation between the offset and the average value of the MeanBase. Random triggers with smaller MeanBase values demonstrate a weaker offset as shown in Fig. 4.37. We chose populations of randomly triggered events with different MeanBase values (top plot), and compared their offset (bottom plot).

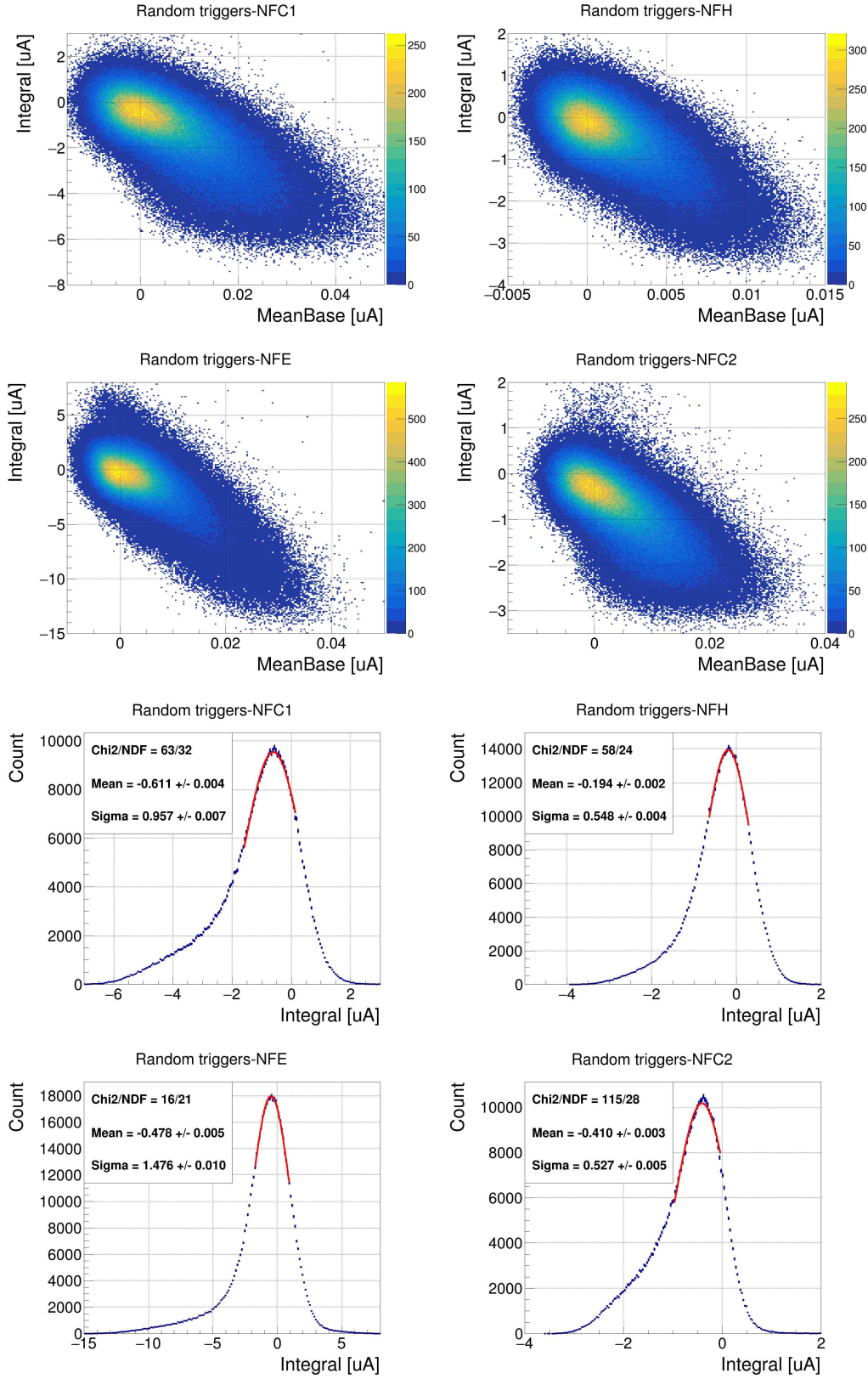


Figure 4.34: Compton data sets. Top: 2d histograms of Integral as a function of Meanbase with the MeanBase peak shifted to zero. Bottom: Integral histogram.

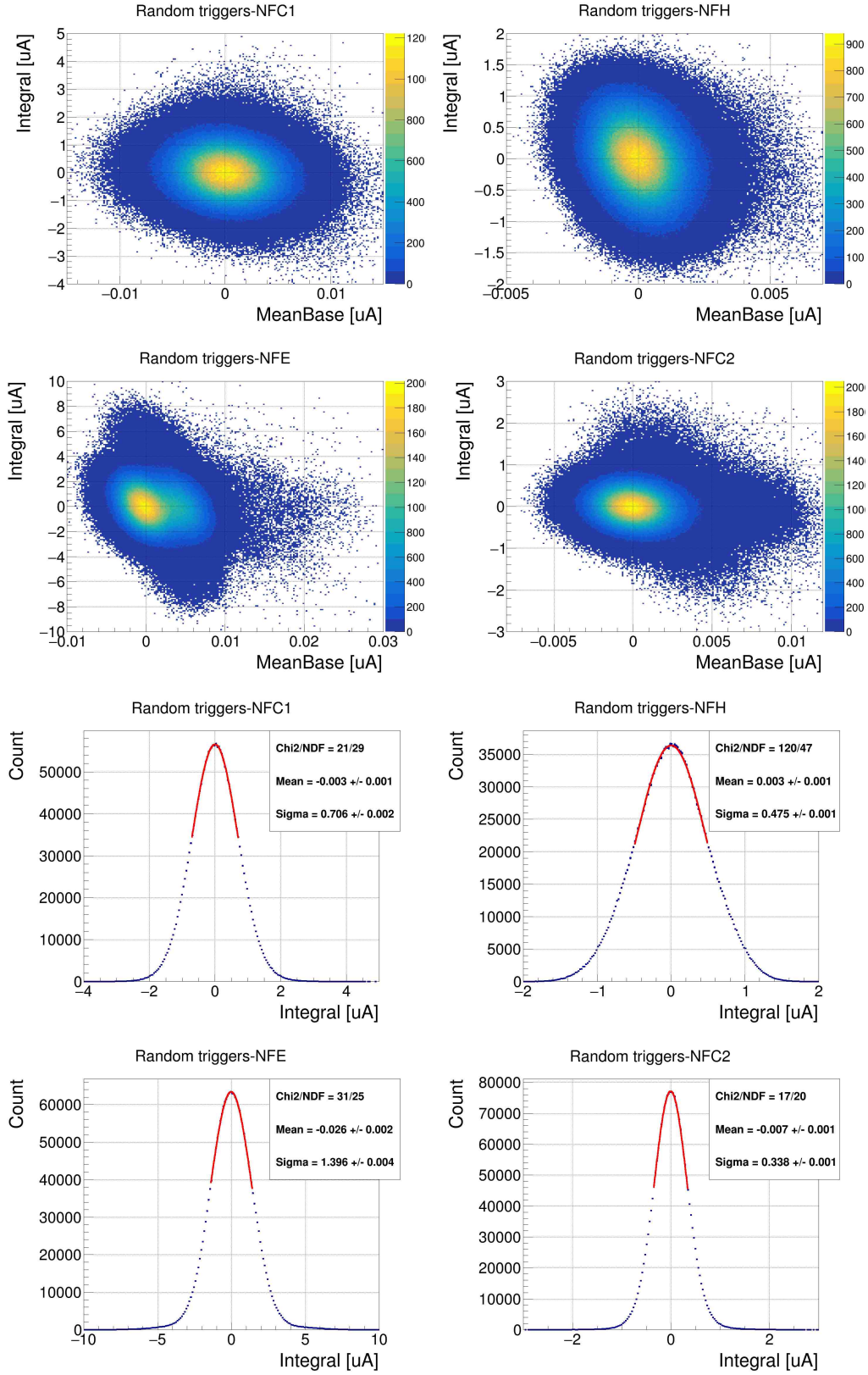


Figure 4.35: Plots are for background data sets. Top: 2d histograms of Integral as a function of Meanbase with the MeanBase peak shifted to zero. Bottom: Integral histogram.

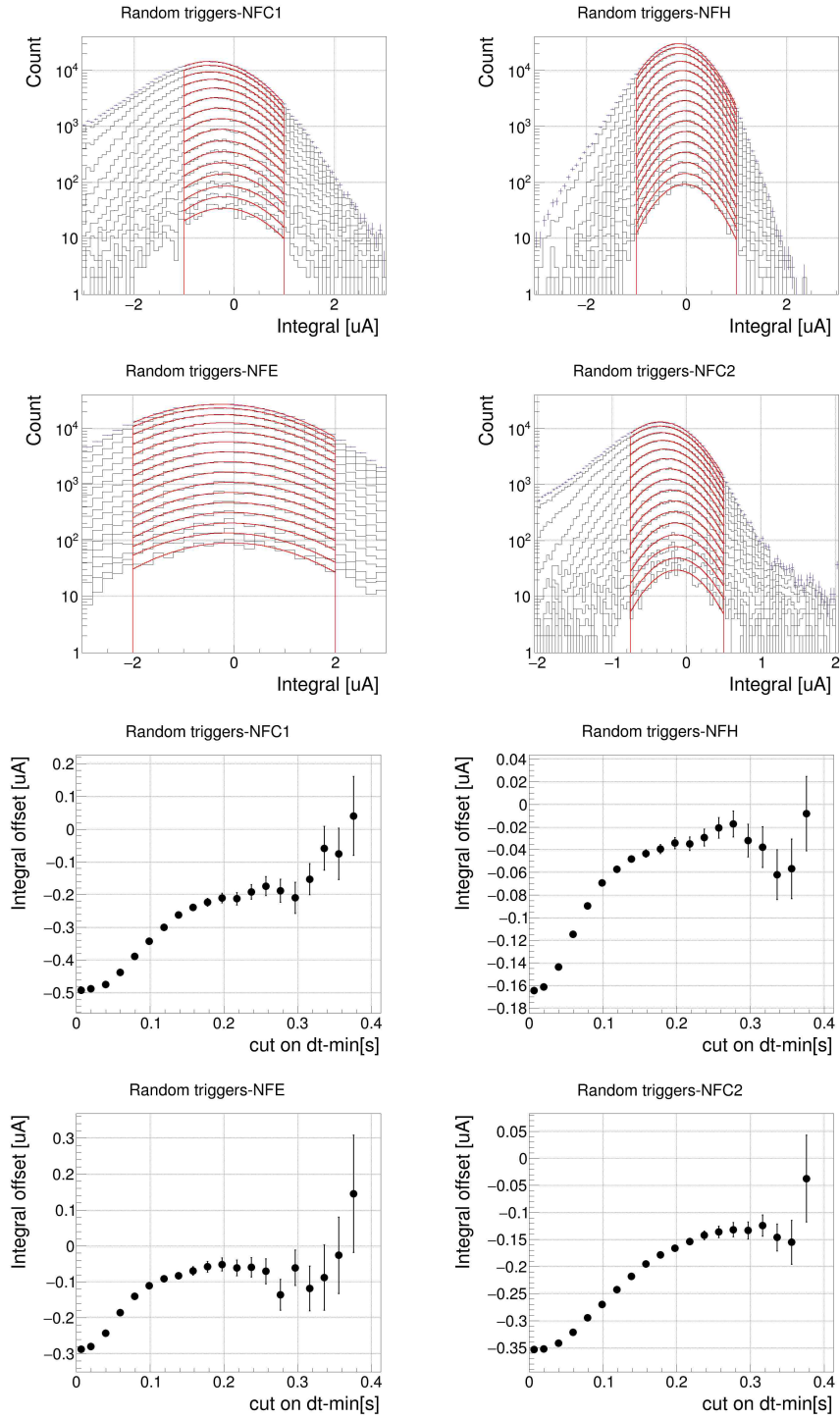


Figure 4.36: Effect of the DT-min cut on the offset. Top: The spectra of passing events, modeled by Gaussian fits, through successively stronger DT-min cuts. Bottom: The center of the Gaussian fits (Integral offset) in the top plot as a function of DT-min cut criteria. The top plots shows fewer fits for better visualization.

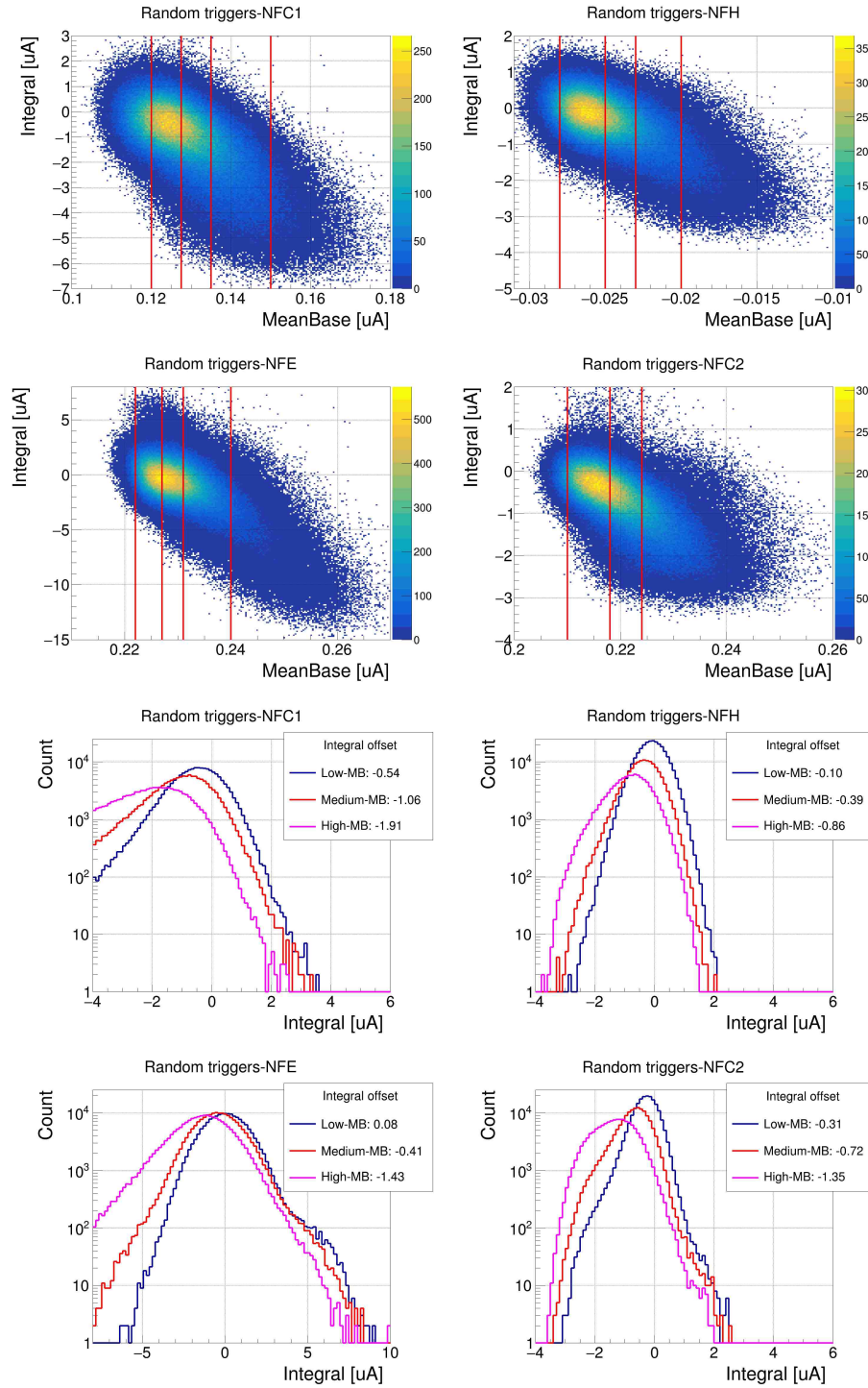


Figure 4.37: Effect of the average MeanBase on the offset. Top: Vertical red lines show regions of the 2d-histograms that were individually projected on the y-axis to find the Integral distribution. Bottom: Projected distributions of Integral values.

We developed a correction function to subtract the Integral offset as a function of MeanBase. To do this, the data was binned based on the MeanBase values, and for each bin, the Integral offset was determined by fitting the Integral distribution with a Gaussian function. The center of the Gaussian fit was used as the Integral offset, and the uncertainty in this parameter was treated as the uncertainty in the offset. This procedure is illustrated for one bin of the NFC1 detector data in Fig. 4.38.

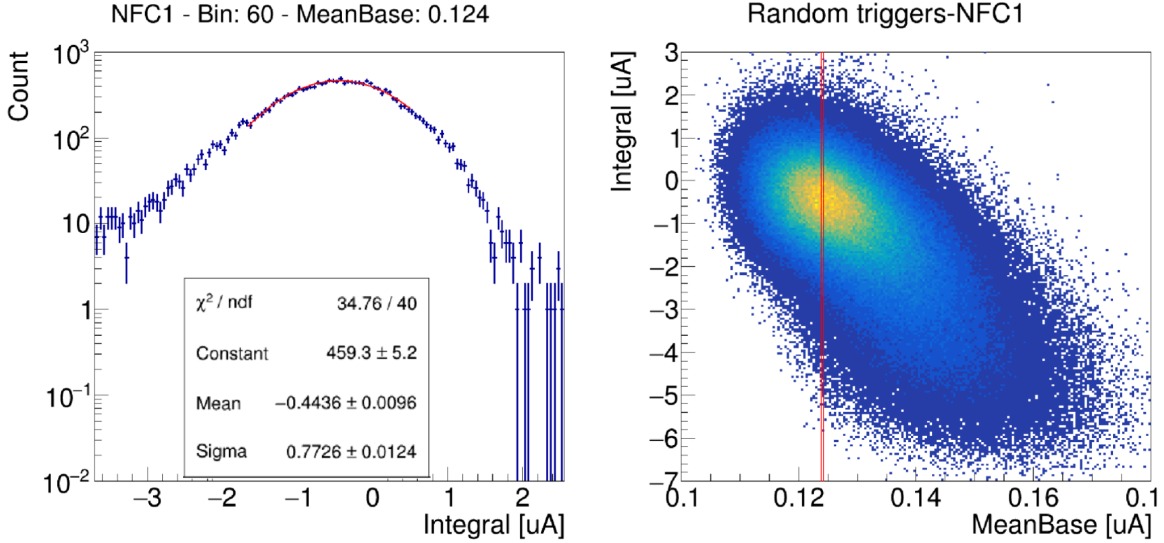


Figure 4.38: Gaussian fit to the distribution of Integral values for events in a MeanBase bin. The point estimates and the uncertainty of the mean value is used to corrected the offset and extract the uncertainty of the correction.

We determined the primary correction function by linearly interpolating the Integral offset values across the MeanBase bins. This function (Fig. 4.39) was then used to subtract the offset, resulting in a corrected Integral. The distribution of the corrected Integral is shown in Fig. 4.40.

The corrected Integral (Fig. 4.40) still shows a small offset. The leftover offset was taken as the systematic uncertainty of the correction, and added in quadrature with the statistical uncertainty of mean values of Gaussian fits in each MeanBase bin. The total 1σ uncertainty band as the function of MeanBase is shown in Fig. 4.41.

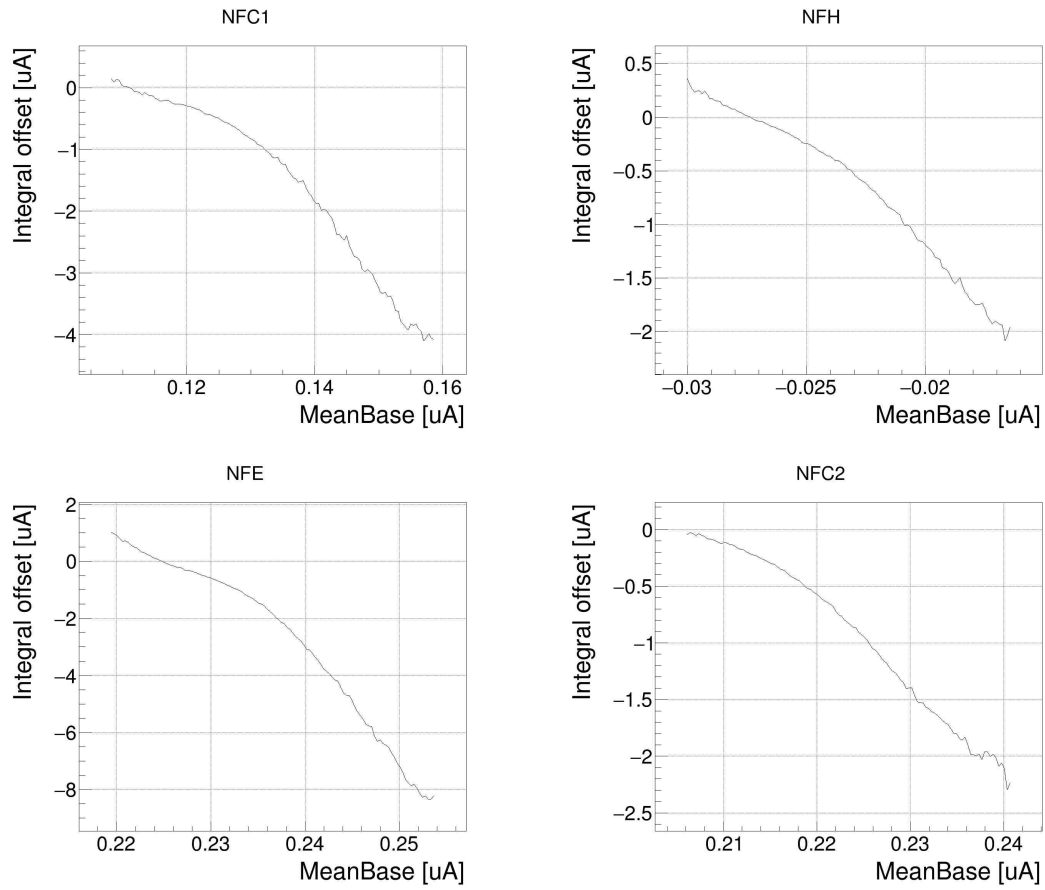


Figure 4.39: Correction function that removes the offset of Integral as a function of MeanBase. The associated uncertainty with this correction is shown in Fig. 4.41.

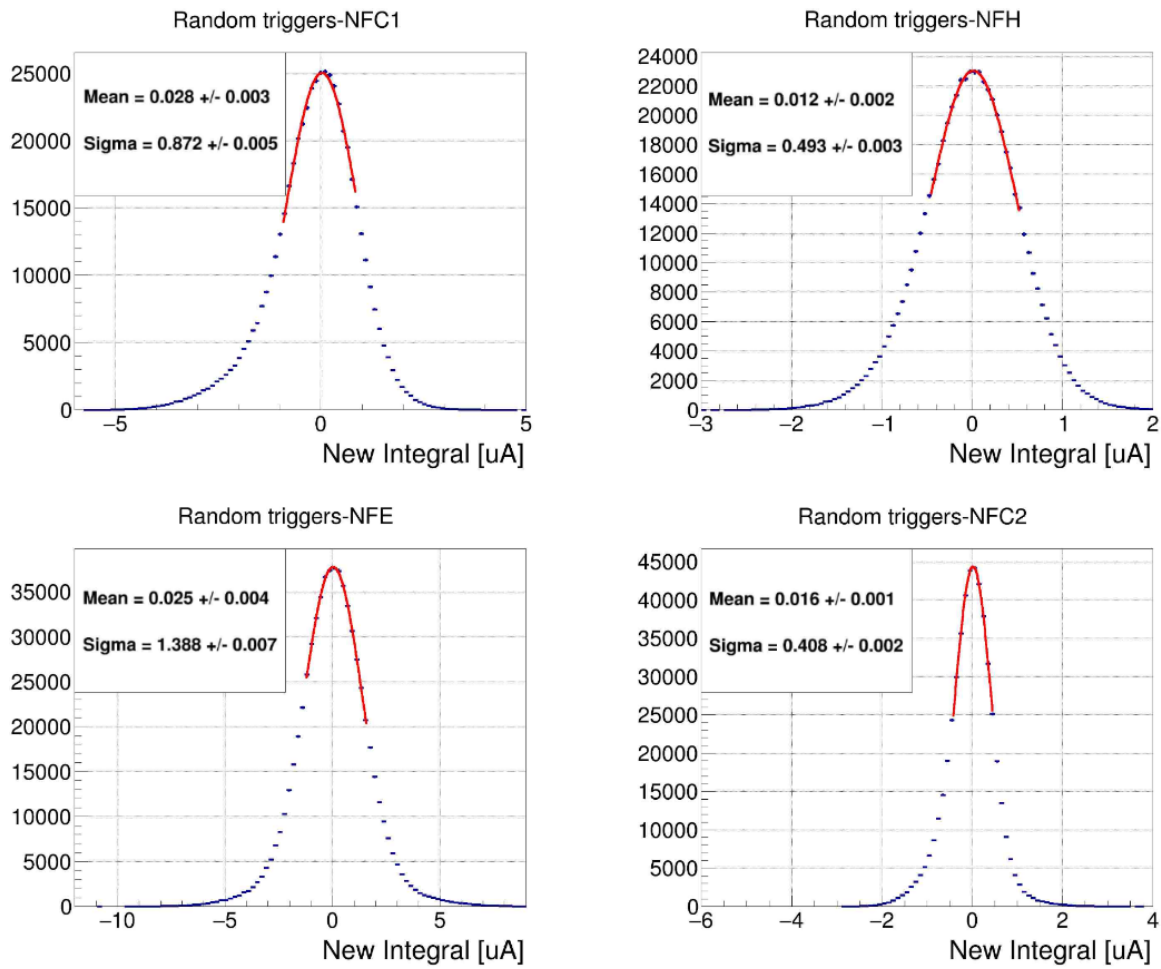


Figure 4.40: Histogram of random triggers as a function of corrected Integral.

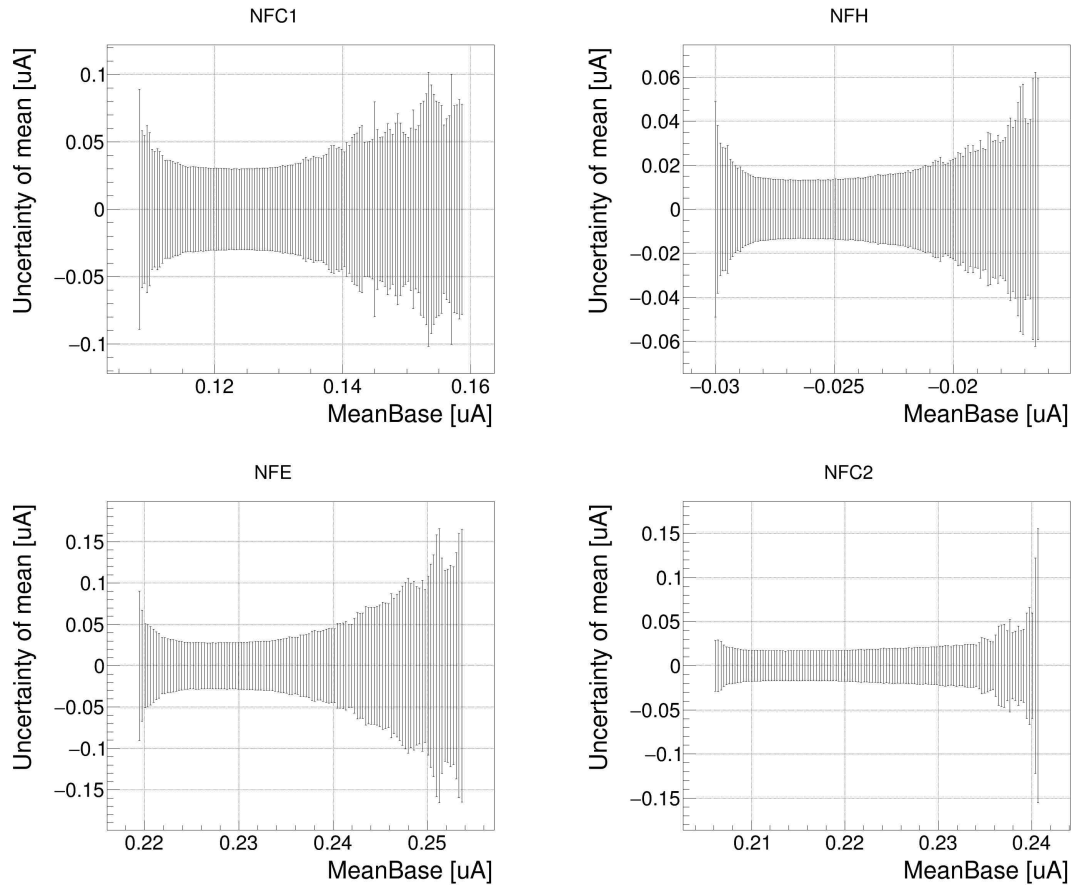


Figure 4.41: The cumulative statistical and systematic uncertainty for the Integral correction as a function of MeanBase.

To determine the total (statistical and systematic) uncertainty of the Integral correction, we generated a population of correction functions by randomly sampling the Integral offset values using their total uncertainties (Fig. 4.41). Each of these functions was then applied to correct the Integral RQ, resulting in a population of corrected Integral spectra. This population was subsequently used to measure the impact of the correction uncertainty on the calibration study discussed in the next chapter. The uncertainty from the Integral correction was found to be negligible compared to other sources of uncertainty. For simplicity, we will omit the term 'corrected' in the following chapter when we refer to the Integral RQ.

We did not observe any offset in the OFL energy estimator; therefore, that did not require any correction. The offset of the OFL was measured indirectly through the distribution of the OF0 RQ, as shown in Fig. 4.42.

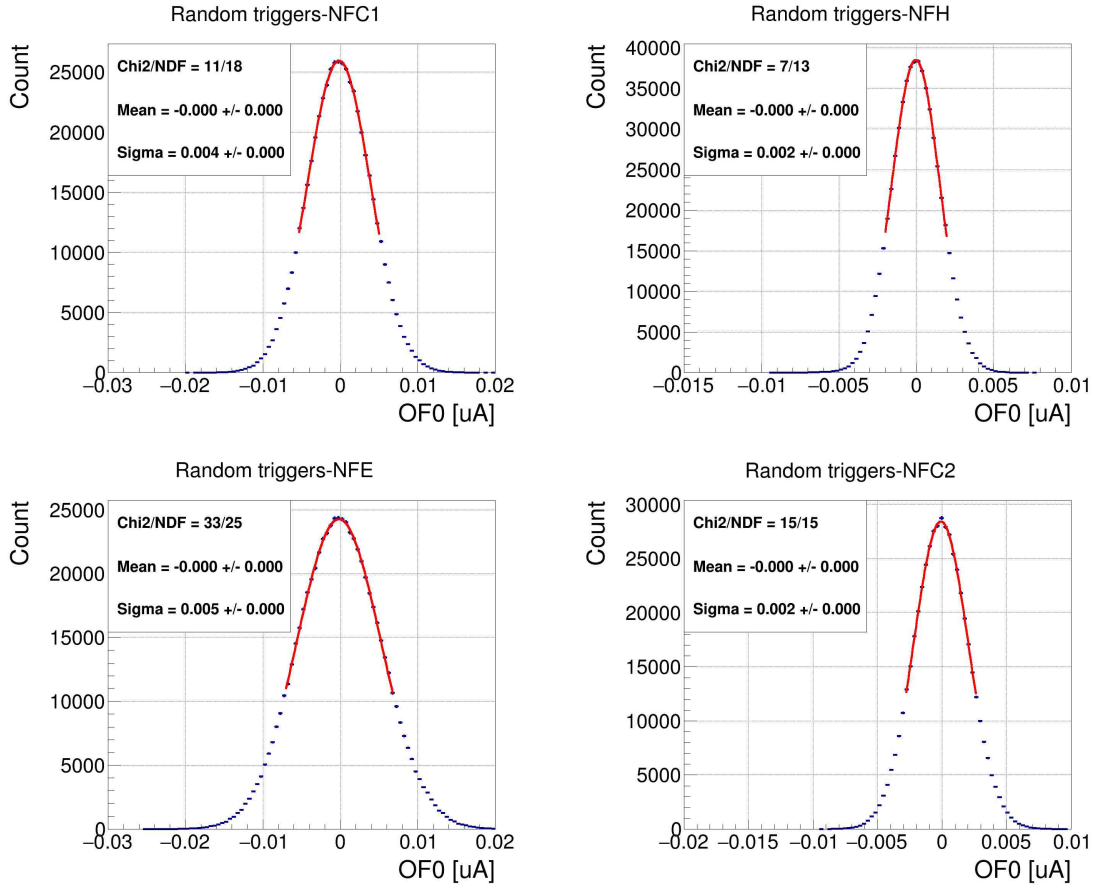


Figure 4.42: Histogram of random triggers as a function of OF0 for the calibration data.

4.8 Pulse amplitude and pulse integral relation

The relation between pulse Amplitude (OFL) and the Integral is modeled using a second-order polynomial of the form $y = ax + bx^2$. The fit to the nominal corrected Integral is used to determine the statistical uncertainties in the coefficients a and b . Additionally, we used the variations of the corrected Integral spectra to find the resulting distribution of the point estimates for a and b . The widths of these distributions were then used to estimate the systematic uncertainties in a and b as shown for detector NFC1 and NFC2 in Fig. 4.43.

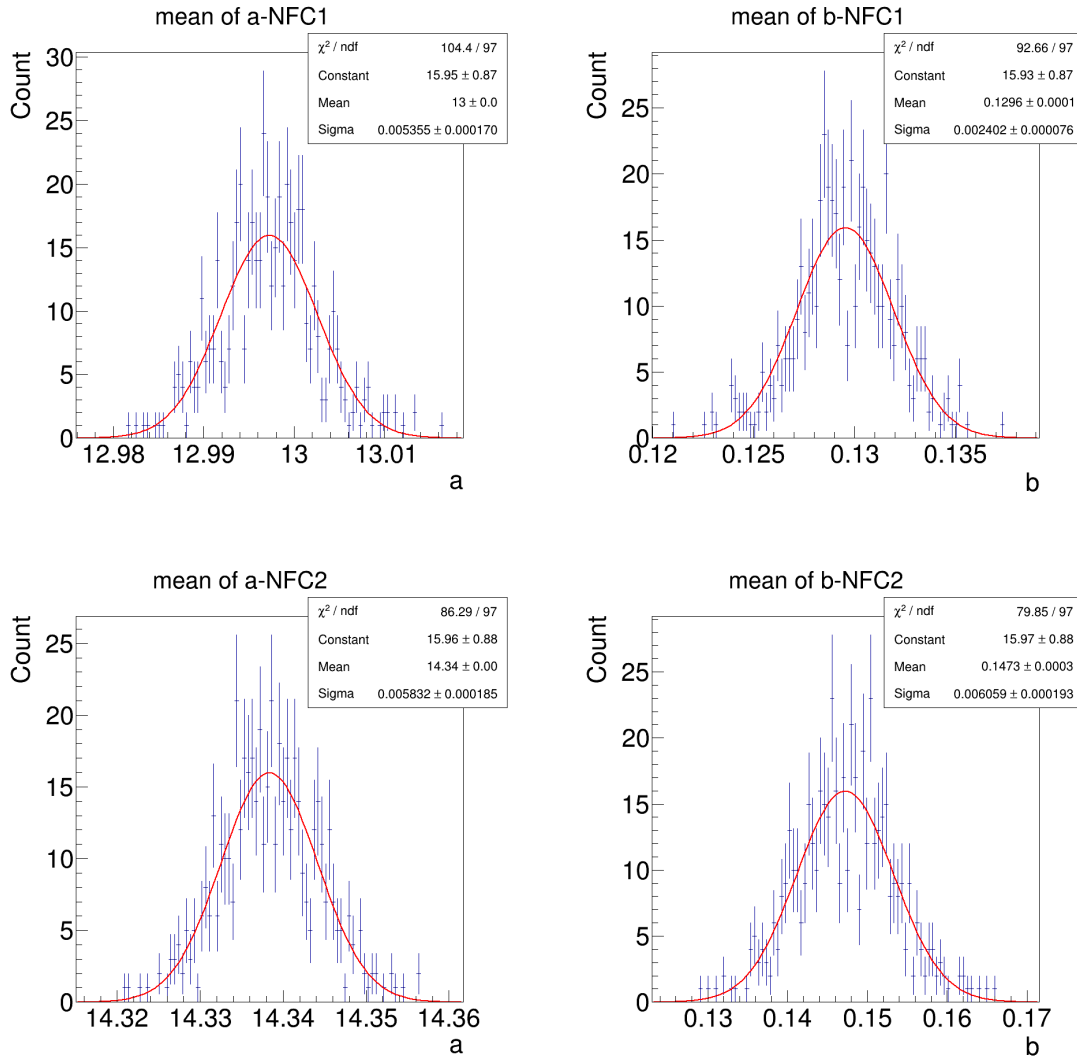


Figure 4.43: The distribution of a and b parameters following variations of the Integral correction.

The relation between pulse Amplitude (OFL) and the Integral RQs is shown in Fig. 4.44. This relation is used in the calibration study discussed in the next chapter.

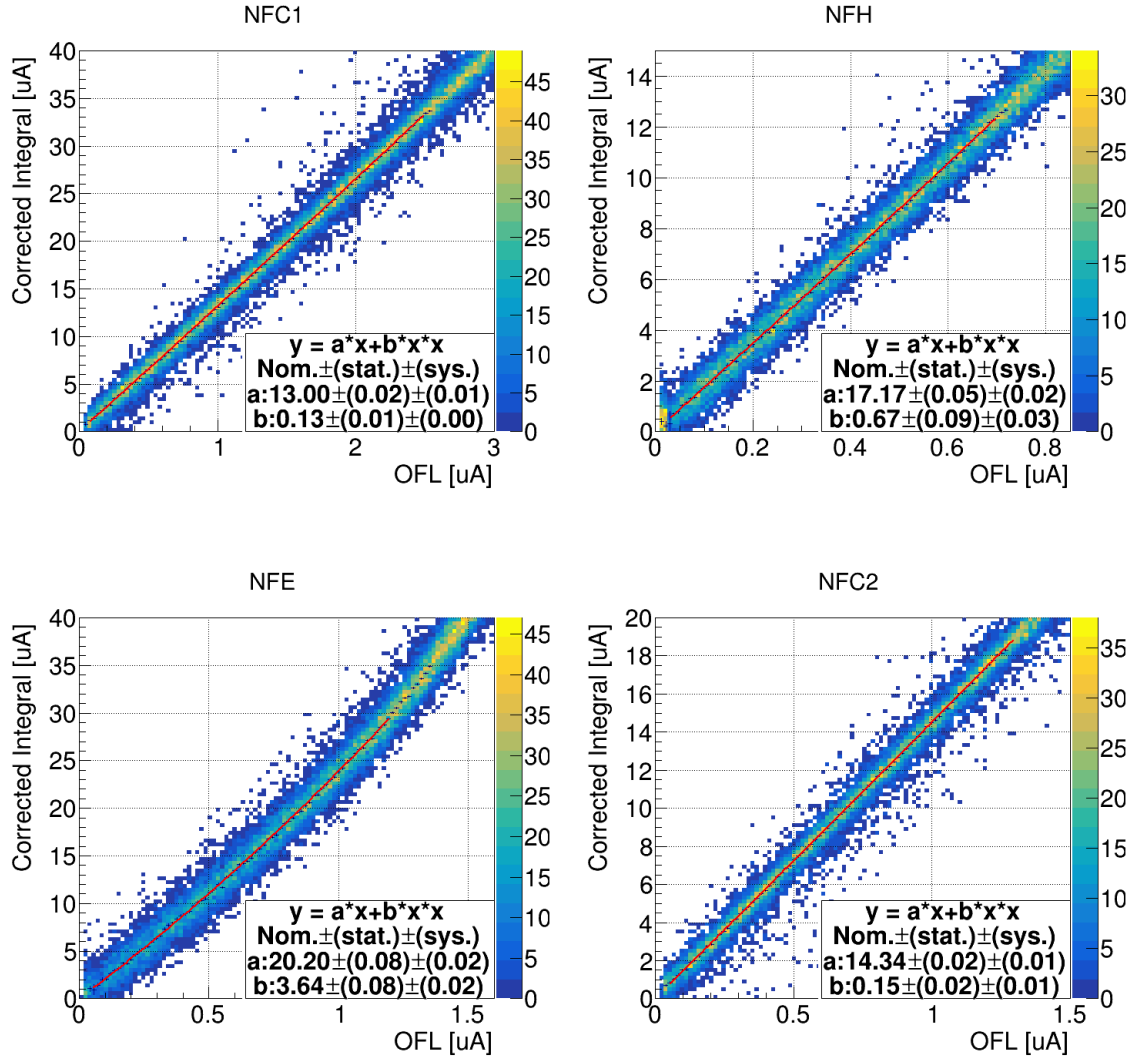


Figure 4.44: The relation between pulse Amplitude (OFL) and Integral.

4.9 Summary

This section primarily discusses the data preparation for the Compton step calibration study, conducted at 0 V crystal bias, which is discussed in the following chapter. The set of cuts studied in this chapter are tailored to the low- and high-energy ranges.

Two populations of rejected events require further understanding. The first population is for the spike like events that showed up in all detectors simultaneously (Fig. 4.23). It is important to identify the exact source of such events. A hypothesis is that they are due to readout electronics. If true, adjusting the electronics will be important for future studies. The reconstructed energies of these events is below 1 keV in total phonon energy which makes them a critical background source for the current DM searches if they go undetected.

The second group of events requiring further investigation consists of the elevated tail events, which were excluded using χ^2 and pulse width cuts. In the 2d histograms of χ^2 and pulse width variables versus energy, these events formed distinct bands within the energy range of interest for the Compton study (Figs. [4.31, 4.28]). However, the discrimination power to isolate these elevated tail events diminishes at lower energies, highlighting the need to understand their origin and assess their potential impact on a dark matter search.

I replaced the Frequency χ^2 at low energies with the Pulse width cut at higher energies. The decision was made to prevent questions regarding the quality of the Frequency χ^2 discriminator for high-energy events with pulse shapes much different compared to the OF processing template (constructed from low-energy events). The number of elevated tail events rejected by either cuts is small. The source of these events has to be studied and better understood. A hypothesis is that such events result from energy depositions in Al fins of the QETs instead of the silicon crystal. This is motivated by the qualitative similarity between the number of elevated tail events and the size of the QET mask in different HVeV detectors. A quantitative comparison of this relation is left for future studies.

The correction to the Integral energy estimator discussed in this chapter is unique. The steps for defining this correction are straightforward and may be valuable for future studies. The bias in the Integral energy estimator was first observed when comparing it to the OFL energy estimator. After applying the correction, the trend of the Integral versus OFL values passes through the origin, as shown in Fig. 4.44, contrasting with the observation prior to the correction.

In the subsequent chapter we use the cleaned Compton calibration data that is collected at 0 V crystal bias to identify the detector calibrations.

Chapter 5

Compton Scattering Calibration at 0 V Crystal Bias

This chapter outlines the statistical workflow to perform the calibration of the 0 V data sets (no **NTL** gain according to Eqn. 2.12) using the Compton scattering signatures as shown in Fig. [4.32, 4.33]. Additionally, it explores and quantifies the data cleaning efficiency for the 100 V data set in the presence of the radioactive source. The efficiency estimation was important to understand the substantial drop in the cleaning efficiency of the 100 V data with respect to the 0 V data. The primary issue is identified to be the high probability of pulse overlaps, known as pileups, which prevents event reconstruction. As we will discuss, the 100 V data sets are particularly susceptible to this problem due to the amplification of the initial energy deposition through the **NTL** gain, resulting in prolonged pulses.

The 0 V calibration is based on three energy signatures: a combined structure from silicon L-steps, the silicon K-step, and the a peak from copper K_α X-ray, at approximate energies of 100 eV and 150 eV (Fig. 3.15), 1.8 keV (Fig. 3.8), and 8.1 keV (Fig. 3.8), respectively. The copper X-ray originates from the detector housing being exposed to gamma rays (Fig. 3.8). The K_β peak of copper is not identifiable in the data, which is consistent with expectations from the detector resolution.

For the L-steps calibration (approximately below 250 eV), we use the pulse height (OFL) as the energy estimator. We assume that a calibration parameter maps OFL to energy following a linear relationship “Energy = calibration.OFL” based on the detector performance understanding. We determine the calibration parameter by fitting the Compton cross section, in units of energy, to the data in the OFL domain. The final unbinned likelihood model has a floating calibration parameter that stretches the Compton simulations (ab initio FEFF cross section curves in Fig. 5.1) for the

best fit to data. Before arriving at the final model, we spent a significant amount of energy to perform a data driven validation of the L-steps simulation. However, we found that the data is statistically limited for a trustworthy validation; therefore, we included extra systematic uncertainty introduced by the cross section model.

At higher energies, such as the K-step and above, the simulation is not directly fitted to the data. Instead, we model the simulation and data individually with an analytical function. We then read the calibration by aligning the signatures in data with the simulation. We identified the K-step in both the pulse area (Integral) and OFL energy estimators and decided to use OFL as it provided a better resolution. For the copper peak, we used the Integral energy estimator, which demonstrated a more linear relationship with respect to energy at higher energies.

5.1 Preliminary studies for L-step fits

It is preferable to use an analytical function to model the calibration signature in both the data and simulation independently. This function should incorporate several nuisance parameters to capture the signature's shape, as well as a parameter for its position. Comparing the shape parameters enables a data-driven validation of the simulation. Once the shape is validated, the calibration can be established by comparing the signature's position in the data with that in the simulation. Initially, we pursued this data-driven approach, but concluded that the data is statistically limited and insufficient for a robust validation. This section outlines the steps leading to this conclusion, and can be skipped if the reader is only interested in the final inference model to find the L-steps in data.

The main challenges we encountered in the L-steps calibration are as follows:

1. There are two steps at approximately 100 eV and 150 eV. While a detector with a few eV resolution should theoretically be able to distinguish them, the small energy gap makes it impractical to model the steps separately in data. As a result, the steps must be fitted simultaneously. This adds complexity to the model and requires a better understanding of how the likelihood function behaves when fitting a two-step structure. Therefore, we performed preliminary studies with toy data before analyzing the main data.
2. Calibration steps are produced by Compton scattering. Since the total cross section for Compton scattering is relatively small, the scattering probability is nearly uniform across the detector. As a result, the calibration is not confined

to specific locations for energy depositions, which aligns with expectations from **DM**. However, this also makes data collection a slow process, a challenge we anticipated but could not overcome due to time constraints at the experimental site. Furthermore, we were unable to use a high-activity gamma source because of data reconstruction limitations. As discussed in subsection 5.5.5, the total event rate of energy depositions in any detector could not exceed a few Hz, resulting in an event rate on the order of mHz in the energy window for the L-steps.

3. Ideally, the primary gamma energy should exceed 100 keV to ensure a sufficient fraction of Compton scatters compared to photoabsorption in silicon, as shown in Fig. 3.1. However, higher-energy gammas also generate longer pulses, which increases the pileup rate and reduces data-cleaning efficiency. Thus, it is essential to find a balance for efficient data collection. The 100 V calibration data (with a radioactive source in place) was especially impacted by the high pileup rate.
4. The theoretical models describing the step shapes are subject to systematic uncertainties, and the simulation packages have not been fully validated. We replaced the Geant4 simulations with FEFF simulations and made efforts to quantify the systematic uncertainties.
5. The energy range of interest for the L-steps displays a dominant background spectrum that resembles the **low-energy excess events** spectrum that is observed in similar detectors in [66, 67]. This background increases sharply at lower energies, making it challenging to distinguish the L-steps.

5.1.1 Comparison of the calibration and background data

A qualitative comparison of the calibration (“CsBa_close”) and background spectra is shown in Fig. 5.1. The x-axis represents the energy, where the 100 V calibration is applied to the 0 V data¹. The selected energy window is expected to include the L-steps; however, the steps are only distinguishable in the data from the NFH detector.

As discussed in Sec. 4.6, data cleaning efficiencies are believed to be constant as a function of energy, though these values have not been explicitly calculated. As such,

¹To a first approximation, the sensor response is expected to be similar for the same amount of phonon energy reaching the **TES**, regardless of the crystal bias.

the spectra presented here are not efficiency-corrected. To account for efficiency differences between datasets, the background spectra are scaled to match the calibration spectra, ensuring consistent event rates in the lowest energy bins. The lowest bin below the L-steps is expected to contain a Compton scattering event population that is three times smaller than the bins above the L-steps (4 electrons compared to 12 electrons available for scattering, see Fig. 3.15). However, this reduction is not observed in the calibration data. Additionally, the background data shows an increasing event rate at lower energies. Therefore, we assumed that the lowest bins are dominated by background events appearing at similar rates in both the background and calibration data which justifies the scaling.

The comparison between the scaled background and the calibration data highlights the importance of background modeling. For the NFH detector, the background clearly extends into the region showing a step-like feature. In other detectors, the steps are not visible, likely because they are obscured by background. This approximate comparison indicates the need for an empirical background modeling.

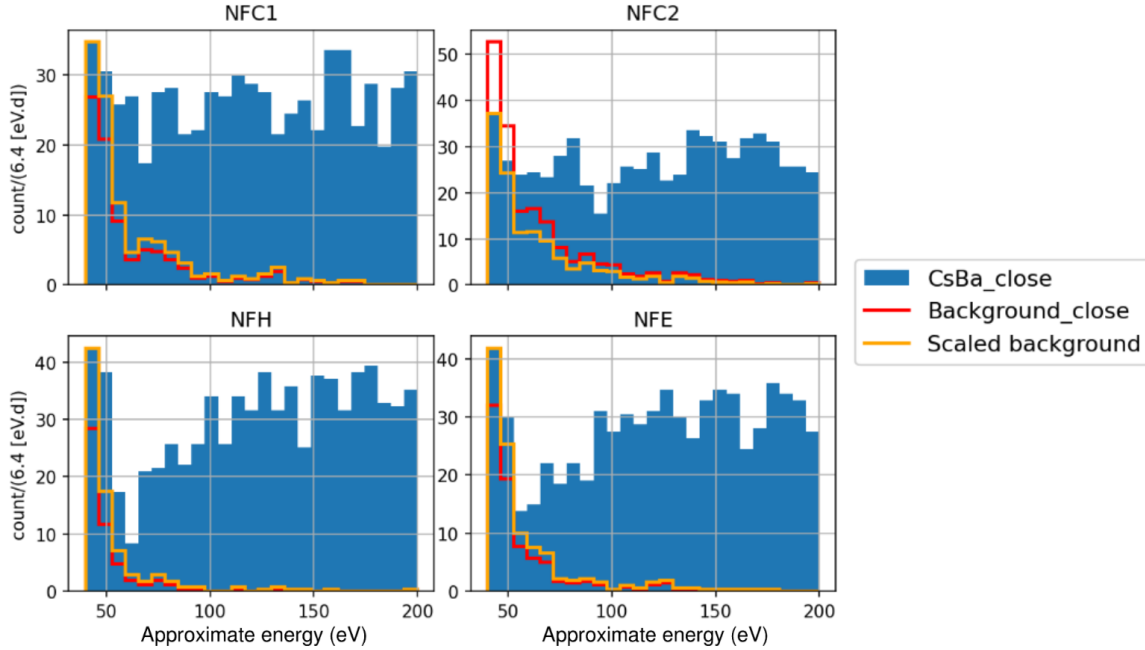


Figure 5.1: Comparison of background and calibration data sets. The blue histogram and the orange line show the calibration and background after data cleaning (without efficiency correction). The red curve shows the scaled background data that matches the calibration data in the lowest energy bin.

Before modeling the background, we analyzed an analytical model to fit the Compton scattering events. For the analysis, we generated toy datasets with an event count

comparable to the experimental data. The following subsection discusses how the Compton scattering event count is estimated using the calibration data.

5.1.2 Approximation for the count of Compton scatters

Simulations suggest that the Compton cross section remains nearly constant between 300 eV and 500 eV, as shown in Fig. 3.15. Furthermore, Fig. 5.1 indicates that the majority of events within this energy range are Compton scatters in the calibration data.

The cross section simulation provides the expected ratio of Compton scattering events between 300 eV and 500 eV to the total number of events below 500 eV. Using this ratio, along with the number of Compton scatters in the calibration data between 300 eV and 500 eV, we can estimate the expected number of Compton scatters below 500 eV.

The relation between the number of observed and expected events is shown in Fig. 5.2. The x-axis shows the number of events below 500 eV and the y-axis shows the number of events within 300 eV to 500 eV. The black horizontal line represents the number of events within 300 eV to 500 eV. The black vertical line represents the observed number of events in the NFH detector, while the vertical line shows the estimated total number of events.

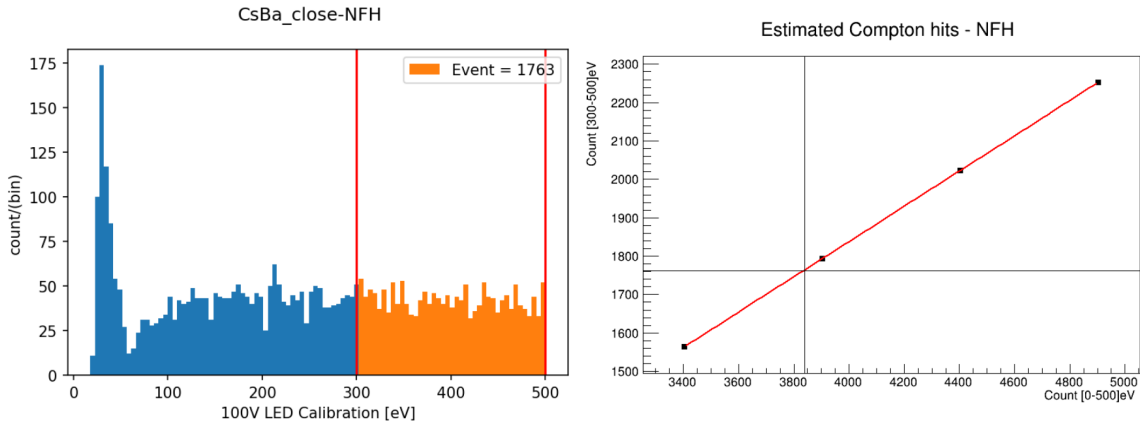


Figure 5.2: Left: The NFH detector data shows approximately 1750 events between 300 eV and 500 eV. Right: Based on the simulation in Fig. 3.15, the total number of Compton scatters below 500 eV is estimated to be approximately 4000 events.

5.1.3 Analytical model for L-steps

The initial PDF to model L-steps consist of two error functions with five floating parameters that is given by

$$\text{PDF}(x|\theta) = \left[\text{base} + (6+k) \frac{1 + \text{Erf}\left(\frac{x-x_1}{\sqrt{2}\sigma}\right)}{2} + (2-k) \frac{1 + \text{Erf}\left(\frac{x-x_2}{\sqrt{2}\sigma}\right)}{2} \right] / \text{Integral}. \quad (5.1)$$

In this model, “base” represents the average number of electrons contributing to the cross section below the initial step. “k” controls the height of the plateau between the first and second steps, with the total height across both steps fixed at 8. “ x_1 ” and “ x_2 ” denote the center points of the first and second steps, respectively, while “ σ ” determines the smearing of the steps. The decision to fix the combined height of the two steps at 8 is based on the electron shell structure of silicon. We expect 8 additional electrons to contribute to the cross section across both steps. The parametrization of the model is illustrated in Fig. 5.3.

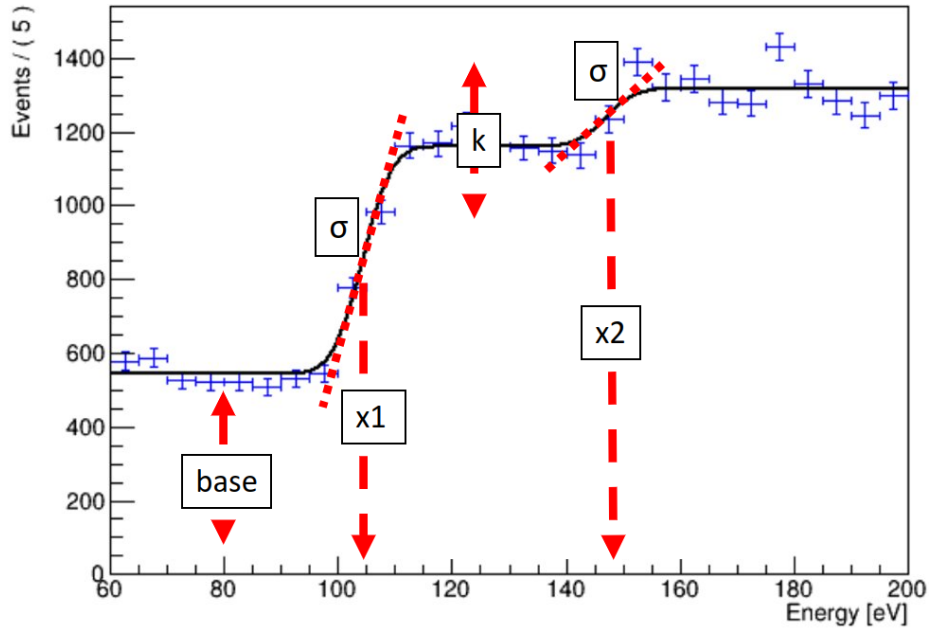


Figure 5.3: The parametrization of the PDF in Eqn. 5.1.

5.1.4 Likelihood and posterior construction overview

We began with the model described in Eqn. 5.1, and generated toy data sets using the parameter values listed in Table 5.1 through rejection sampling [68]. This model

Parameter	Value	Info
base	4	Number of silicon valence electrons.
k	0	6 electrons in L_3+L_2 , and 2 electrons in L_1 shells.
σ (resolution)	5	Based on previous measurements with HVeV detectors.
x_1	99	Approximation for the binding energy of L_2 , L_3 .
x_2	150	Approximation for the binding energy of L_1 .

Table 5.1: The truth information to produce toy data sets from Eqn. 5.1.

was used to construct an unbinned likelihood function that defined as

$$L = \prod_i \text{PDF}(x_i|\theta), \quad (5.2)$$

where the index i runs over the events within the window used to normalize the PDF, and θ represents a vector of floating parameters (base, k , x_1 , x_2 , and σ). To build the posterior distribution with the Bayes' theorem

$$\text{Posterior}(\theta|\text{data}) = \frac{L(\text{data}|\theta) \cdot \text{prior}(\theta)}{\text{Evidence}}, \quad (5.3)$$

where priors were chosen to be uniform **PDF**s centered around the nominal parameter values. The position of the step is not distinguishable by eye in the calibration data; thus, the priors for the step positions should be broad enough to encompass the true positions.

Ideally, the fitting model should be parameterized to minimize strong correlations between parameters. Additionally, the size of the data determines the number of unknown parameters that the model can accurately estimate. For smaller datasets, the information may be insufficient to precisely estimate all unknown parameters. At the expected statistics of 4000 events, the **PDF** in Eqn. 5.1 resulted in posteriors with strong non-Gaussian credible intervals, significant correlations, and biased estimators. To mitigate this, we gradually fixed some of the floating parameters to reduce statistical uncertainties with constraints derived from simulations. Ultimately, we found that all shape parameters should be fixed for well-behaved posteriors and unbiased estimators. The steps we followed are summarized below:

1. Select an analytical model.
2. Generate toy datasets from the analytical model and fit them. Since this is a fit of the true PDF to the data, point estimates are expected to be unbiased, and credible intervals should be valid.

3. Introduce extra constraints if the uncertainties are strongly non-Gaussian, points estimates are biased, or credible intervals are not valid.

5.1.5 Markov Chain Monte Carlo

The posterior study in the previous subsection is conducted using **Markov chain Monte Carlo (MCMC)** sampling. We evaluated several **MCMC** packages, including **emcee** and **BAT**. Ultimately, we selected the Metropolis-Hastings algorithm implemented in **BAT** due to its faster sampling time for the posterior introduced in Eqns. [5.1, 5.3]. The **emcee** package [69], which provides a pure-Python implementation of several affine-invariant **MCMC** algorithms, is particularly popular in the astrophysics community. In contrast, **BAT**, originally written in C++, is more widely recognized among particle physicists. We used the new Julia-based implementation of the **BAT** [70], which employs the Brooks-Gelman test to verify the convergence of chains before drawing samples. A conceptual overview of **MCMC** algorithms to clarify the meaning of the terms used in this paragraph is provided in Appendix B.

5.1.6 Posterior validations

The initial findings suggest that the priors on parameters x_1 , x_2 , and k , as defined in Table 5.1, should exclusively confine the parameters to individual steps. For example, setting the priors for x_1 and x_2 within the energy range of 75 eV and 165 eV, and allowing k to vary between -6 and 2, results in a posterior distribution that is multi-modal rather than Gaussian as shown in Fig. 5.4. This is expected as the steps associated with these parameters can be interchanged without affecting the overall shape of the resulting analytical model.

The degeneracy can be lifted by confining x_1 to be within 75 eV and 120 eV, and x_2 to within 120 eV and 165 eV, and k to be within -2 and 2, as shown in Fig. 5.5. Although practical for toy data sets, confining the priors for the real data is highly questionable since we cannot see the steps; also, we do not know the calibration in advance.

As shown in Fig. 5.5, the posterior distribution of the model with restricted priors still displays significant non-Gaussian credible intervals. Furthermore, the choice of priors for x_1 and x_2 seems arbitrary, with no clear rationale for the specific cutoff points selected for each parameter (e.g., why 120 eV instead of 130 eV?). This arbitrariness becomes even more concerning when fitting uncalibrated data that lack distinct step-like features. These findings indicate a need for reparameterizing the

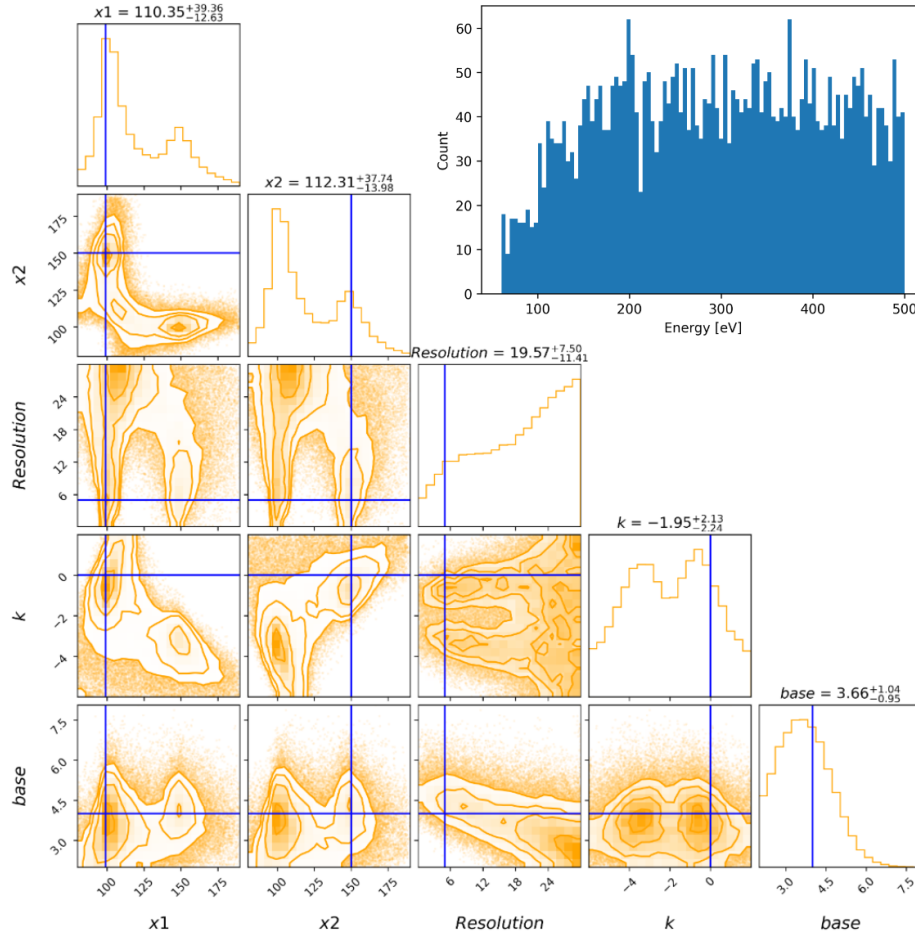


Figure 5.4: Posterior of the flexible model, and toy data consisting of 4000 events that was used to construct the likelihood. Blue lines show the parameter values that were used to generate the toy data (true values).

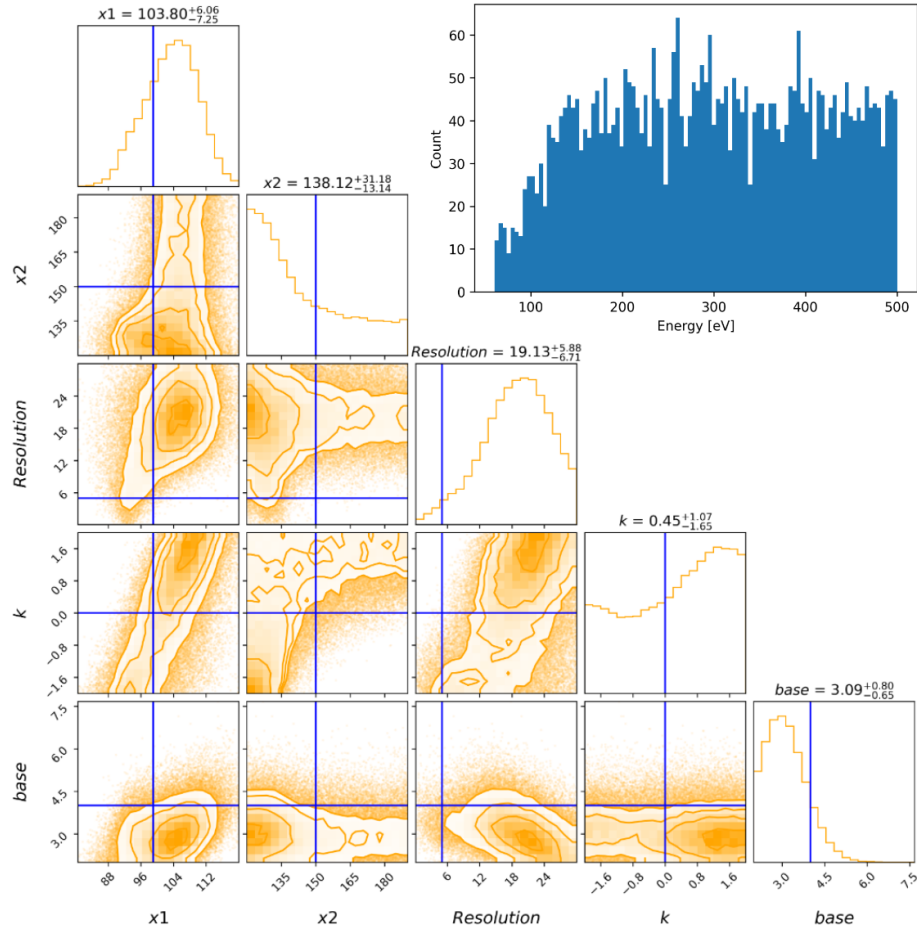


Figure 5.5: Posterior of a flexible model with priors restricted to individual steps, and toy data consisting of 4000 events that was used to construct the likelihood. The blue lines indicate the true parameter values.

model. Additionally, the non-Gaussian shapes suggest that incorporating information from simulations is necessary to eliminate some of the floating parameters of the double-step model.

We fixed the parameters k and $base$ using values derived from the simulation fit. However, the posterior results remained unsatisfactory, particularly for x_2 and the resolution. The different behavior of the fits for x_1 and x_2 were expected, as the height of the second step is smaller than that of the first step by a factor of approximately 3. Consequently, the second step is more susceptible to Poisson fluctuations in the data. To address this, we redefined x_2 as λx_1 . This new parameterization allows the prior on x_1 to cover a broader range, and enables leveraging the simulation to define a prior for the second step's position relative to the first. In summary, this reparameterization offers the following advantages:

1. This approach allows the simulation to constrain λ , under the assumption of a linear detector response. Note that the multiplicative factor remains calibration-independent as long as a linear calibration is assumed.
2. It resolves the issue related to the arbitrary selection of priors for x_1 .

The assumption of a linear response is supported by the observation that the χ^2 distribution in the 40 eV to 300 eV energy range remains flat across all four detectors, as shown in Fig. 4.28. This flatness indicates a consistent pulse shape within this window. Following the model reparameterization, we fixed λ , resulting in two floating parameters. We then examined the posterior distributions for non-Gaussian behaviors. The qualitative comparisons were satisfactory, as demonstrated with toy data in Fig. 5.6. For a more rigorous quality check, we performed pull tests [71] to evaluate the point estimates and credibility intervals.

5.1.7 Bayesian inference and pull tests

There are several conventions for reporting point estimates and credible intervals in Bayesian inference. In this study, we selected the **maximum a posteriori (MAP)** as the point estimator and employed the **highest density interval (HDI)** to determine the credible intervals, as illustrated in Fig. 5.7. The **MAP** estimator identifies the mode of the posterior distribution as the best fit, in contrast to the **maximum likelihood estimation (MLE)** point estimates commonly used in frequentist analyses. According to the **HDI**, the 1σ credible interval is defined as the region of the posterior distribution containing the densest 68% of the probability mass. This approach differs from other

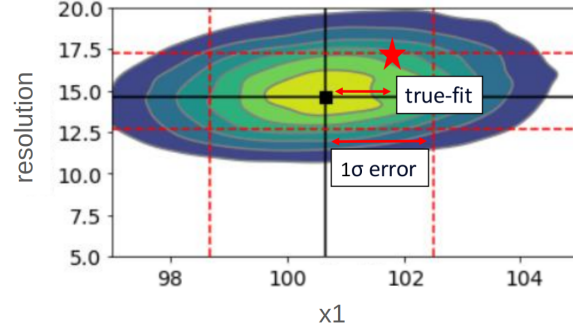


Figure 5.6: Posterior distribution of the reparameterized model, with the parameters $base$, k , and λ fixed. The red star indicates an example point representing the true values used to generate the sample points for this posterior. The pull tests will be explained in the following subsection.

conventions, such as using equal-tailed posterior intervals with equal probability mass values.

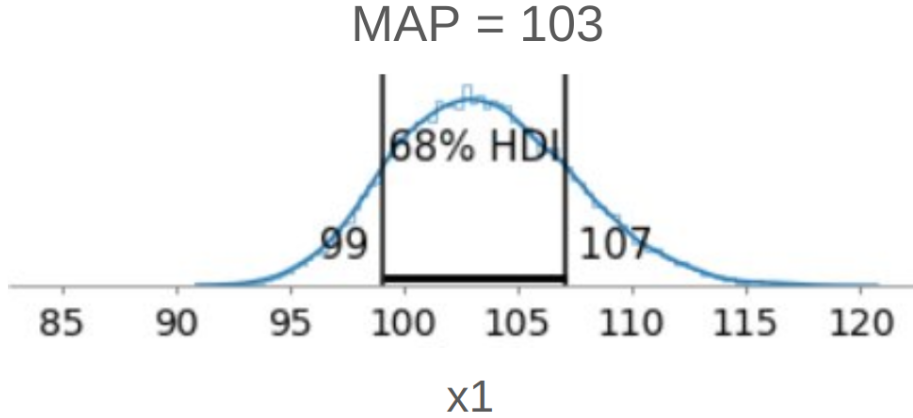


Figure 5.7: Illustration of **MAP** and **HDI** definitions in Bayesian inference. The **MAP** estimator identifies the mode of the posterior distribution as the best fit, while the **HDI** report the region containing the densest portion of the posterior distribution.

Using the definitions provided, we performed pull tests [71] to assess the validity of the point estimates and the coverage of the credible intervals. Although coverage is not a requirement in Bayesian inference, it is a desirable characteristic from the frequentist statistics that ensures reproducible results [72].

The pull of the fit can be defined as

$$g = \begin{cases} \frac{\text{True value} - \text{Best fit}}{\text{Right side of HDI interval}} & \text{if Best fit} \leq \text{True value} \\ \frac{\text{Best fit} - \text{True value}}{\text{Left side of HDI interval}} & \text{otherwise} \end{cases} \quad (5.4)$$

where the denominator uses the range of asymmetric credible intervals as reported by the **HDI**. For a reliable point estimate and credible interval, one would expect the distribution of g values, accumulated by fitting toy datasets, to follow a Gaussian distribution centered at zero with a width equal to one. In other words, the Best fit values should, on average, match the “True values” used to generate the toy datasets. Additionally, the 1σ credible interval should encompass the “True value” 68.1% of the time (right coverage).

The results of the pull test for the x_1 and resolution parameters, which are the only floating parameters in the final model, are shown in Figs. [5.8, 5.9], respectively. The toy datasets used to construct the posteriors are similar to those discussed in Fig. 5.6. For each parameter, the first plot displays the distribution of **MAP** values, the second plot presents the distribution of the average of the left and right sides of the **HDI**², and the last plot shows the pull distribution.

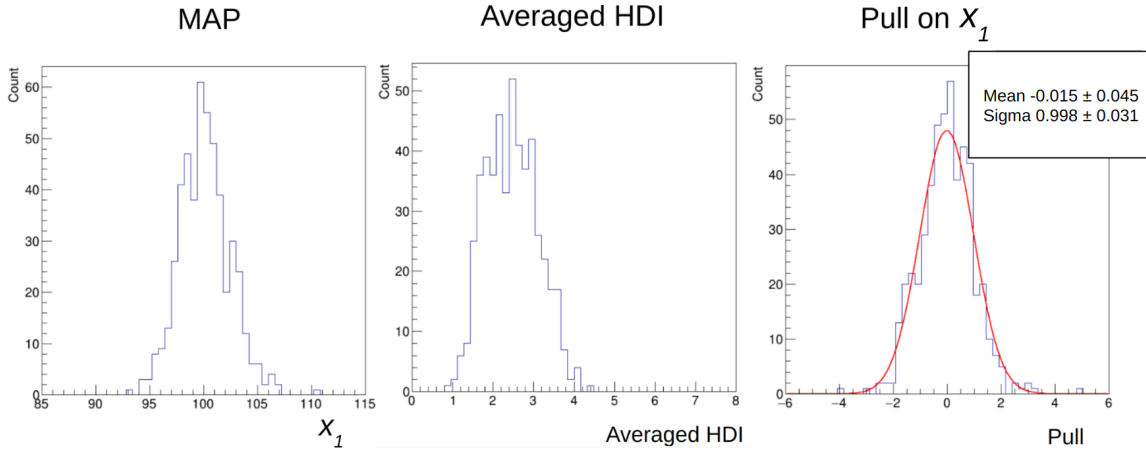


Figure 5.8: Pull test results for parameter x_1 . Left: Distribution of **MAP** values. Middle: Average of the left and right sides of the **HDI**, Right: Pull distribution.

The pull tests align with a normal distribution, indicating that the constructed inference model is well-behaved for the double-step **PDF**, given the expected data size. Similar pull tests on earlier models with additional floating parameters for step shapes resulted in biased Gaussian distributions and incorrect coverage values. We also confirmed that tests at higher statistics perform better, as demonstrated by an example fit with an extreme event count of 500k, shown in Fig. 5.10.

The primary takeaway from the validations thus far is that the limited data size presents statistical challenges, preventing the inference model from performing reli-

²The left and right **HDI** bounds are averaged for ease of visualization.

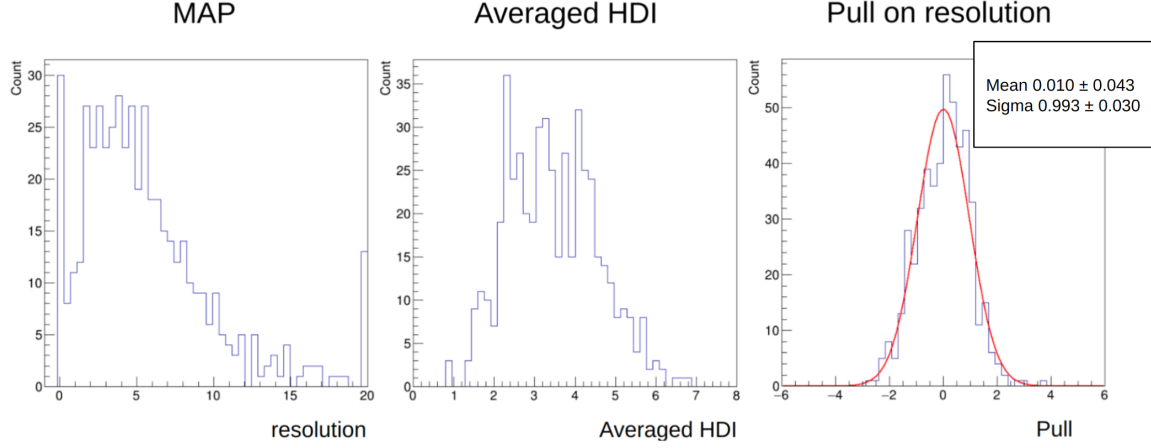


Figure 5.9: Pull test results for parameter resolution. Left: Distribution of **MAP** values. Middle: Average of the left and right sides of the **HDI**, Right: Pull distribution..

ably. We considered two potential solutions: first, studying the shape parameters by combining the data from all **HVeV** detectors, or alternatively, skipping the data-driven validation of the simulation and continue with shape parameter constraints. Following the latter approach, we could also fit the simulation directly to the data, rather than relying on an analytical model. These options will be briefly discussed in the following subsections.

5.1.8 Study shape parameters with combined data sets

The shape parameters can be studied by constructing an inference model that uses data from all **HVeV** detectors. This approach is based on the fact that Compton step shapes depend on the detector's target material, which is silicon for all **HVeV** detectors. While we expect the shape parameter values to be consistent across detectors from the physics perspective, the inference process may still yield varying shape parameters. This is because the response of L-step fits to data from detectors with different resolutions is not immediately obvious. Since we had no prior knowledge of the resolution of detectors, we chose not to combine the information from various detectors.

To study the concern described in the previous paragraph, we profiled the fit parameter values as a function of the smearing applied to the FEFF cross section curves (Fig. 5.1). The smearing factors control the width of the Gaussian smearing function. The resulting outputs, shown in Fig. 5.11, indicate that the best-fit values for the shape parameters depend on the resolution. Consequently, if the resolution

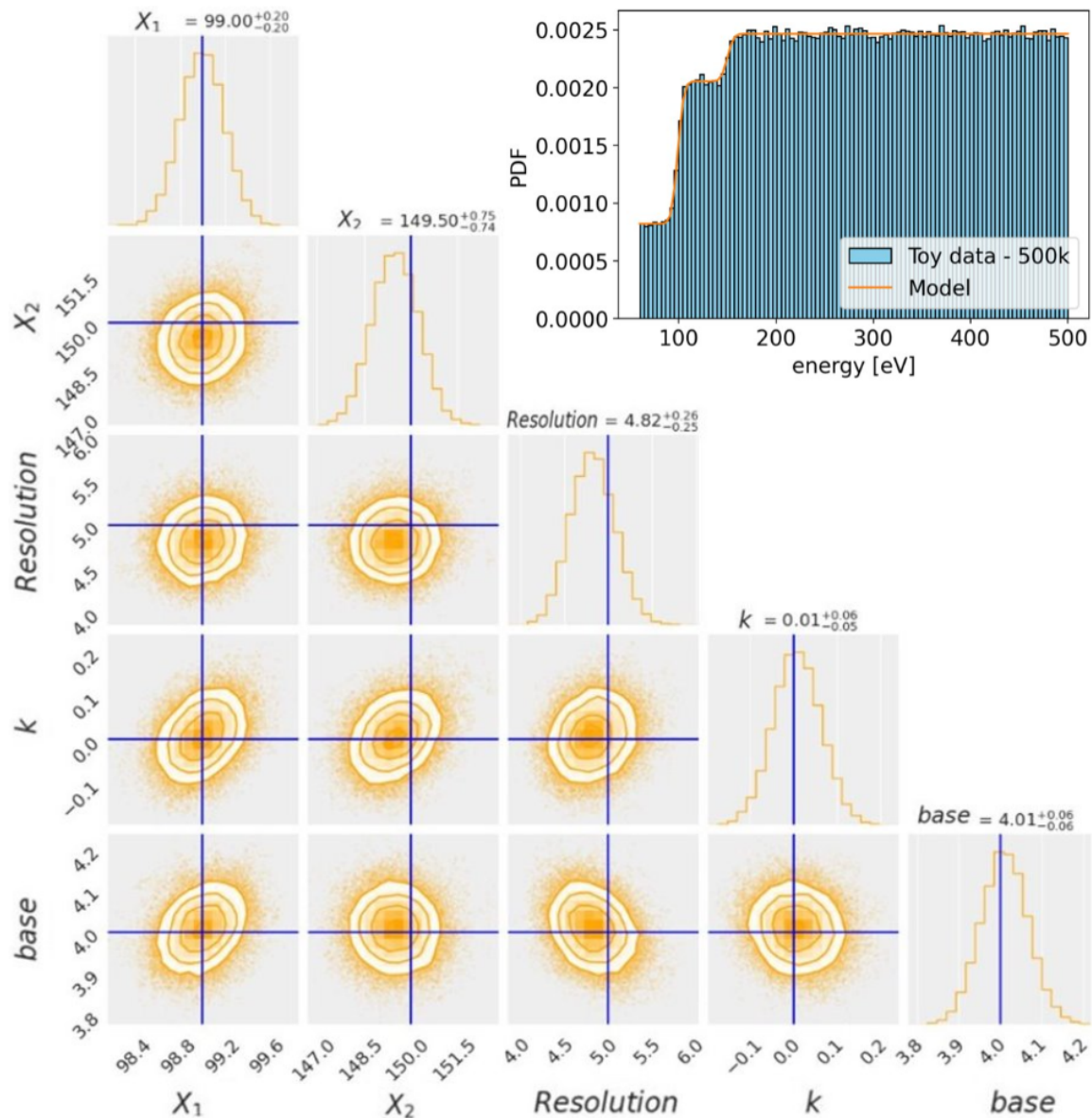


Figure 5.10: Posterior of a flexible model with priors restricted to individual steps, and toy data of 500,000 events that was used to construct the likelihood. The blue lines indicate the true parameter values.

varies between detectors, consistent shape parameter values cannot be expected.

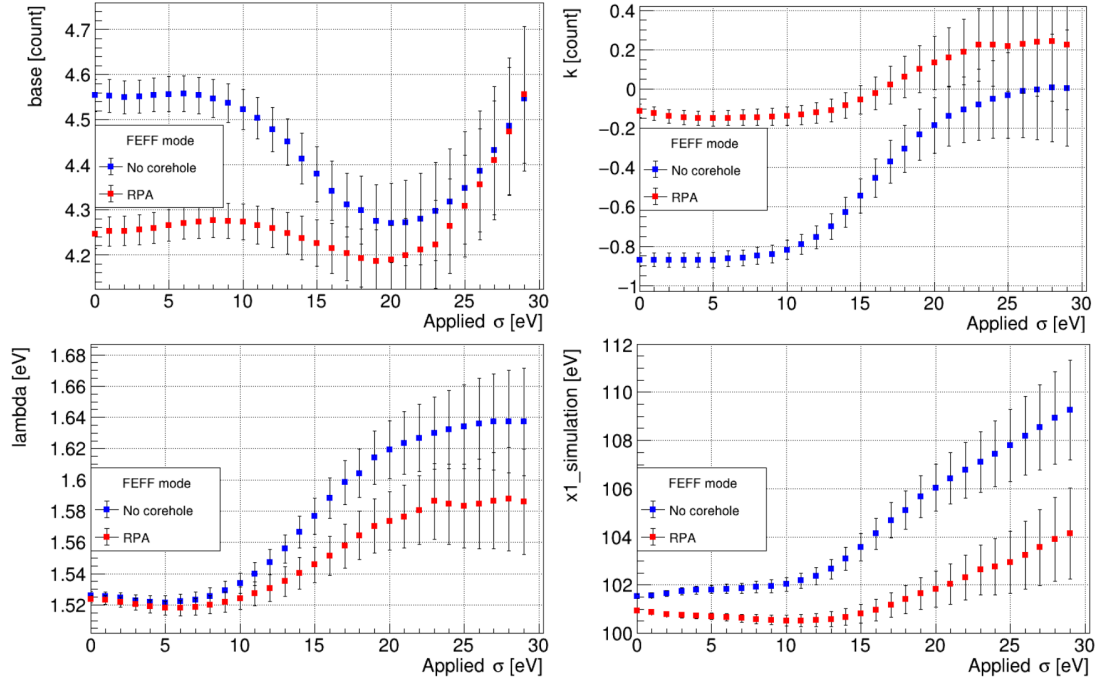


Figure 5.11: Systematic changes in best-fit values of a double-step model shape parameters as a function of smearing factor applied to FEFF simulations.

We ruled out the study of the shape parameter through combining the information from all **HVeV** detectors. The results in Fig. 5.11 raise another concern: given the dependence of the shape parameters on the smearing factor, what shape parameter do we choose to constrain the analytical model? Ideally, the uncertainty in detector resolution should be propagated into the shape parameter values; however, since the resolution is unknown, this introduces a non-trivial source of systematic uncertainty in the calibration.

Additionally, while the pull test for the “resolution” parameter in Fig. 5.9 appears to behave, we observe a cluster of fits at both ends of the **MAP** window, constrained by the boundaries of the uniform prior. This observation may raise questions regarding the choice of the prior.

To bypass these issues, we decided to depart from the analytical model and a Bayesian inference. Instead, we opted to fit the FEFF cross section (Fig. 5.1) directly to the data. Furthermore, we switched from a Bayesian approach to a frequentist study.

5.1.9 Statistical uncertainty estimates

To conclude this section, we address one more question: how much data is required to reduce the statistical uncertainty of the L-step fits below a certain threshold? This question is crucial for planning future calibration campaigns. We estimate the statistical uncertainty of the calibration fits using the constrained model with only two floating parameters which are x_1 and resolution.

We generated multiple groups of toy datasets using the spectrum from the Geant4 simulation that is illustrated in Fig. 3.15³. For each group, the simulation spectrum was first smeared with a Gaussian resolution model, and then sampled to construct the toy datasets. Toy data sets were individually fitted to arrive at Fig. 5.12.

The left plot displays the distribution of the left side of the HDI intervals (HDI-left) for the L-step fits to a subset of toy datasets. A Gaussian fit to this distribution provides one of the data points in the right plot. The mean value of the Gaussian function represents the uncertainty in the size of the HDI-left, while the width represents the uncertainty of this quantity. In the right plot, the x-axis represents the smearing factor applied to the simulation, the y-axis shows the number of events in the toy datasets, and the z-axis indicates the average size of the HDI-left along with its associated 1σ uncertainty. The result for the HDI-right intervals was close and is not reported here.

³At the time, FEFF simulations were not yet available.

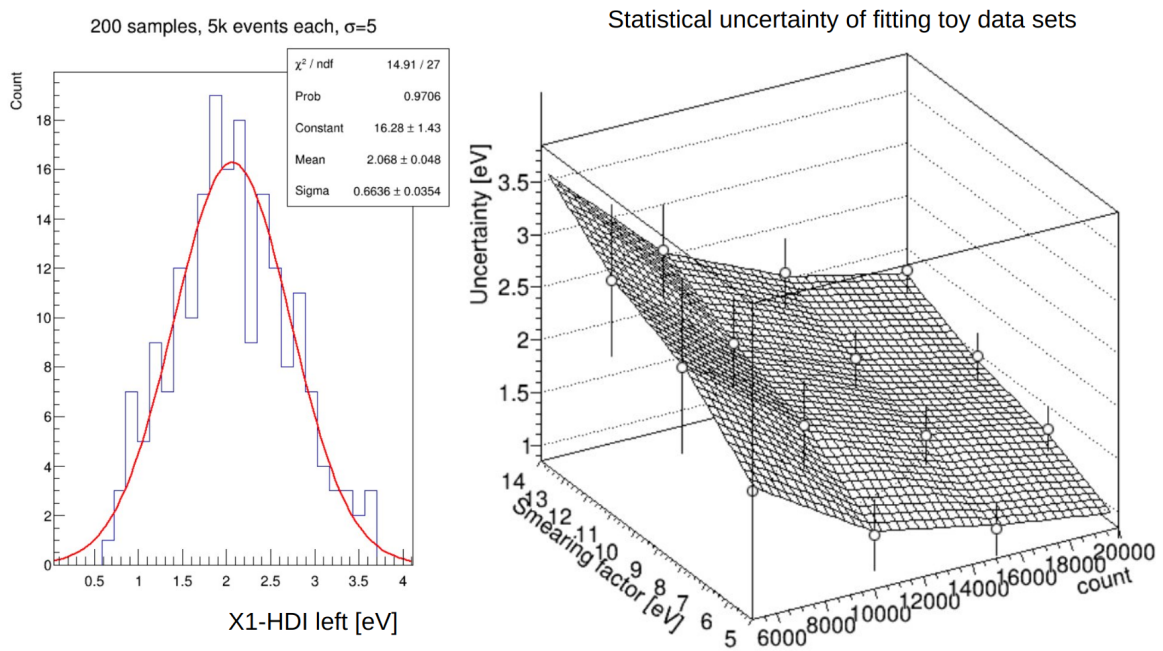


Figure 5.12: Statistical uncertainty measurements as a function of the Compton scattering count and detector resolution. The smearing factor was applied to the simulation prior to generating the toy datasets.

5.2 L-steps fits at 0 V

This section focuses on the experimental data and discusses the final inference model used to fit L-steps. It begins by constructing an empirical background model, then describes the strategy for fitting the L-steps, and finally presents the results.

5.2.1 Empirical background models

Previous studies by other groups have indicated that the shape of the unknown rising background, known as **low-energy excess events (LEE)**, may vary over time since the detector cool down [67]. Consequently, before proceeding with background modeling, we compared the spectra of background data sets collected at different time intervals using **Kolmogorov-Smirnov (KS)** tests. Specifically, we compared three sub-data sets from the “0V bg close” label (Fig. 4.9), recorded on Feb 21, Feb 29, and Mar 14 all in 2022, which we refer to as bg1, bg2, and bg3, respectively. The first two, bg1 and bg2, are close in time to the calibration data, whereas bg3 was collected approximately 20 days later. The p-values from the **KS** tests show that the spectral shapes for bg1 and bg2 are consistent. However, the result for bg3 is less conclusive. In the energy range of 40 eV to 70 eV (Fig. 5.13), the high p-values indicate consistency across all data sets. However, this consistency reduces when the energy range is expanded to 40 eV to 100 eV (Fig. 5.15). The **KS** test results for these two energy windows are shown in Figs. [5.14, 5.16].

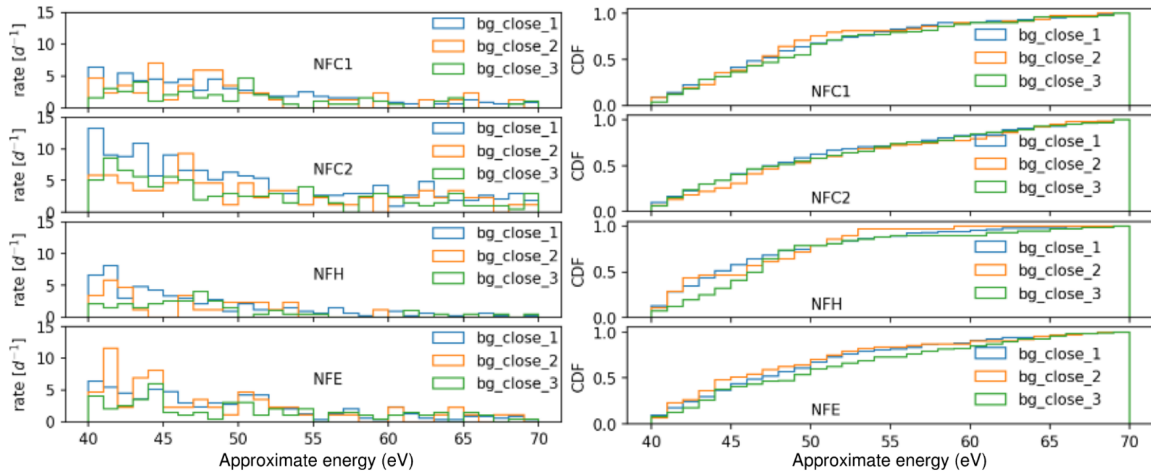


Figure 5.13: Comparison of the three background data sets (bg1, bg2, and bg3) in the energy range of 40 eV to 70 eV. The left panel shows the event rate spectra, and the right panel shows the CDF. The x-axis shows an approximate calibration according to the 100 V data sets that is applied to the 0 V data sets.

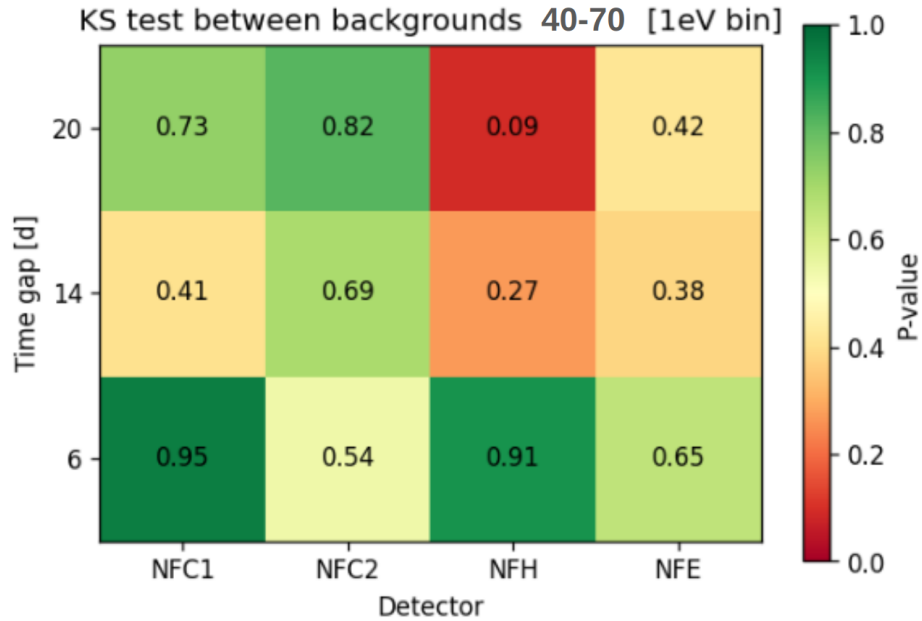


Figure 5.14: The **KS** test p-values for the comparison of background data sets in the 40 eV to 70 eV energy range. From the bottom to top, the first row compares bg1 and bg2, the second row compares bg2 and bg3, and the third row compares bg1 and bg3. The results indicate consistency within this window.

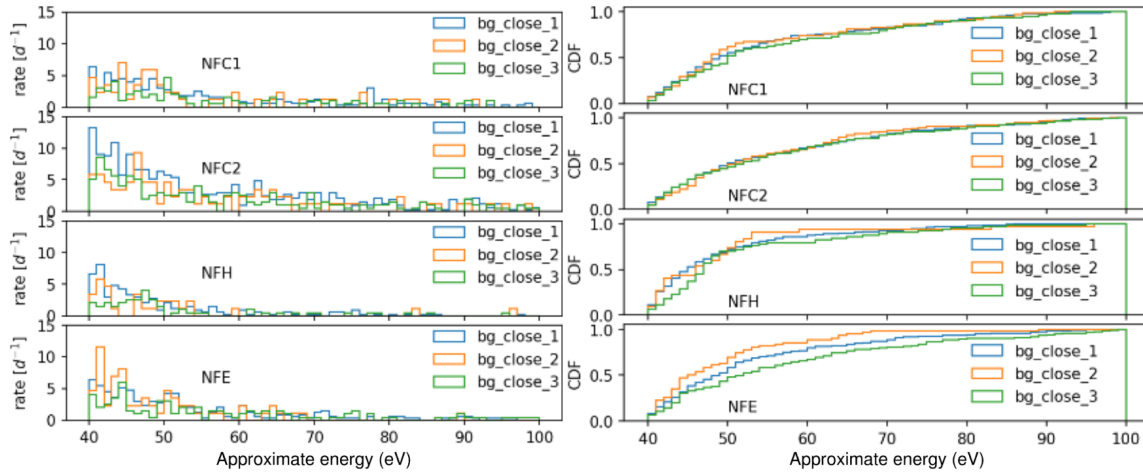


Figure 5.15: Comparison of the three background data sets (bg1, bg2, and bg3) in the energy range of 40 eV to 100 eV. The left panel shows the event rate spectra, and the right panel shows the CDF. The x-axis shows an approximate calibration according to the 100 V data sets that is applied to the 0 V data sets.

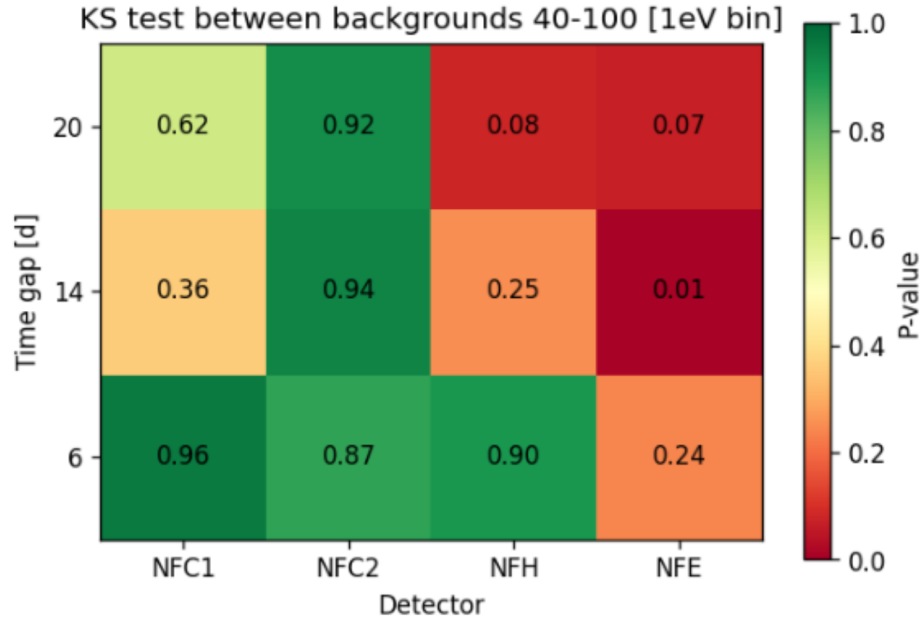


Figure 5.16: The KS test p-values for the comparison of bg data sets in the energy window of 40 eV to 100 eV. From the bottom to top, the first row compares bg1 and bg2, the second row compares bg2 and bg3, and the third row compares bg1 and bg3. The result shows consistency between bg1 and bg2. However, bg3 is not consistent with the other two across all detectors.

Based on the background spectra comparisons, we constructed an empirical background model using the closest data sets to the calibration data, bg1 and bg2. After testing several models, as shown for the NFC1 data in Fig. 5.17, we selected the simplest one, characterized by energy^A , to describe the rising background shape. All models include a component for Compton scattering. The chosen model closely matches the kernel density estimate. The background data exhibits characteristics similar to LEE spectra reported in other experiments with different detector materials. A recent study [73] employed a similar analytical model, characterized by $A \cdot \text{Energy}^\alpha + B \cdot \text{Energy}^\beta$, to fit the LEE in their dataset.

The double-exponential model with an additional Gaussian smearing parameter, shown in Fig. 5.17, was discarded due to strong correlations. Modeling the background with exponential components, rather than the chosen parameterization of the form energy^A , simplifies the computation to include a Gaussian resolution model. This is because the convolution of an exponential function with a Gaussian resolution model has an analytical solution.

We chose not to apply the resolution smearing to the selected background model. Introducing an additional resolution parameter would complicate the model and appear arbitrary without knowing the true shape of the background spectrum.

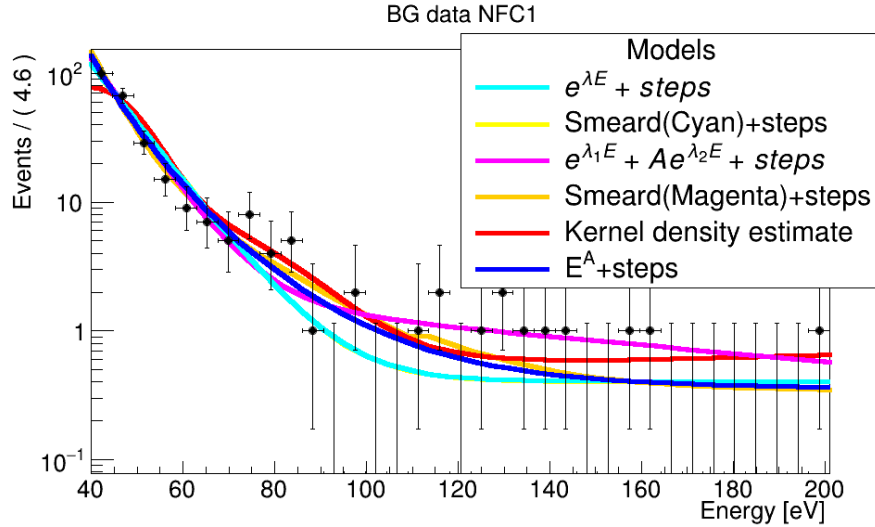


Figure 5.17: Comparison of different background models. The data points represent the NFC1 detector data, while the curves correspond to the various models tested. The selected background model, shown in blue and characterized by $\text{energy}^A + \text{steps}$, closely matches the kernel density estimate in red. Other models, including exponential and smeared versions, are shown as indicated in the legend. The x-axis shows an approximate calibration according to the 100 V data sets that is applied to the 0 V data sets.

5.2.2 Direct fit of FEFF cross section to data

The energy estimator used for L-step calibration is the pulse height (OFL). We assume that the calibration parameter maps OFL to energy following a linear relationship that is given by

$$\text{OFL} = \frac{1}{\text{calibration}} \times \text{Energy}. \quad (5.5)$$

We determine the calibration parameter by fitting the Compton cross section from FEFF simulations (Fig. 5.1) in units of energy to the data in the OFL domain. The unbinned likelihood model used for the fit includes a floating calibration parameter that stretches the Compton simulations to match the data.

The calibration parameter is subjected to several sources of uncertainty, including:

1. The size of the data set (statistical uncertainty).
2. Nuisance parameters in the likelihood model (systematic uncertainty).
3. The choice of FEFF simulation settings. We accounted for the uncertainty in modeling or ignoring the core-hole potential effects, as discussed in Sec. 3.2 (systematic uncertainty).
4. The choice of the analytical function for empirical background modeling (systematic uncertainty).

The combined statistical and systematic uncertainty from nuisance parameters can be measured by profiling the likelihood over the calibration parameter. The statistical uncertainty is dominant in this study. We only discuss the systematic uncertainty due to the FEFF simulations that are shown in Fig. 5.1. The systematic uncertainty associated with the choice of analytical function for empirical background modeling was evaluated and found to be negligible.

We were unable to identify L-steps visually due to limited data, and the presence of a strong energy-dependent background. To estimate the approximate window for Compton steps, we applied the calibration for a 100 V data set to the 0 V calibration data. This step was performed prior to a formal calibration to avoid introducing additional sophistication due to the look-elsewhere effect. For the approximate calibration, we used the location of the first e^-h^+ peak at 100 V crystal bias. This approach is valid because the coefficient mapping the TES response to energy is expected to be, to first order, independent of the crystal bias. At 100 V, the mean OFL value for the first e^-h^+ peak corresponds to approximately 100 eV energy deposition, which is close to the energy range for L-steps.

For the calibration, we used a likelihood function with two terms to model the background and calibration data simultaneously. Each term consists of the the same underlying **PDFs** following

$$\begin{aligned} \text{PDF}_k(A_{\text{OF}} | C, \sigma, d, N_k^{\text{LEE}}, N_k^{\text{Comp}}) &= \frac{N_k^{\text{Comp}}}{N_k^{\text{LEE}} + N_k^{\text{Comp}}} \cdot \text{PDF}^{\text{Comp}}(C \cdot A_{\text{OF}} | \sigma) \\ &+ \frac{N_k^{\text{LEE}}}{N_k^{\text{LEE}} + N_k^{\text{Comp}}} \cdot \text{PDF}^{\text{LEE}}(A_{\text{OF}} | d). \end{aligned} \quad (5.6)$$

where A_{OF} shows the uncalibrated energy deposition values that are measured by the detector given by the **OF** amplitude, C is a calibration constant in units of $[\text{eV}/\mu\text{A}]$ following Eqn. 5.5, σ is the Gaussian smearing width in units of eV that is applied to the Compton cross section, d is the exponent factor that determines the shape of **LEE**, and $N_k^{\text{LEE}}(N_k^{\text{Comp}})$ is the number of **LEE** (Compton) events which is different between the calibration and background data sets, as indicated by the index k . The number of **LEE** events is chosen to be independent between the calibration and background data sets because the data cleaning efficiencies and the livetimes are not the same. Note that N_k^{LEE} and N_k^{Comp} factors depend on the shape parameters as they are obtained through the integration of the Compton and background models; those dependencies are not shown explicitly to simplify the notation.

The likelihood function that models the background and calibration data simultaneously follows

$$\begin{aligned} L &= \text{Pois}(N_{\text{calib}} | N_{\text{calib}}^{\text{LEE}} + N_{\text{calib}}^{\text{Comp}}) \prod_i^{N_{\text{calib}}} \text{PDF}_{\text{calib}}(x_i | C, \sigma, d, N_{\text{calib}}^{\text{LEE}}, N_{\text{calib}}^{\text{Comp}}) \\ &\times \text{Pois}(N_{\text{bg}} | N_{\text{bg}}^{\text{LEE}} + N_{\text{bg}}^{\text{Comp}}) \prod_j^{N_{\text{bg}}} \text{PDF}_{\text{bg}}(x_j | C, \sigma, d, N_{\text{bg}}^{\text{LEE}}, N_{\text{bg}}^{\text{Comp}}), \end{aligned} \quad (5.7)$$

where N_{calib} (N_{bg}) is the observed number of events in the calibration (background) data, and x_i (x_j) goes over the pulse amplitude of the events in the calibration (background) data sets. The Poisson terms constrain the expected number of energy depositions according to the observed event counts.

The resolution parameter (σ) controls the smearing of the simulation on the true energy scale [eV]. The calibration parameter (C) introduces a stretch factor to the simulation's x-axis, transforming the domain of the smeared cross section from energy [eV] to the units of the data in OFL [μA]. The underlying assumptions for a linear stretch factor to represent the calibration are:

- The calibration is linear.
- Zero OFL [μA] corresponds to zero energy [eV].

Throughout the minimization process, each iteration adjusts the smearing factor and the stretch value to identify the best fit. We used the likelihood model described to fit a pair of background and calibration data for each detector.

We expanded the basic likelihood function described above to also include the trigger efficiency function. The trigger efficiency functions are shown in Fig. 5.18. The trigger efficiency curves are measured by applying the triggering algorithm, described in Sec. 4.4, to noise traces after injecting artificial pulses with known amplitudes. The resulting plots display the ratio of triggered events to all injected events as a function of pulse amplitude. The trigger efficiency is modeled by the function

$$f(A_{\text{OF}} | p1, p2) = \frac{1}{1 + \exp\left(-\frac{A_{\text{OF}} - p1}{p2}\right)}, \quad (5.8)$$

where $p1$ and $p2$ control the shape of the function. The result follows

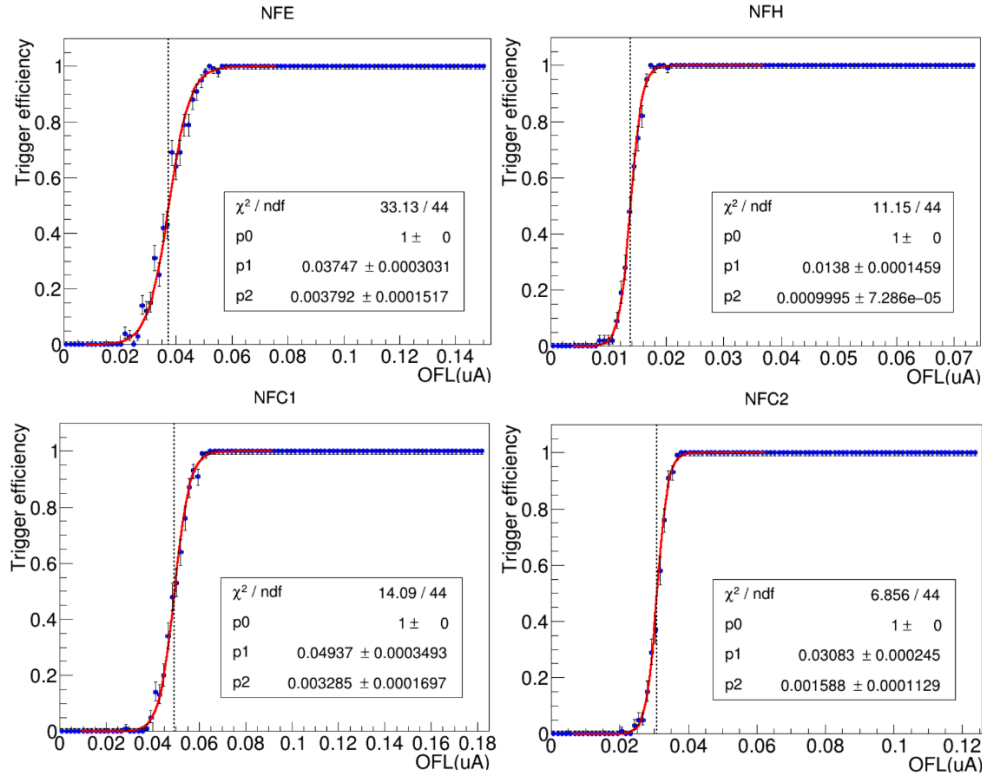


Figure 5.18: The trigger efficiency function for HVeV detectors. Courtesy of Sudipta Das.

For each detector, we multiplied the PDFs in Eqn. 5.7 by the trigger efficiency function to construct corrected PDFs. The fit parameters for the efficiency function, $p1$ and $p2$, are treated as floating parameters in the final likelihood function. However, they are constrained by a multivariate Gaussian PDF to account for the uncertainty and correlations between $p1$ and $p2$, based on the standalone modeling of the trigger efficiency (Fig. 5.18). Therefore, the final calibration likelihood function is

$$\begin{aligned}
L = & \text{Multivariate_Gaussian}(p1, p2) \\
& \times \text{Pois}(N_{\text{calib}} \mid N_{\text{calib}}^{\text{LEE}} + N_{\text{calib}}^{\text{Comp}}) \prod_i^{N_{\text{calib}}} \text{PDF}_{\text{calib}}^{\text{eff}}(x_i \mid C, \sigma, d, N_{\text{calib}}^{\text{LEE}}, N_{\text{calib}}^{\text{Comp}}, p1, p2) \\
& \times \text{Pois}(N_{\text{bg}} \mid N_{\text{bg}}^{\text{LEE}} + N_{\text{bg}}^{\text{Comp}}) \prod_j^{N_{\text{bg}}} \text{PDF}_{\text{bg}}^{\text{eff}}(x_j \mid C, \sigma, d, N_{\text{bg}}^{\text{LEE}}, N_{\text{bg}}^{\text{Comp}}, p1, p2),
\end{aligned} \tag{5.9}$$

where

$$\text{PDF}_k^{\text{eff}}(A_{\text{OF}}) = \frac{\text{PDF}_k(A_{\text{OF}}) \times \text{Efficiency}(A_{\text{OF}} \mid p1, p2)}{\int_{\text{fit range}} \text{PDF}_k(A_{\text{OF}}) \times \text{Efficiency}(A_{\text{OF}} \mid p1, p2) dA_{\text{OF}}}. \tag{5.10}$$

In addition to the calibration, we also aimed to find the FEFF spectrum that aligns more closely with the data. To achieve this, we adjusted the Compton spectrum in the fit to depend on a floating parameter, “mu”, that linearly morphs between FEFF spectra, as shown in Fig. 5.19-left. We then performed a simultaneous fit of four detectors, with the morphing parameter shared across all detectors. Finally, we profiled the likelihood over “mu” to determine the statistical and systematic uncertainties. As shown in Fig. 5.19-right, the blue curve represents the likelihood without profiling (statistical uncertainty), while the orange curve shows the profiled likelihood (total uncertainty). Even after combining the data from all four detectors “mu” has a significant uncertainty. As seen in Fig. 5.19-right, the data prefers the FEFF simulation without core-hole modeling, but is compatible with either FEFF models. That leaves us without a clear indication of which model to choose.

The fit results of the FEFF “No core-hole” spectrum to the data from various HVeV detectors according to the likelihood function in Eqn. 5.9, are shown in Fig. [5.20, 5.21, 5.22, and 5.23]. Also, the summary of the profile likelihood uncertainties for the calibration parameters is shown in Fig. 5.24.

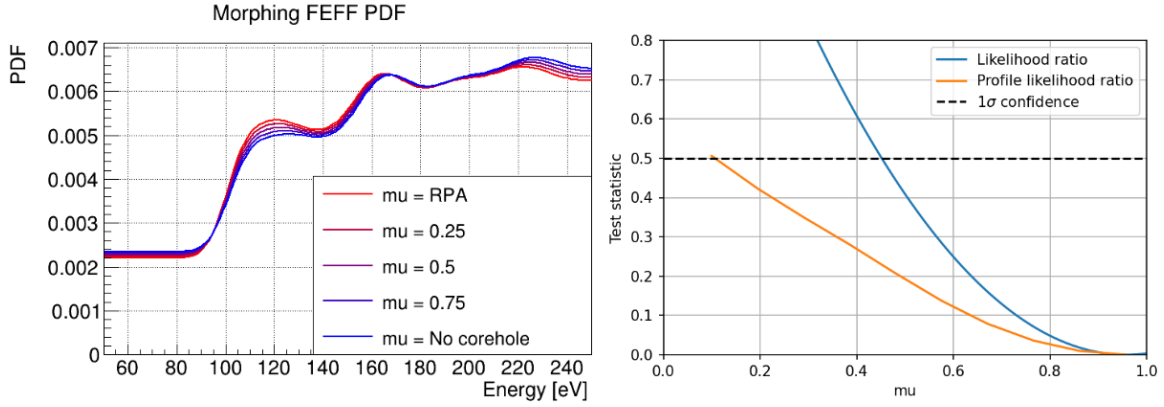


Figure 5.19: The Compton L-step model with a morphing parameter “ μ ” in the range 0 to 1. At boundaries 0(1) the PDF corresponds to the core-hole(No core-hole) PDFs. We use 4 copies of this PDF to perform a combined fit of the calibration data across 4 detectors where μ is shared between all detectors. That fit returns the likelihood (blue), and the profile-likelihood (orange) shown on the right.

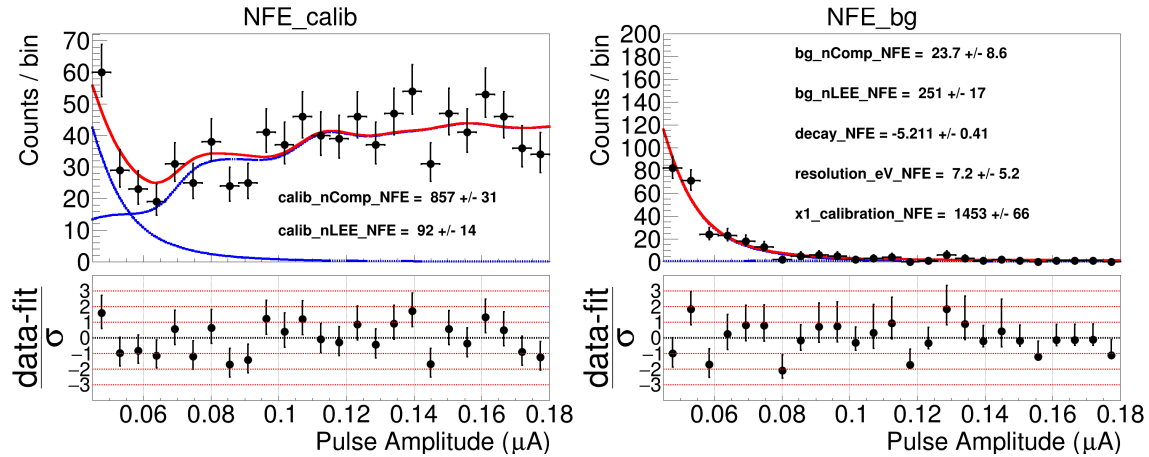


Figure 5.20: Fit of FEFF “no core-hole” cross section to the NFE data. The “x1_calibration” parameter is the calibration coefficient discussed previously; that means, multiplying OFL [μA] by x1_calibration yields Energy [eV].

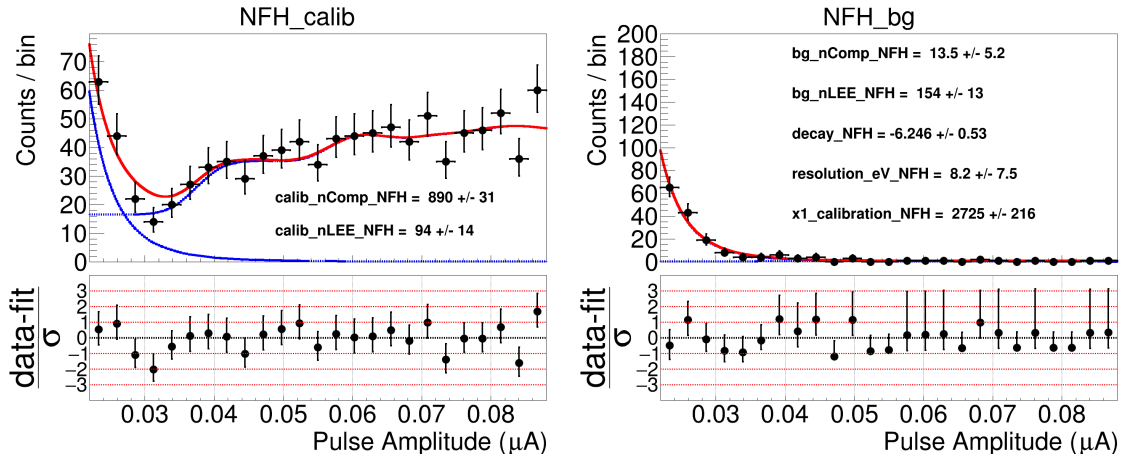


Figure 5.21: Fit of FEFF "no core-hole" cross section to the NFH data. The "x1_calibration" parameter is the calibration coefficient discussed previously; that means, multiplying OFL [μA] by x1_calibration yields Energy [eV].

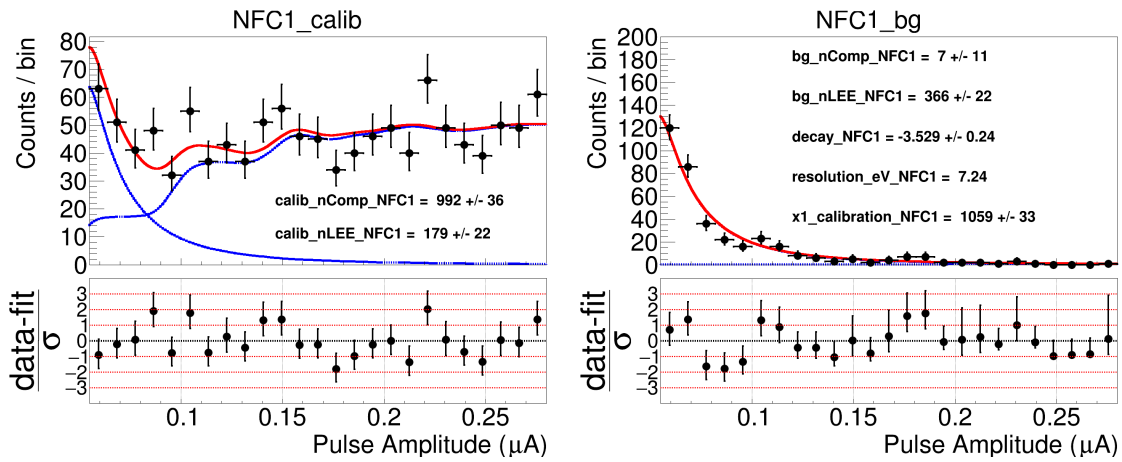


Figure 5.22: Fit of FEFF "no core-hole" cross section to the NFC1 data. The "x1_calibration" parameter is the calibration coefficient discussed previously; that means, multiplying OFL [μA] by x1_calibration yields Energy [eV].

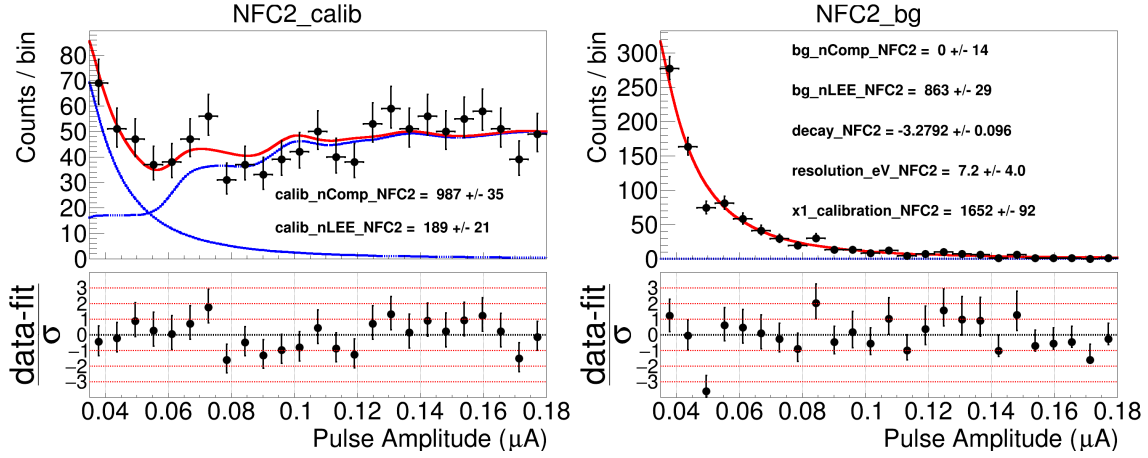


Figure 5.23: Fit of FEFF “no core-hole” cross section to the NFC2 data. The “x1_calibration” parameter is the calibration coefficient discussed previously; that means, multiplying OFL [μA] by x1_calibration yields Energy [eV].

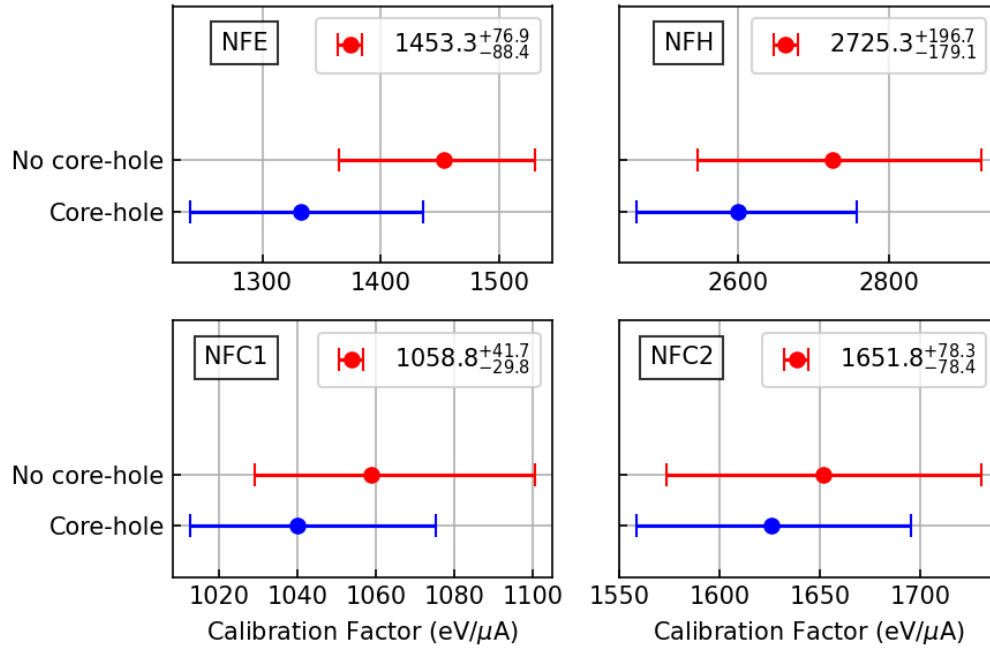


Figure 5.24: A summary of calibration parameters for the different fits with uncertainties according to profile likelihoods.

The calibration parameter values and their major uncertainties are reported in Table 5.2. A peer-reviewed paper by the DAMIC-M collaboration suggests that the “No core-hole” spectrum provides a better match to their silicon Compton step data, although they do not provide supporting evidence for this claim [49]. Our data are compatible with both FEFF cross sections, but show a slight preference for the “No core-hole” model. Consequently, we used the “No core-hole” fits for the nominal results. Given the limited evidence favoring this model, we included half of the difference between the calibration parameter values, shown in Fig. 5.24, as systematic uncertainties.

We profiled the likelihoods to determine the statistical and systematic uncertainties of the calibration parameters. The differences between the left and right 1σ uncertainties were small. Therefore, we report the larger side of the asymmetric uncertainties as an approximation in Table 5.2.

The systematic uncertainties from the choice of background function is disregarded for all detectors. Those uncertainties were found to be even smaller than those due to the choice of the FEFF cross section.

For each detector, we combined the uncertainties listed in Table 5.2 in quadrature for subsequent studies.

Table 5.2: Calibration factors in units of [eV/uA].

Detector	Calib. factor (eV/uA)	PL Unc. (Stat. $\pm$ Sys.)	FEFF Unc. (Sys.)
NFE	1453.3	76.9 (62.3, 45.1)	60.5
NFH	2725.3	196.7 (129.7, 147.9)	63.3
NFC1	1058.8	41.7 (40.4, 10.5)	9.5
NFC2	1651.8	78.3 (76.1, 18.3)	13.1

To close this subsection, we conducted Kolmogorov-Smirnov (KS) tests to evaluate the quality of the fits for the background and calibration data sets as shown in Fig. [5.25,5.26].

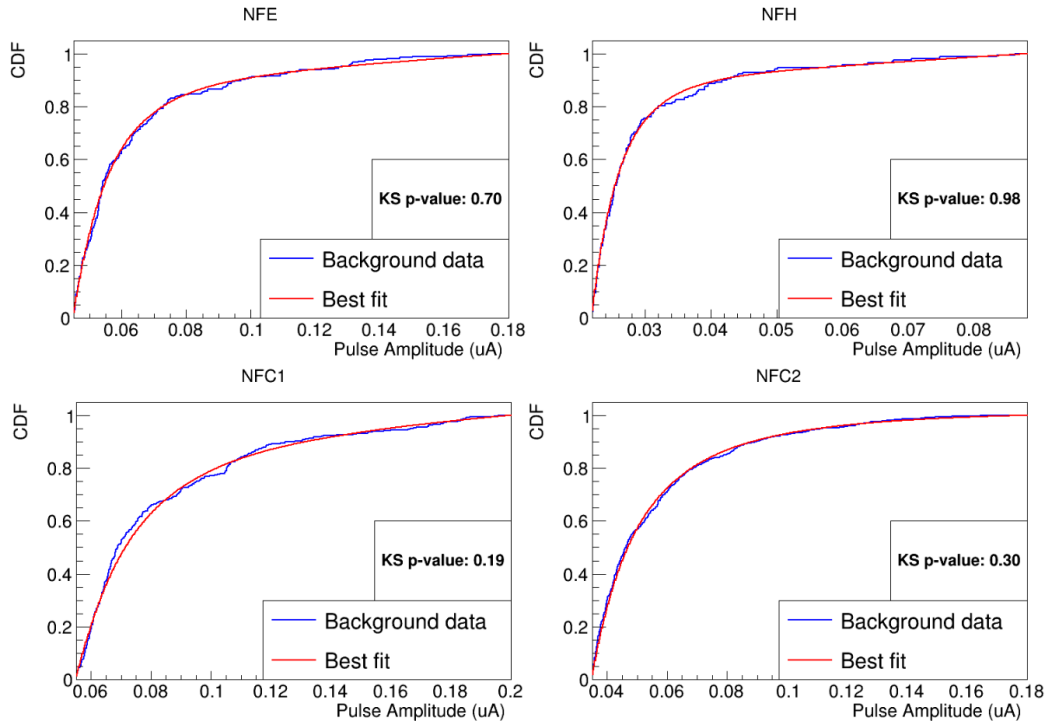


Figure 5.25: KS tests between the background data and best fits.

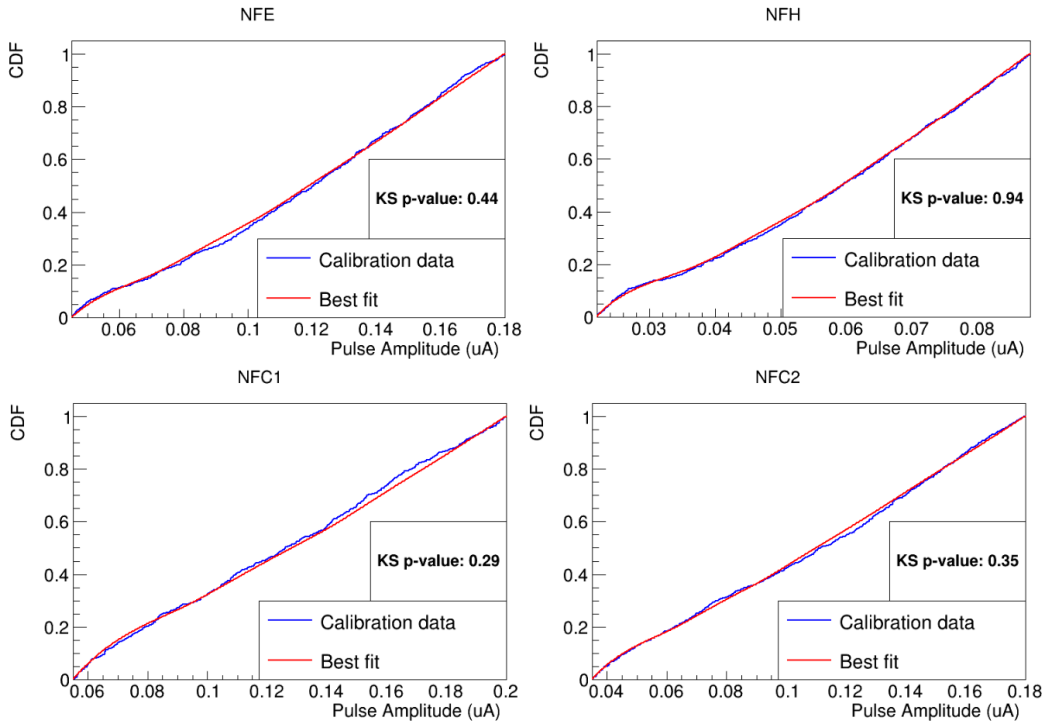


Figure 5.26: KS tests between the calibration data and best fits.

5.3 K-step and higher energy signatures at 0 V

At higher energies we did not analyze the data from NFE. This detector has the smallest volume of TES among detectors which makes it saturate faster and become less sensitive at high energy depositions as discussed in Sec. 2.1.

In addition to the L-steps, we observed the Compton K-step, a peak corresponding to the copper K_α X-ray from the detector housing, a Compton edge representing the maximum energy deposited by gamma rays in backscatters, and a photopeak when gamma rays deposit their entire energy through absorption, either immediately or after a few scatters within the same detector. These signatures are distinguishable in Fig. 4.33, except for the absorption photopeak, which requires zooming in on the plot. We were unable to distinguish the K_β peak due to smearing from the detector resolution.

We fit these signatures independently in both the simulation and the data using analytical functions. The positions of these signatures were then used to map the corresponding energies in the simulation to the energy estimator values in the experimental data. The location of the Compton K-step was identifiable in both the pulse amplitude and pulse integral energy estimators. However, we chose the pulse amplitude estimator due to its superior resolution. At higher energies, the pulse amplitude estimator lacked sufficient resolution to distinguish energy signatures. This is due to a systematic change in the pulse shape relative to the OF reconstruction template. Therefore, we could find the copper X-ray peak only in the spectra of the pulse integral energy estimator.

The positions of an energy signature in the spectrum of the Integral energy estimator is subjected to an additional systematic uncertainty due to the Integral bias correction (see subsection 4.7.1). This uncertainty was assessed for the copper peak. We generated multiple adjusted Integral spectra based on the uncertainty of the correction, and fitted each one individually to determine the distribution for the position of the copper peak. For every detector, this uncertainty was found to be an order of magnitude smaller than the fit uncertainty. Therefore, we ignored the integral correction uncertainty in the calibration.

5.3.1 Compton K-step and copper k_α peak

We modeled the Compton K-step with a **PDF** constructed from

$$f(E | x_0, \sigma, k, \text{base}) = k \left[1 + \text{erf} \left(\frac{E - x_0}{\sqrt{2}\sigma} \right) \right] / 2 + \text{base}, \quad (5.11)$$

where x_0 represents the offset of the step, σ determines the slope (or resolution), k is proportional to the height of the step, and base is proportional to the height of the pre-step region.

Moreover, we modeled the copper peak with a combination of a Gaussian **PDF** and a flat background. The modeling of the experiment data for both signatures is shown in Fig. 5.27.

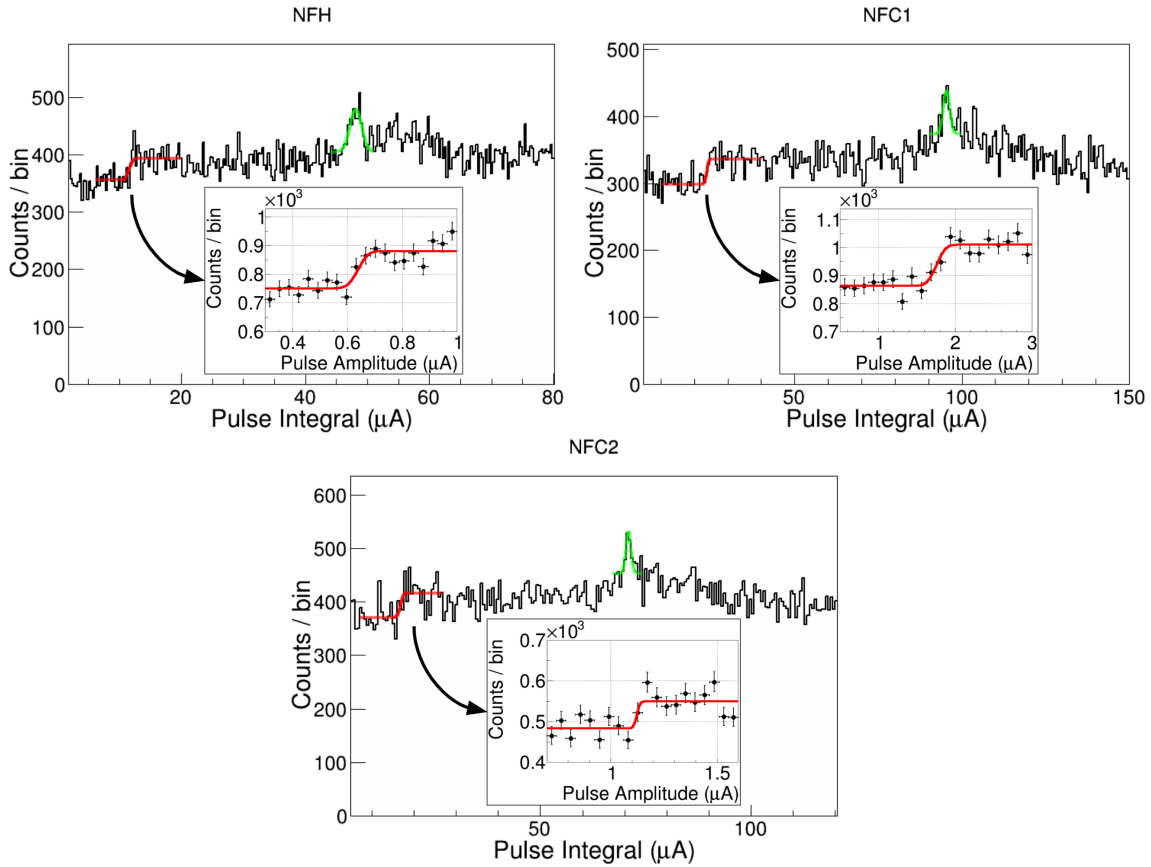


Figure 5.27: The spectra of the calibration data in the $\mathcal{O}(\text{keV})$ energy range for the NFH, NFC1, and NFC2 detectors. The inset plot shows the K-shell Compton step feature in the OFL energy estimator. Courtesy of Sudipta Das.

We fitted the Geant4 simulation using the same model applied to the data. The **HVeV** detectors have a baseline resolution of $\mathcal{O}(3)$ eV and are expected to achieve a resolution of $\mathcal{O}(2\%)$ of the measured energy at high energy depositions [25]. To

account for this, we smeared the simulation data with $r(E) = 3 + 0.02E$ where E represents the energy. We also varied the coefficient of the energy-dependent term in the resolution model to assess any systematic shift in the fit values of energy signatures. The uncertainty in positions due to the simulation smearing was small and not propagated. A smeared simulation along with the K-step and copper peak fits is shown in Fig. 5.28. The systematic uncertainty in the position of the energy signatures as a function of simulation smearing is shown in Fig. 5.29.

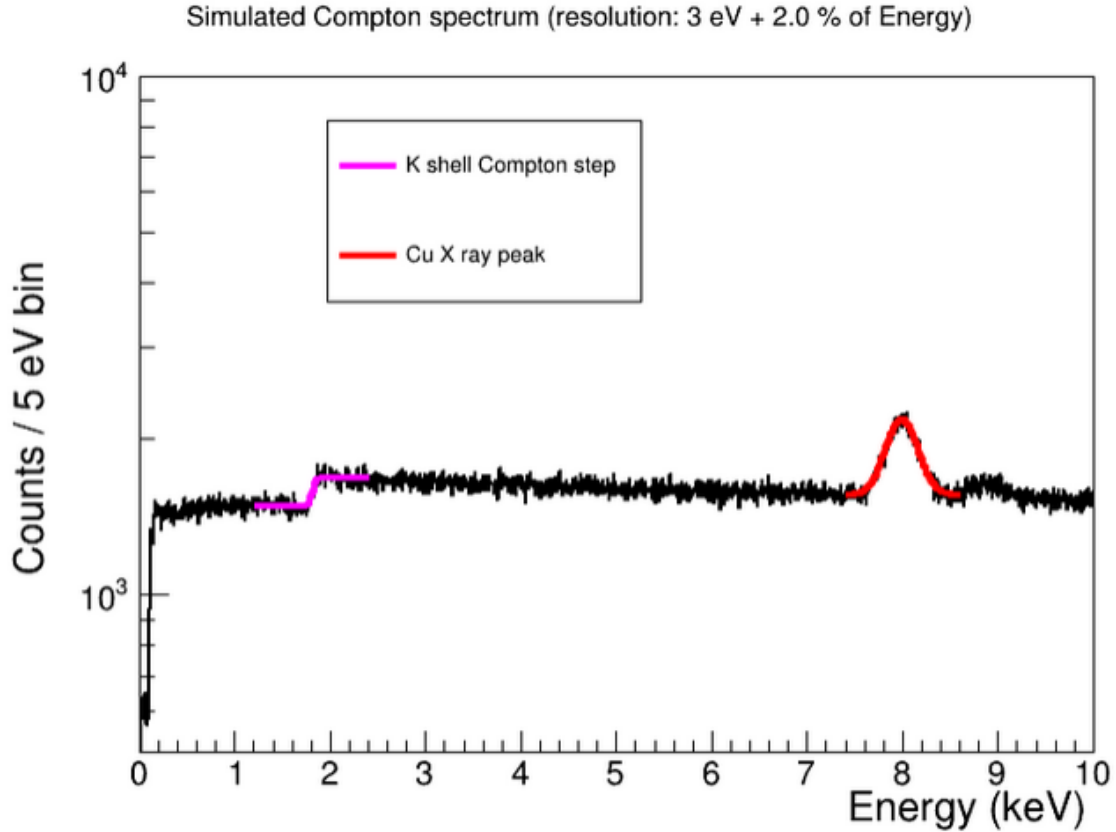


Figure 5.28: The smeared Geant4 simulation and energy signature fits. Courtesy of Sudipta Das.

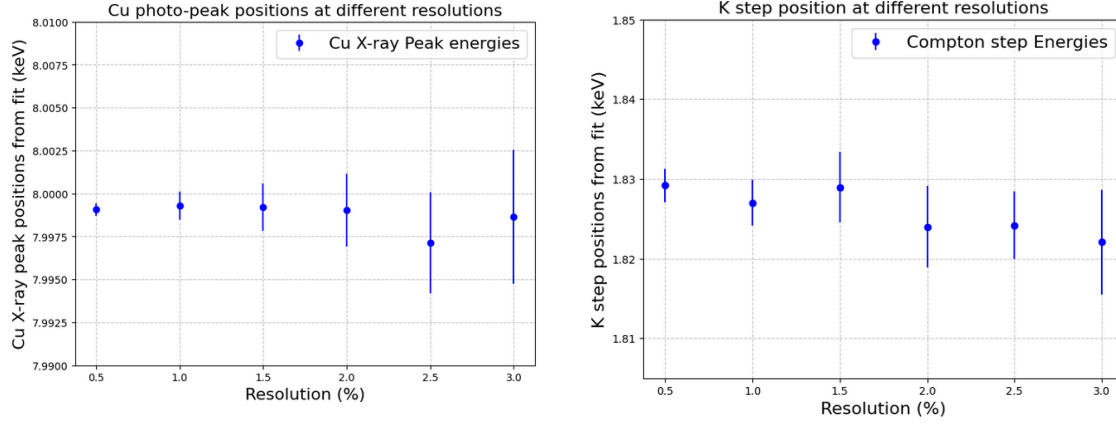


Figure 5.29: Uncertainty of the energy signature fits as a function of smearing that is applied to the simulations spectrum. The x-axis shows the linear term in the resolution function of the form $r(E) = 3 + a \cdot E$ [eV]. Courtesy of Sudipta Das.

5.3.2 Compton edge and photopeak

The position of the Compton edge and photopeak are not used in the final calibration results. However, they are used for an approximate calibration used for the pileup rate study in Sec. 5.5. The study in Sec. 5.5 is not a precision measurement; therefore, we did not investigate the systematic uncertainties in the Compton edge and photopeak fits.

The photopeak is modeled with a combination of a Gaussian function and a linear polynomial. Also, following [74], the Compton edge is modeled with a PDF that is constructed from

$$f_{\text{Compton edge}} = p_0 \cdot \text{Erfc} \left(\frac{x - p_1}{\sqrt{2} \cdot p_2} \right) + p_3 \cdot \text{Exp} \left(-\frac{(x - p_1)^2}{2 \cdot p_2^2} \right). \quad (5.12)$$

The Compton edge fits are shown in Fig. 5.30, and the photopeak fits are shown in Fig. 5.31.

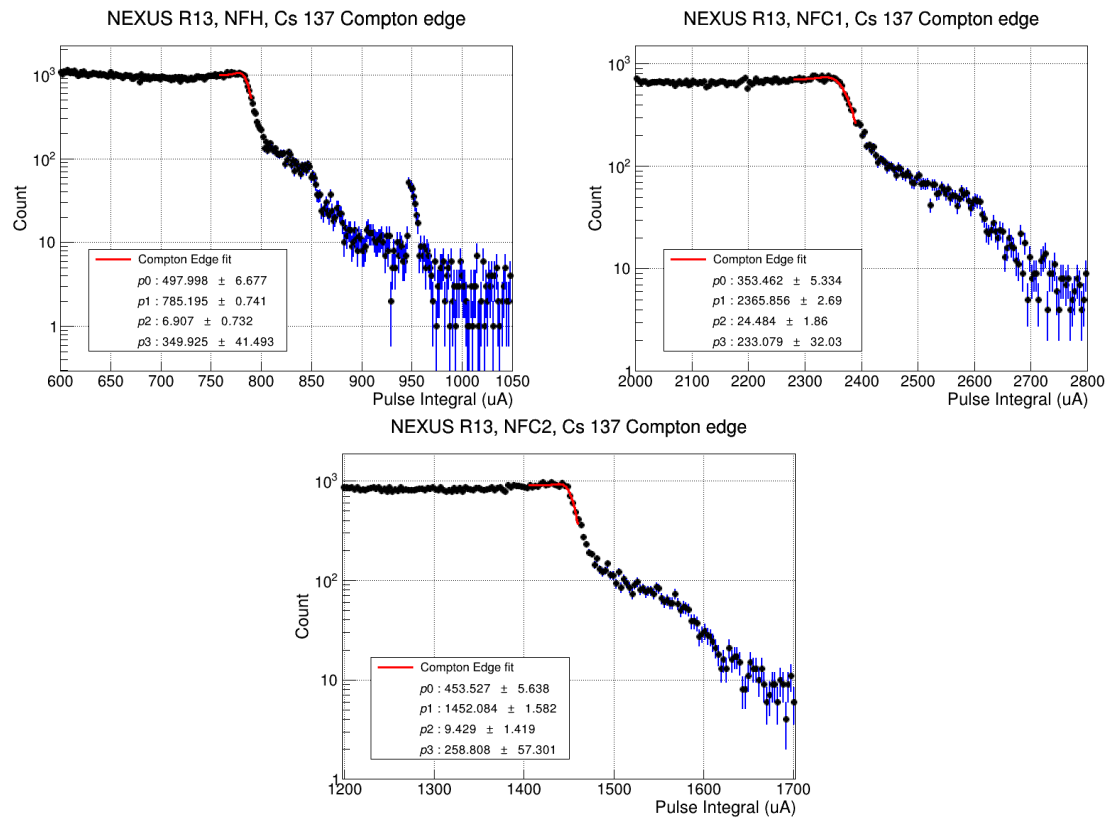


Figure 5.30: The fit of the Compton edge in the calibration data. Courtesy of Sudipta Das.

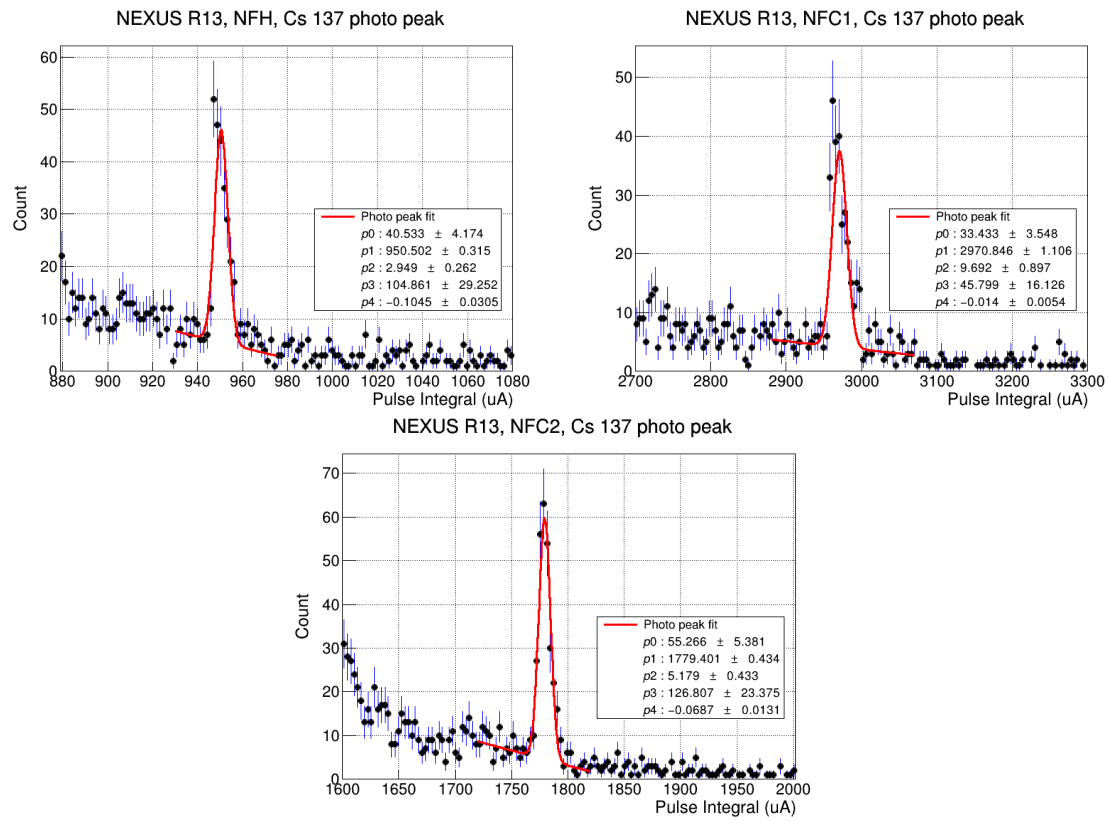


Figure 5.31: The fit of the photopeak in the calibration data. Courtesy of Sudipta Das.

5.4 Calibration function of the 0 V

The calibration coefficients derived from the L-step fits assume a linear calibration at low energies. We selected pulse amplitude values at 100 eV and 150 eV to represent the L-step positions and determined their uncertainties based on the uncertainty in the calibration coefficients. A linear function, $f(E) = a \cdot E$, constrained to pass through the origin, was fitted to these points for each detector. These linear fits provided the calibration functions up to 250 eV for the pulse Amplitude energy estimator (OF).

We converted the pulse amplitude values for both the L-steps and the K-steps into pulse integral values using the relation in Fig. 4.44. Since the uncertainties from this transformation were negligible compared to those in the amplitude values, we considered only the amplitude uncertainties. For each detector, we fitted the combined L-steps, K-step, and copper peak energy values as a function of pulse integral using a second-degree polynomial constrained to pass through the origin. These quadratic fits produced the calibration functions for the pulse integral energy estimator, valid up to 8 keV.

Following [58], the final calibration function is defined as

$$E = \begin{cases} E_{OF}, & \text{if } E_{OF} \leq 150 \text{ eV} \\ (1 - c)E_{OF} + c \cdot E_{Integral}, & \text{if } 150 < E_{OF} \leq 250 \text{ eV} \\ E_{Integral}, & \text{if } E_{OF} > 250 \text{ eV} \end{cases} \quad (5.13)$$

where E_{OF} is given by the linear calibration function at low energies, $E_{Integral}$ is given by the second-degree polynomial for the Integral, and c is an energy dependent factor that introduces a transition from the linear function to the second-degree polynomial function. The c factor is defines as

$$c = \frac{E_{OF} - 150 \text{ eV}}{100 \text{ eV}}. \quad (5.14)$$

The resulting calibration function is shown in Fig. 5.32.

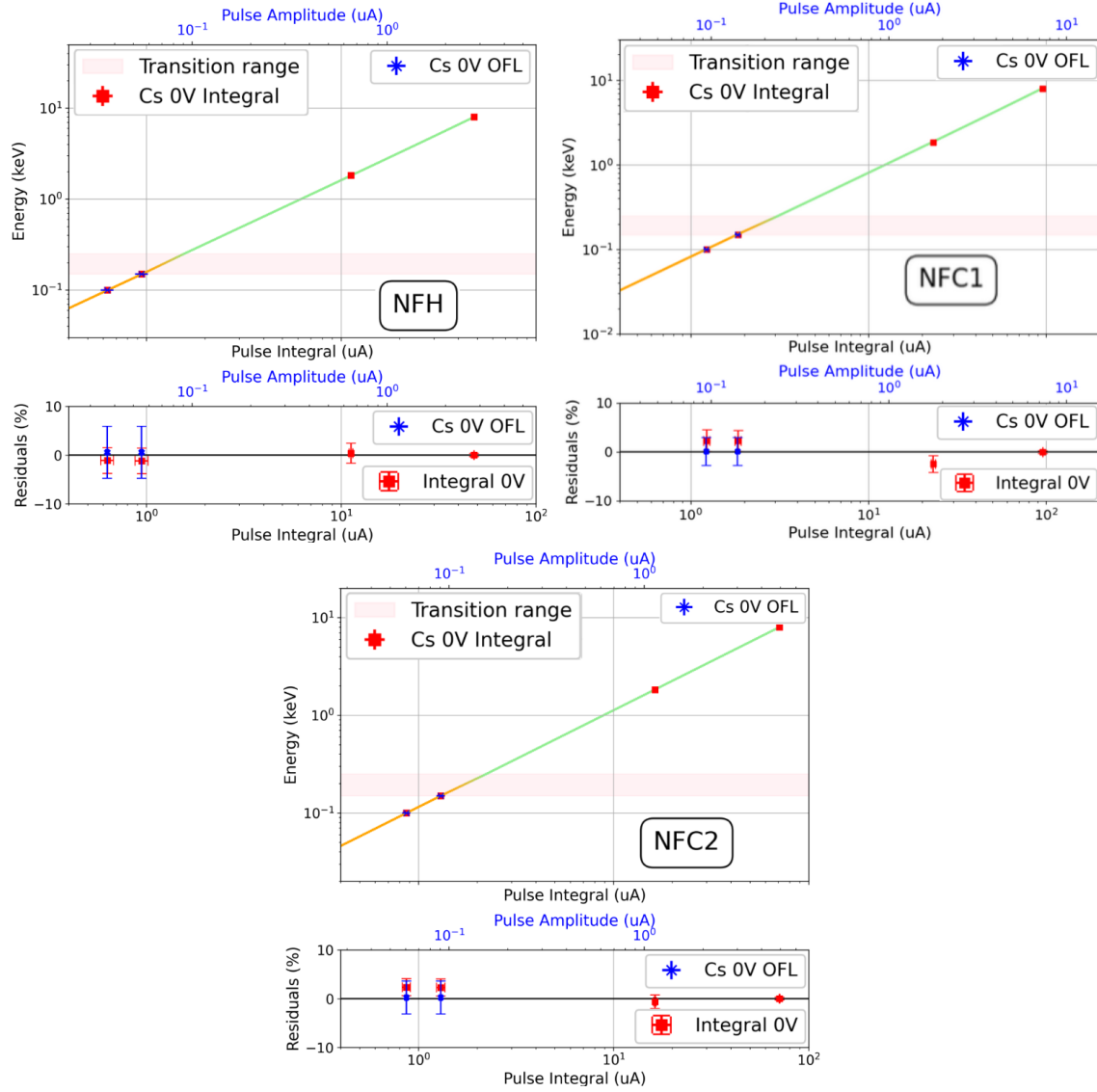


Figure 5.32: The detector calibration curves are shown according to Eqn. 5.13. The residuals represent the differences between the calibration line and the data points. The uncertainty in the residuals is calculated by measuring the difference between the upper and lower bounds of the calibration lines and data points. Courtesy of Sudipta Das.

5.5 Compton calibration at 100 V

The data sets shown in Fig. 4.9 include a subset highlighted in cyan. This data was collected in April 2022 with a 100 V crystal bias while the radioactive source was in place. The livetime of the 100 V data is comparable to the 0 V calibration data discussed in previous sections; thus, we expected to observe the Compton calibration signatures. However, no signatures were visible due to the significant fraction of data removed during the cleaning process.

We followed a data cleaning procedure similar to the description in Chapter 4. The cleaning efficiency for the 100 V data was unexpectedly low, requiring further investigation. This section discusses the issue. The analysis presented is not intended as a precision measurement, so uncertainties are not included. Furthermore, this study focuses on the NFC1 detector, with the expectation that the conclusions will be the same for the other detectors.

5.5.1 Comparison of 0 V and 100 V data sets

At the 100 V bias, the **Neganov-Trofimov-Luke (NTL)** gain boosts the energy transfer to the **TES** for ionizing recoils (subsection 2.2.2). This additional energy prolongs the time required for the **TES** to return to its equilibrium temperature compared to operating the detector at 0 V. As a result, pulses become longer which increases the probability of pulse overlaps (pileups). The processing code cannot reconstruct overlapping events; therefore, we apply cuts to remove them.

We examined patterns associated with pileups in the distribution of the OFL versus Integral energy estimators. The comparison plots for the 0 V and 100 V data sets are shown in Fig. [5.33,5.34]. In each figure, the left plot shows the distribution before the data cleaning, and the right plot shows the distribution after the data cleaning.

The 0 V plots shows a prominent band both before and after data cleaning. However, the pattern is different at 100 V; many events are shifted to regions above the primary band, the band that persists even after the data cleaning. At 100 V, a few randomly selected events from the structures above the primary band consistently showed portions of adjacent pulses within the reconstruction window of the selected events.

These observations indicated a high pileup rate at 100 V. For future studies, estimating the pileup rate before planning a calibration run would be beneficial. Therefore, we aimed to understand and quantify the pileup rate.

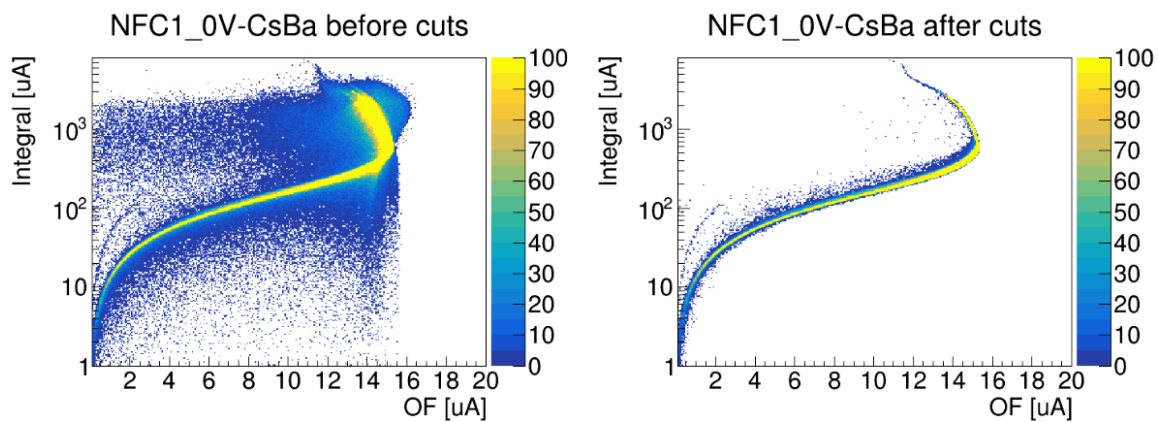


Figure 5.33: Two dimensional distribution of OFL versus Integral for the 0 V data set.

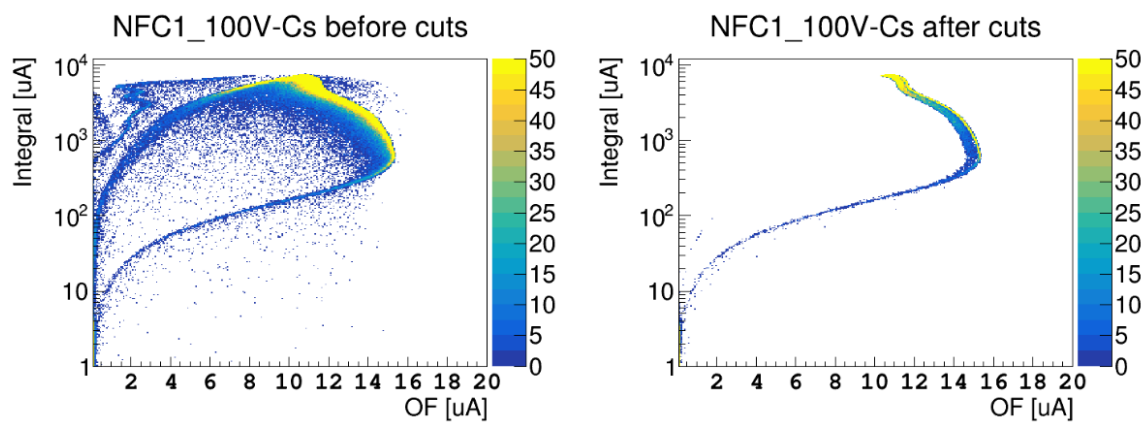


Figure 5.34: Two dimensional distribution of OFL versus Integral for the 100 V data set.

5.5.2 Time gap distribution of adjacent events

The Poission probability is given by

$$P(N|\lambda) = \frac{e^{-\lambda t}(\lambda t)^N}{N!}, \quad (5.15)$$

where N is the number of energy depositions in the detector in a time window t , and λ is the event rate. For uncorrelated energy deposition in the detector, $\lambda = \sum_{i=1}^m \lambda_i$, where m goes over various sources for the events. We will continue assuming that energy depositions in our detectors are not correlated in time. Indicated by Eqn. 5.15, the probability of seeing no event in a time window t is given by

$$P(0|\lambda) = e^{-\lambda t}. \quad (5.16)$$

And the PDF of having no event in a time window t is

$$\begin{aligned} \text{Norm} : \int_0^\infty e^{-\lambda t} dt &= \frac{1}{\lambda}, \\ \text{PDF} : \lambda e^{-\lambda t}. \end{aligned} \quad (5.17)$$

The relation shows the correspondence between the Poisson distribution of particles hitting the detector, and the exponential distribution of the time gaps between consecutive events.

5.5.3 No-pileup probability

The goal is to determine the probability of standalone events, those that do not overlap with others. We refer to this as the no-pileup probability.

For each triggered event, pileup can occur due to either a preceding or a subsequent event. The triggered event is be pileup free in the front, if the trigger point of the subsequent event falls outside of the reconstruction window. For the back pileup, merely checking the trigger point of the adjacent events is not sufficient. The pileup may still occur if a prolonged pulse from a second preceding event extends all the way into the reconstruction window of the triggered event. The preceding and subsequent pileup scenarios are illustrated previously in Fig. 4.19.

We can derive an analytical function for the no-pileup probability. As a first approximation, we determine the probability that **adjacent** events do not overlap. A derivation for this probability is given in Appendix C. A shorter reasoning that leads

to the same probability follows:

1. Randomly choose 1 event.
2. The probability for the random event to have an energy E_1 is $p(E_1) = \phi(E_1) dE$, where $\phi(E)$ is **PDF** for the energy distribution of events.
3. The probability of having no pileup in the front of the chosen event is $p(\text{Gap} > T_1) = \int_{T_1}^{\infty} \lambda e^{-\lambda t} dt$, where Gap is the time difference between the chosen and the subsequent events, T_1 is the length of the chosen event with energy E_1 , and the integral is over the distribution of time gaps according to Eqn. 5.17.
4. So, the total probability of selecting a random event with no pileup in the front is $\sum_i \phi(E_i) \Delta E \int_{T_i}^{\infty} \lambda e^{-\lambda t} dt$, where T_i is the time length of the events as a function of energy. In the continuous limit, we can define a pulse length profile following $f(E_i) = T_i$. Therefore, the no-pileup probability reduces to $\int_{E_0}^{E_1} \phi(E) e^{-\lambda f(E)} dE$, where E_0 and E_1 are the minimum and maximum pulse energies.
5. The front and back no-pileup probabilities are independent. Also, it is simple to show that the back no-pileup probability, when we only consider the immediate events, follows the same equation that we found for the front. Therefore, the total no-pileup probability is

$$P(\text{no-pileup}) = \left[\int_{E_0}^{E_1} \phi(E) e^{-\lambda f(E)} dE \right]^2, \quad (5.18)$$

and the effective rate for the no-pileup events follows

$$R = \lambda \left[\int_{E_0}^{E_1} \phi(E) e^{-\lambda f(E)} dE \right]^2, \quad (5.19)$$

which is the same as Eqn. C.7.

The derivation here fully accounts for the front no-pileup probability, but it approximates the back no-pileup probability as it only considers the immediate preceding event. In practice, we expect this first-order approximation to be accurate for a small population of prolonged pulses. We will validate this expectation with the help of **Monte Carlo (MC)** simulations. The simulation also goes beyond the first order approximation and accounts for any pileup from the back.

As indicated by Eqn. 5.18, the no-pileup probability depends on three components:

1. The probability density function (**PDF**) of energy depositions, $\phi(E)$.
2. The total rate of events hitting the detector.
3. The detector pulse length profile, $f(E)$.

An approximation of the first item can be obtained from Geant4 simulations. The second item can be estimated either from simulations or the processed data. Determining the pulse length profile as a function of energy ($f(E)$) is not straightforward. Although there are approximate analytical models for the detector pulse shapes, which is described in various sources such as [30], these approximations are only valid for low-energy depositions where the **TES** response remains linear. We employed a data-driven method to determine $f(E)$ at all energies.

5.5.4 Pulse length profile

There are various methods to construct pulse templates. One approach is to select high-quality pulses at a specific energy, and average them to create the template. It would be ideal to construct pulse templates at different energies, and measure their lengths to determine $f(E)$. However, that is not practical for the calibration data set with a 100 V crystal bias. At 100 V, high-energy Compton scattering pulses are boosted to energies beyond the known calibration range. Additionally, the tails of high-energy events extend far beyond the reconstruction window, which is optimized for low-energy events. As a result, we cannot determine the energies of high-energy pulses, nor can we fully reconstruct them or apply standard quality checks to identify good pulses for the template construction.

First, we start with the 0 V calibration data. The pulse integral and amplitude distribution in Fig. 5.33 indicate that most events are concentrated in the main cluster with minimal or no pileup. Therefore, we can leverage the observation to construct pulse templates at various energies following:

1. Apply an approximate calibration to the data. Note that we have high-energy calibration signatures from the ^{137}Cs source up to approximately 662 keV (subsection 5.3.2).
2. Select narrow energy windows at various energies, and identify pulses that fall within these windows.

3. Generate 2D-histograms for each energy window with the x-axis representing the length of a pulse, y-axis representing the height of a pulse, and z-axis (color bar) representing the count in each cell.
4. For pulses falling within each energy window, align them by their trigger points, subtract their baselines, and put them in the corresponding 2D-histograms.
5. Pulses pass through some cells in the 2D-histograms. Increment the value of these cells by one.
6. Identify the most populated cells in the 2D-histograms. These cells provide the pulse template at the corresponding energy.

The described algorithm does not rely on data cleaning to extract the average pulse shapes at various energies. Additionally, it is expected to be robust against anomalies, provided that the dominant population of pulses are of good quality.

The approximate calibration function for detector NFC1 that is used to group pulses is shown in Fig. 5.35. It is a second-degree polynomial that goes through the origin.

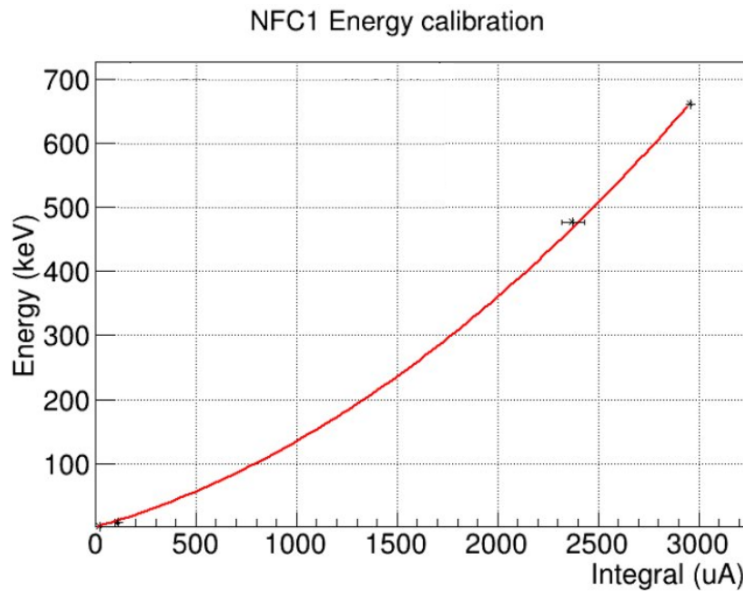


Figure 5.35: An approximate high-energy calibration function for detector NFC1. This function uses the positions of the Compton k-step at ~ 1.8 keV, and the ^{137}Cs Compton edge and photopeak at ~ 477 keV and ~ 662 keV, respectively. Courtesy of Sudipta Das.

A sample histogram of raw pulses at approximately 669 keV is presented in Fig. 5.36-top. The red line shows the most populated bins. Pileup events, which

appear in the center of the histogram, are adjacent to the selected events within this energy window. Selecting the most populated cells effectively rejects the pileup events. In the bottom panel, two additional templates extracted at lower energies are displayed.

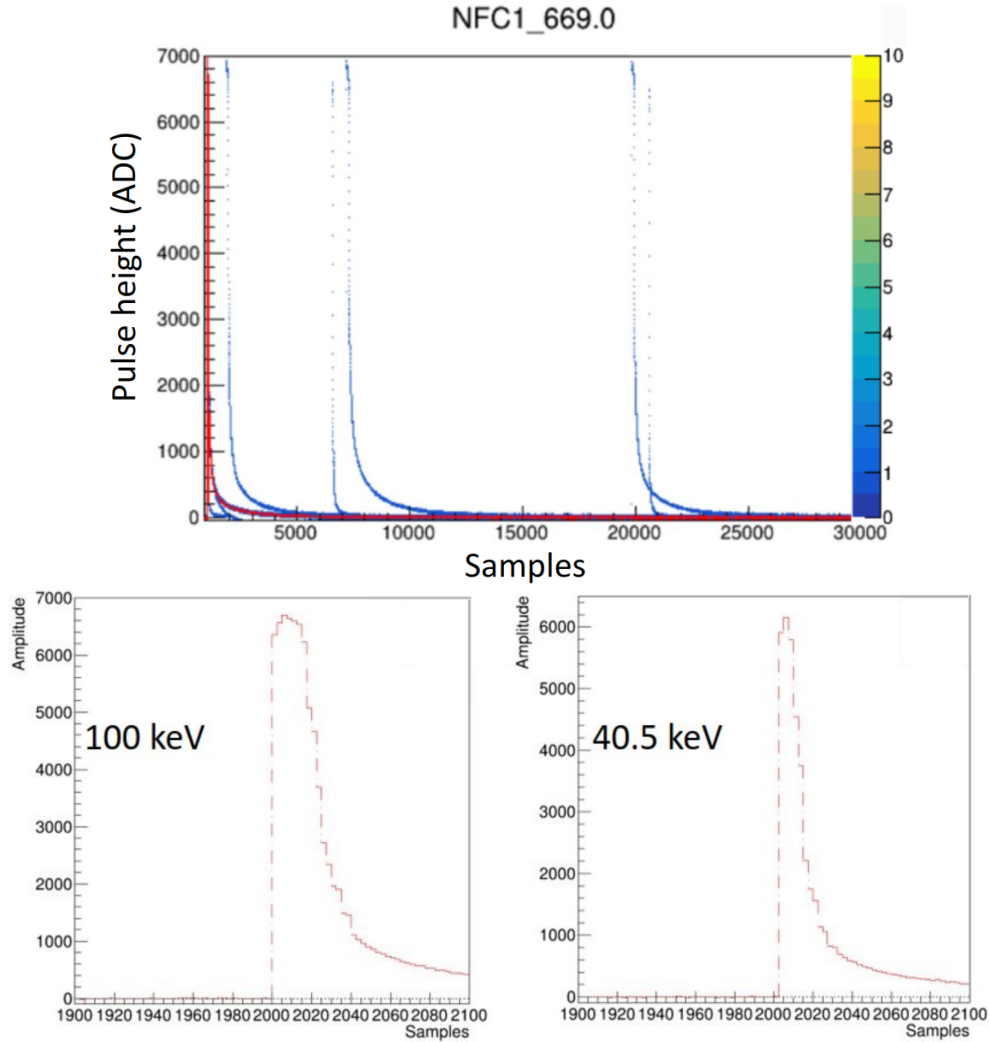


Figure 5.36: Histograms of the raw data traces and extracted pulse templates at various energies. In all plots, the y-axis shows the digitized pulse amplitude from the detector readout, and the x-axis shows the time samples (1 sample = $6.4 \mu\text{s}$). Top: Pulses within 0.5 keV around ~ 669 keV are accumulated in the histogram. The red line represents the most populated cells, serving as the pulse template at this energy. Bottom: Two additional zoomed-in templates are shown. At 100 keV, the TES response becomes highly non-linear, as indicated by the flat-top pulse.

We measured the template lengths at various energies to develop the pulse length profile. To determine the template endpoint, we scanned the pulse tail from left to right and identified the first window where the variance dropped below the variance observed before the rising edge. The first sample within this window was chosen as the pulse endpoint. The starting point of the template was set at the event trigger. This method is illustrated in Fig. 5.37.

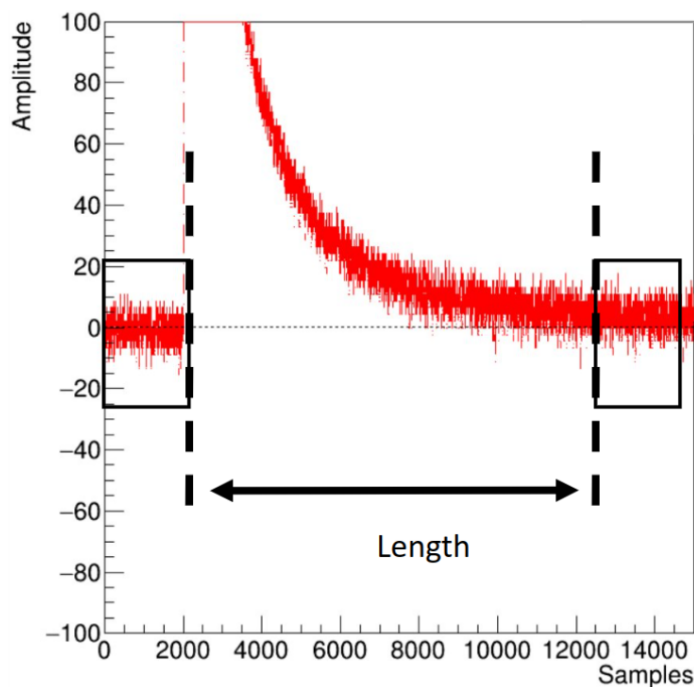


Figure 5.37: Illustration of the pulse length measurement using the extracted template as shown in Fig. 5.36. On the x-axis (1 sample = $6.4 \mu\text{s}$).

Finally, we modeled the pulse length profile using an analytical function, as shown in Fig. 5.38. Subsequent checks showed that some 2D-histograms lacked a sufficient number of pulses to construct robust templates, resulting in length measurements that deviated from the trend. Due to the number of bins in the 2D-histograms, and the computational cost required to improve these measurements, we chose not to refine the templates further. Instead, we manually excluded points that deviated from the trend. It is important to note that:

1. Including any of the rejected length measurements above the cut line would shift the profile upward, thereby reducing the no-pileup probability. Even with the optimistic assumption that we used, the cleaning efficiency for the 100 V calibration data remains very low, suggesting that including the rejected length measurements would not alter the conclusion.

2. We observed a trend with a constant slope above the threshold of approximately 50 keV to 100 keV. In this energy range, the template also develops a flat-top shape (see Fig. 5.36-bottom), indicating the saturation of the TES. The TES saturation happens when it gets too close to the normal state resistance due to an excessive heat. The constant slope trend informed the choice of the model (Fig. 5.38), which features an asymptotic constant slope.
3. The asymptotic constant slope allows us to use the same pulse length template for the 100 V data set. Although energy depositions are boosted at high voltage, this should not affect the pulse length profile function.

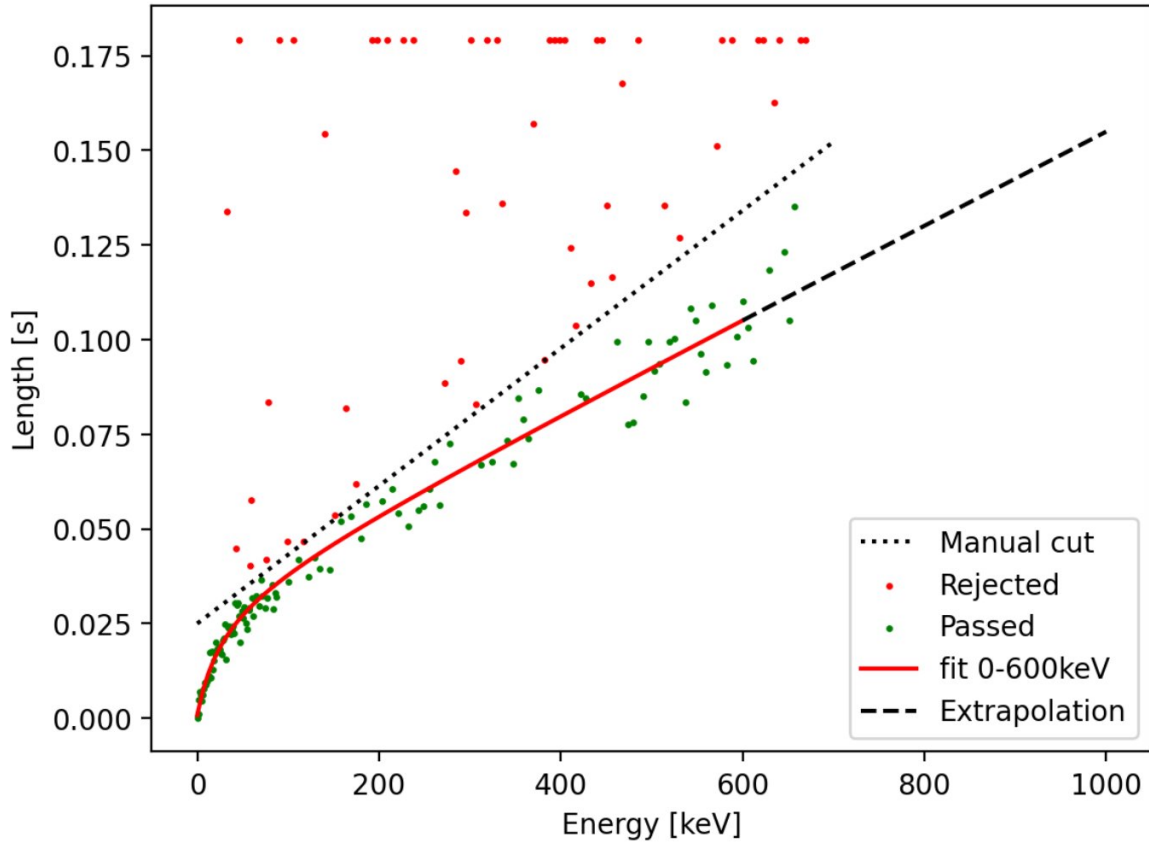


Figure 5.38: Pulse length profile. An analytical function, $f(x, a, b, c) = ax/(x+b)+cx$, is fitted to data over the energy range from 100 eV to 600 keV. Further details regarding the cut and the rejected points are discussed in the main text.

5.5.5 Pileup probability numerical modeling

Two **Monte Carlo (MC)** algorithms were employed to numerically model the no-pileup probability. The first algorithm performs the calculation with an adjustable precision regarding the number of prior events considered to identify pileups (refer to Fig. 4.19). The second algorithm finds the no-pileup probability with the full precision.

Both algorithms handle the front-pileup probability with a full precision. The criterion for detecting front pileup is that no additional trigger should occur within the post-trigger processing window. For instance, overlapping events are accepted as long as the subsequent event falls outside the reconstruction window of the triggered event. For this criterion, the pulse length profile for the front pileup was replaced with a constant value equal to half the size of the processing window in Eqn. 5.18. For the back-pileup, any event with the tail of a preceding pulse falling in its reconstruction window is considered a pileup event. To implement this, half the size of the processing window was added to the pulse length profile (remember that the pulse length starts from the rising edge in the length profile). In both cases, the treatment of the processing window for front- and back-pileup probabilities assumes the trigger point is centered within the processing window.

We used the adjusted pulse length profiles in Eqn. C.6. Subsequently, the individual terms for the front- and back-pileup probabilities were multiplied to obtain the total no-pileup probability.

For the **MC** simulations, we selected a time span of 1000 seconds and populated it with events based on the energy distribution from the Geant4 simulation. For each event, we assigned a pulse length according to Fig. 5.38. We then calculated the ratio of no-pileup pulses. This process was repeated 1000 times to obtain a distribution for the ratio.

For an event rate of 15 Hz and 0 V crystal bias the result of **MC** studies is summarized in Fig. 5.39.

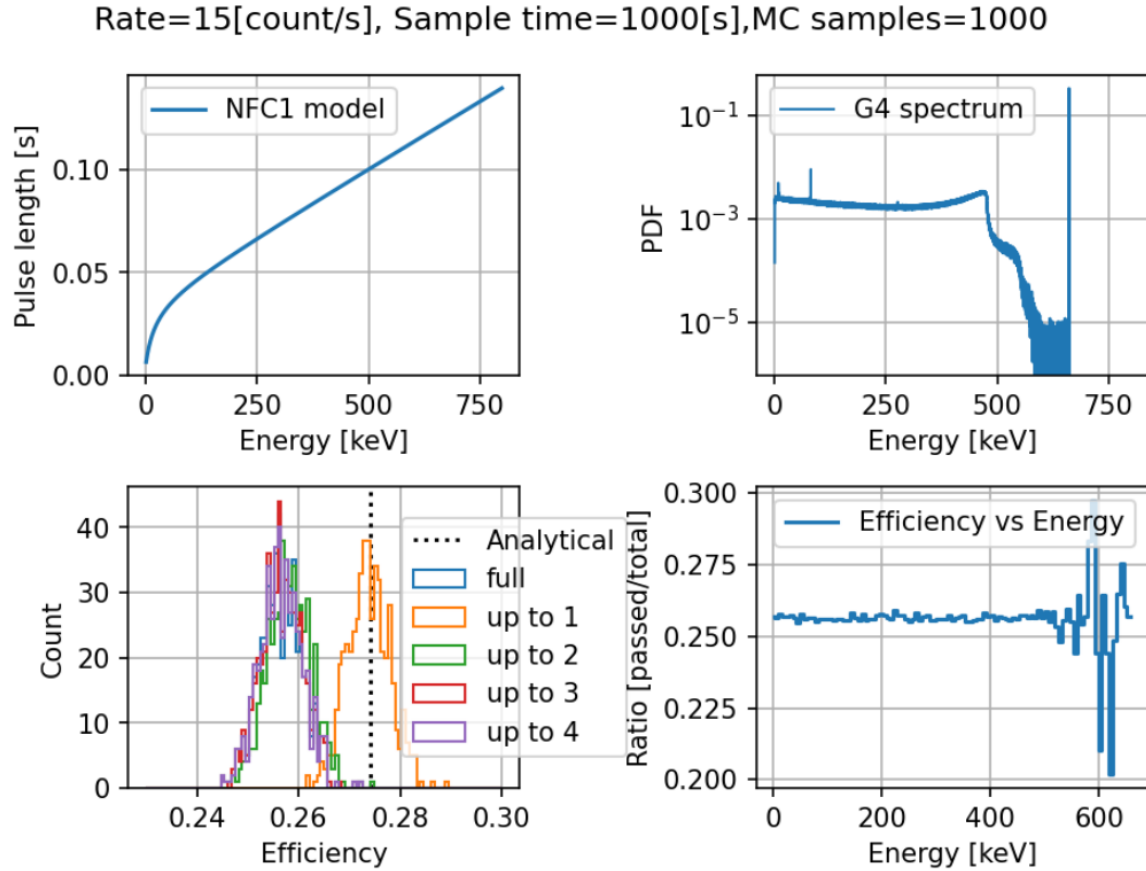


Figure 5.39: Top left: Pulse length profile. Top right: Geant4 simulation spectrum. Bottom left: The x-axis represents the no-pileup probability. The dashed line is calculated using the analytical function in Eqn. C.6. The blue distribution shows the no-pileup ratio distribution from the MC simulation that considers all orders of pileups from the back. The other colors represent the no-pileup probability when only a limited number of preceding events are checked for pileups. The agreement between the analytical model and the orange distribution serves as a cross-check. Bottom right: The no-pileup probability according to the full MC simulations as a function of energy. This plot demonstrates that the quality cuts used to remove pileups do not introduce an energy-dependent efficiency.

After the preliminary MC simulation, we scan the efficiency for various event rates between 1 Hz and 30 Hz for a crystal bias of 0 V as shown in Fig. 5.40.

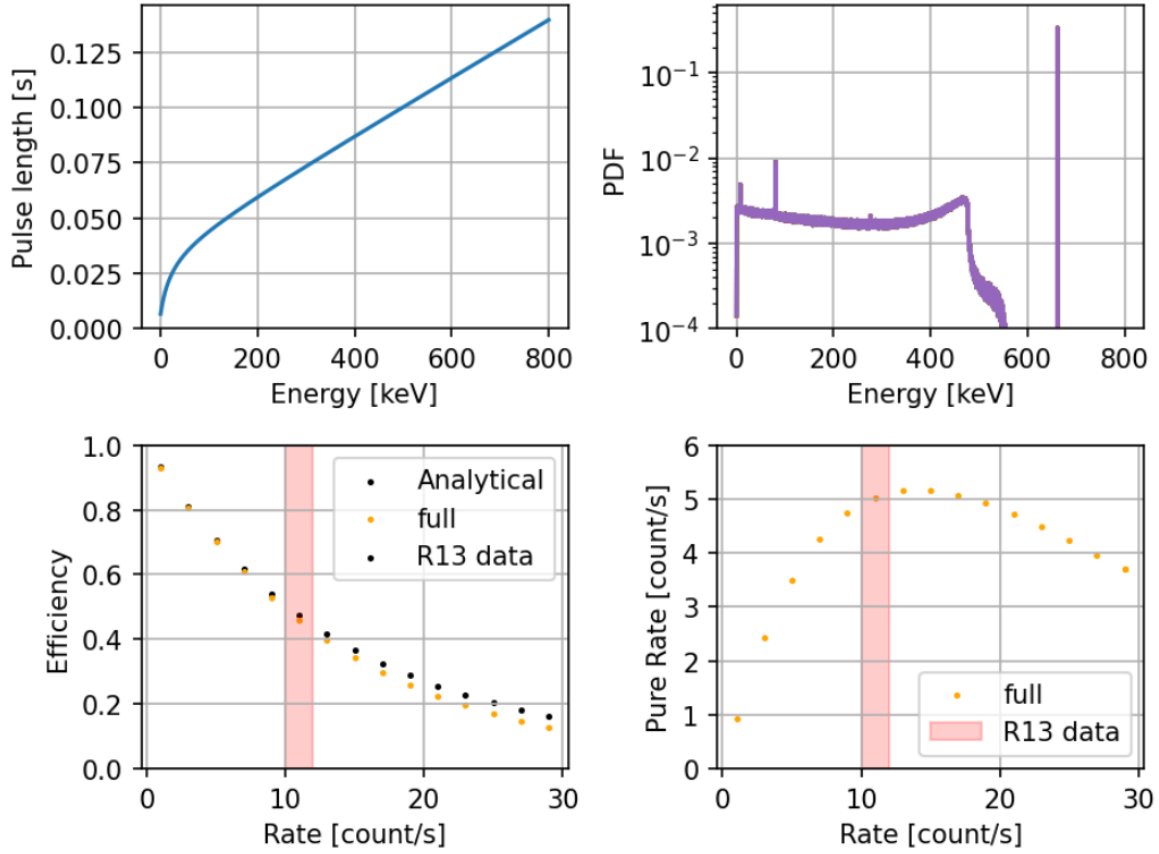


Figure 5.40: Top left: Pulse length profile. Top right: Geant4 simulation spectrum. Bottom left: No-pileup efficiency as a function of event rate. The black and orange dots represent the efficiency calculated using the analytical function and the full MC simulations, respectively. The shaded red area indicates the estimated event rate for the NFC1 detector in the experimental data. Bottom right: Effective event rate, defined as the product of the event rate and efficiency, plotted against the event rate. The shaded red area indicates that the data collection was conducted near the optimal event rate.

Finally, we conducted an event rate scan for the 100 V data as shown in Fig. 5.41. In the Geant4 simulations, energy depositions were scaled according to NTL gain. We did not consider the discrete nature of e^-h^+ pair production. The experiment data shows an excess of events around the first e^-h^+ peak at 100 eV. We modeled this by adding a Gaussian peak to the Geant4 spectrum, adjusting its amplitude to achieve a qualitative match with the experimental data. The no-pileup efficiency did not change significantly by changing the amplitude in the vicinity of the chosen value.

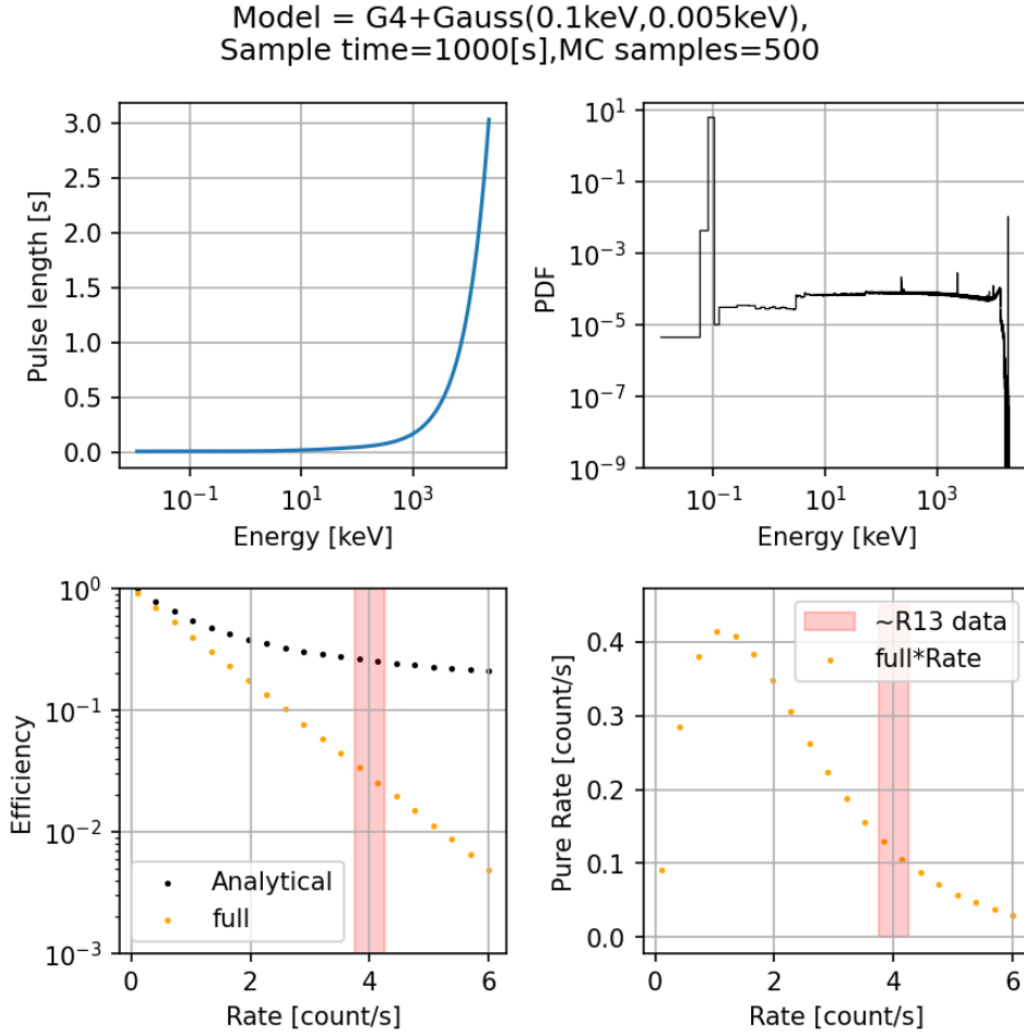


Figure 5.41: Top left: Pulse length profile. Top right: Geant4 simulation spectrum. Bottom left: No-pileup efficiency as a function of event rate. The black and orange dots represent the efficiency calculated using the analytical function and the full MC simulations, respectively. The shaded red area indicates the estimated event rate for the NFC1 detector in the experimental data. Bottom right: Effective event rate, defined as the product of the event rate and efficiency, plotted against the event rate. The shaded red area indicates that the data collection was away from the optimal event rate.

5.6 Summary

This chapter outlines the statistical methods used to identify the locations of calibration energy signatures, primarily focusing on Compton steps in silicon. This chapter also describes the development of a calibration function based on these signatures. The calibration procedure is applied to the 0 V data sets from four **HVeV** detectors. Additionally, this chapter introduces a method to estimate the fraction of overlapping events in a data set as a function of energy deposition rate and distribution, and the detector response time to energy depositions (pulse length profile).

The data sets in the calibration study are relatively small, containing approximately 4000 Compton scatter events below 500 eV, making it challenging to distinguish the L-steps (achieve converging L-step fits). From the experience gained in validating the results presented in subsection 5.1, constraining the detector resolution in L-step fits can improve the convergence of the fits and reduce the calibration uncertainty. Based on the results shown in Fig. 5.12, I recommend targeting 20,000 Compton scattering events below 500 eV in future calibration studies, rather than the current 4,000 events.

A major challenge in modeling the L-steps was accounting for the background spectrum. One approach was to subtract the background from the calibration data. That requires consistent calibration and background spectra, weighted by their live-times and data cleaning efficiencies. The simultaneous fit function introduced in this chapter relies solely on the shape of the Compton cross section and **LEE** models, thereby avoiding the need for a direct background subtraction from the calibration spectrum. This approach significantly simplifies the analysis.

The likelihood fit for the L-steps assumes consistency in the shape of the **LEE** spectra between the calibration and background data sets but makes no assumptions about the number of **LEE** events across the data sets. The **LEE** events pose a significant background for low-mass dark matter searches with cryogenic crystal calorimeters, and their underlying physics is not well understood. In a follow-up study, it would be interesting to compare the shape and event count of **LEE** events in the presence and absence of a radioactive source.

In addition to the comparison of the **LEE** with and without the radioactive source, a future study can compare the **LEE** spectra across different **HVeV** detector designs. One hypothesis suggests that the relaxation of thermally induced stress between the crystal and contacting objects may trigger the **LEE** [75]. Based on this, it could be argued that **QETs** in contact with the crystal may also contribute to the **LEE**. We

observed that the shape of the **LEE** in NFH decreases more rapidly than in NFE, despite more **QET** coverage in the NFH. A summary of the **LEE** shape measurements is provided in Table 5.3, and the corresponding fits are shown in Figs. [5.20, 5.21, 5.22, 5.23].

Detector	QET aluminum coverage (mm) ²	Exponent
NFC2	31.8	-3.28 ± 0.10
NFC1	31.8	-3.53 ± 0.24
NFH	21.6	-6.25 ± 0.53
NFE	8.5	-5.21 ± 0.41

Table 5.3: Measurements for the exponent of the background models across different **HVeV** detectors. The model follows is $E^{-\text{Exponent}}$

The no-pileup probability, discussed in Sec. 5.5, offers a framework for estimating the data cleaning efficiency in future calibration runs. In this study, we used a Cs source with primary gammas of approximately 662 keV energy. Utilizing a gamma source with lower-energy photons could enhance data cleaning efficiency, as shorter pulse durations (from lower energy depositions) lead to fewer pileups. However, a competing factor is the probability of gammas passing through intermediate materials between the radioactive source and the detectors, as lower energy gammas generally have a reduced mean free path in materials. As outlined in Sec. 5.5, a combination of Geant4 simulations and approximate detector response modeling should provide guidance on optimal source placement relative to the detectors, which controls the Compton events rate, to maximize the data cleaning efficiency.

We successfully calibrated the Compton data with a 0 V crystal bias. However, the 100 V calibration data after the cleaning stage was found to be insufficient to see the Compton energy signatures. The **NTL** gain at 100 V extended pulse durations, leading to a high pileup rate, which in turn caused many events to be rejected. This issue can be prevented in future studies with greater attention to pileup rate.

At this stage, the Compton calibration scheme is fully developed. In the next chapter, we calibrate the **HVeV** detectors at a 150 V crystal bias using a well-established calibration scheme with optical photons (2 eV) from LEDs. We also compare the LED calibration with the Compton calibration to evaluate the response of our detectors at different crystal voltages. Note that the LED calibration discussed in the next chapter applies exclusively to the **HVeV** R&D detectors used in this thesis; it is not applicable to the SuperCDMS SNOLAB detectors, which motivated the development of the Compton scattering calibration. More information regarding the LED calibration is provided in the following chapter.

Chapter 6

LED Calibration at 150 V crystal bias

In addition to the 0 V Compton calibration described in Chapter 5, each detector was also calibrated at a 150 V crystal bias using 2 eV photons from **light-emitting diode (LED)** modules. The energy deposited by 2 eV photons is small, necessitating enhancement through the **NTL** gain (Eqn. 2.12) to raise the energy of their calibration signatures above the triggering threshold. This contrasts with the Compton scattering signatures, which occur at 100 eV (L-steps) and higher energies without any crystal bias.

We compared the 0 V and 150 V calibrations to compare the detector performance under different crystal biases. To a first approximation, the readout signal should be similar when the total phonon energy reaching the **TES** is equivalent. However, we observed a stronger detector response at 150 V compared to 0 V for the same expected amount of final phonon energy. The leading hypothesis is that, at 0 V bias, some **e⁻h⁺** pairs do not fully recombine, resulting in less energy reaching the **TES** than anticipated. This chapter summarizes the analysis leading to this observation.

The installation of the **LED** source required expanding the detector housing and modifying the readout cables. These changes can be identified by comparing Fig. 4.7 and Fig. 4.5. These modifications impacted the performance of the detectors and required significant amount of work to isolate and correct the changes in the detector performance.

The calibration of **HVeV** detectors with optical photons with energies ranging from approximately 1.6 eV to 3.2 eV has been extensively discussed in the literature [25, 32, 56, 63]. This chapter provides a brief overview of the **LED** calibration procedure, and discusses the challenges specific to this study.

Leveraging the **N**TL gain, the **L**ED calibration in this study extends up to approximately 3 keV in total phonon energy. The keV-range **L**ED calibration was conducted for the NFC1, NFC2, and NFH detectors. The NFE detector was excluded due to its smaller **T**ES volume that makes the NFE detector get saturated faster compared to other detectors at higher energy depositions [25].

6.1 LED data

The operating principle of **L**EDs is shown in Fig. 6.1. A semiconductor material is doped with positive and negative charges on either side, separated by a depletion region. When a forward-bias is applied, electrons in the conduction band recombine with holes in the valence band, emitting light with energies equal to the band gap. The number of photons emitted in this processes follows the Poisson statistic

$$p(k; \lambda) = \frac{\lambda^k e^{-\lambda}}{k!}. \quad (6.1)$$

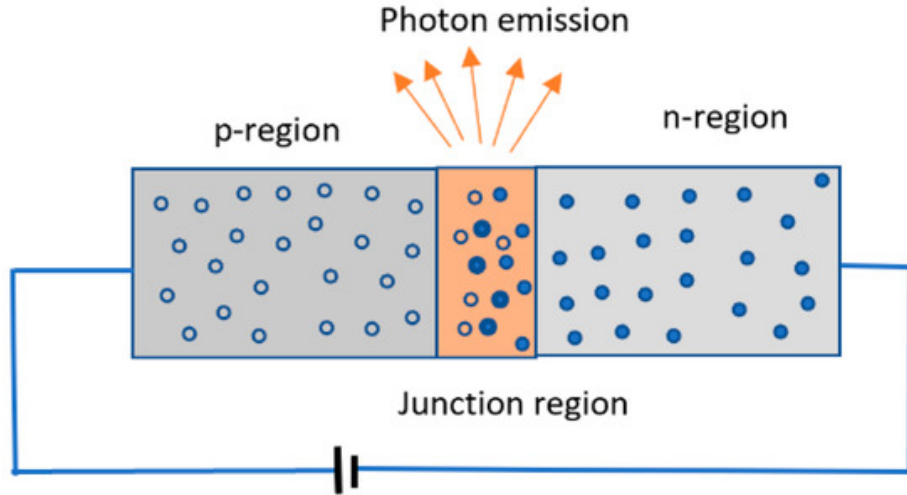


Figure 6.1: A schematic illustrating the operating principle of **L**EDs [76].

We used **L**EDs that emitted 2 eV photons (620 nm). The uncertainty in the photon energy was measured to be much smaller than the resolution of the detectors. The **L**ED was driven by different voltage signals, resulting in varying mean numbers of emitted photons (λ) across the data sets. For lower λ values, there was a nonzero probability that a voltage signal would lead to zero emitted photons.

The voltage was applied at a constant frequency to ensure equal time intervals between consecutive **L**ED events. Subsequently, the detector readout triggering logic

employed the constant frequency to trigger even in the absence of a signal above the trigger threshold. The triggered events are then processed similar to the 0 V calibration data sets which is detailed in Subsection 4.4.2.

A photon with an energy of 2 eV falls between the silicon band gap, and the average energy required to generate one **electron-hole** (e^-h^+) pair. As noted in [36], photons at these energies produce no more than a single e^-h^+ pair. Due to the detector timing resolution, **LED** pulses with multiple photons appear as a single energy deposition. Consequently, the total phonon energy in a reconstructed pulse is governed by the number of e^-h^+ pairs in a pulse.

An external electric field across the crystal increases the gap size between the total phonon energies for consecutive numbers of e^-h^+ pairs, as described by the equation:

$$E_t = E_r + n_{e^-h^+} \times eV_{\text{external}}. \quad (6.2)$$

Hence, the spectrum of the energy estimator will show distinct peaks, each representing a specific number of e^-h^+ pairs. This assumes a detector energy resolution that is significantly smaller than the energy gaps between the peaks. An example of the **LED** calibration data for the NFC2 detector is shown in Fig. 6.2.

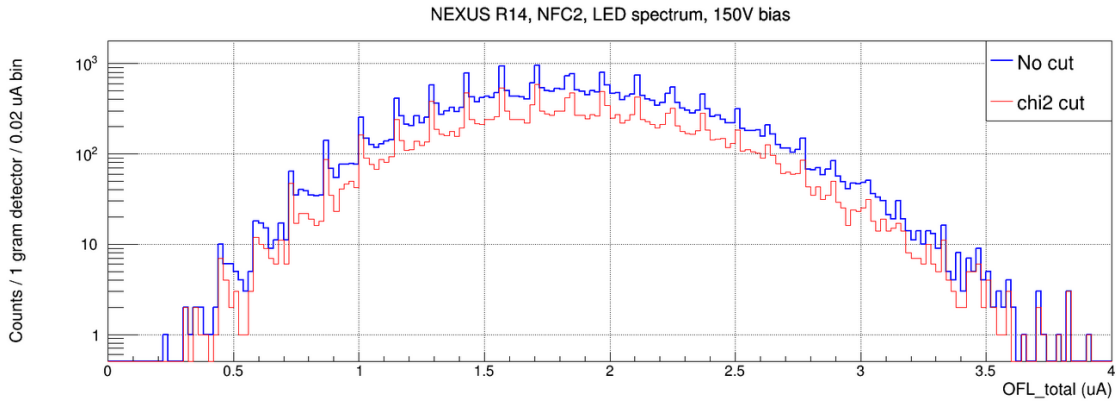


Figure 6.2: A common **LED** data spectrum. Individual peaks represents the consecutive number of e^-h^+ pairs. Courtesy of Sudipta Das.

6.2 Data cleaning

An event selection based on the **optimal filter** (OF) χ^2 values, similar to the one described in 4.5.6, is the only cut applied to the **LED** data sets. For the **LED** data,

the cut is extended beyond the detector's linear energy response. Consequently, the distribution of χ^2 values increases with energy due to a systematic deviation between the shape **OF** template and the pulses in the data. The χ^2 distribution for one of the **LED** data sets for detector NFC2 is shown in Fig. 6.3. The data cleaning cut rejects any event above the line. The effect of the cut is shown in Fig. 6.2.

The cut is constructed by fitting the e^-h^+ peaks with Gaussian functions, and selecting events within 3σ of the Gaussian mean values. Next, the mean (yellow dots in the left panel of Fig. 6.3) and standard deviation of the χ^2 distribution are obtained for each group of events through individual Gaussian fits. The 2σ upper threshold of the χ^2 distribution for each group is then determined (red dots in the left panel). Finally, these threshold points were fitted with a high-degree polynomial to define the cut function. The left panel in Fig. 6.3 illustrates the polynomial's degree, where p0 represents the constant term.

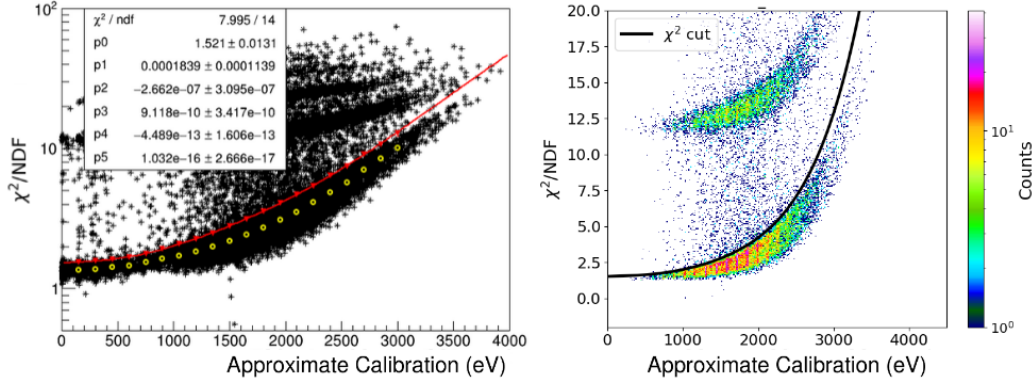


Figure 6.3: The **LED** data and the definition of the χ^2 cut for detector NFC2. The left and right panels show the same data, with the right panel zoomed in and the box removed to display the data and the cut. Left: Each black point represents a reconstructed event. Yellow dots indicate the mean value, and red dots represent the upper 2σ threshold of the χ^2 distribution for events under each e^-h^+ peak. More details are provided in the text. Right: Same as the left panel, but shown as a 2D-histogram. Events above the black line are rejected. Courtesy of Sudipta Das.

Data clusters above the primary band contain additional pulses within the reconstruction window of each triggered event. For example, one event from the second cluster of Fig. 6.3 is shown in Fig. 6.4.

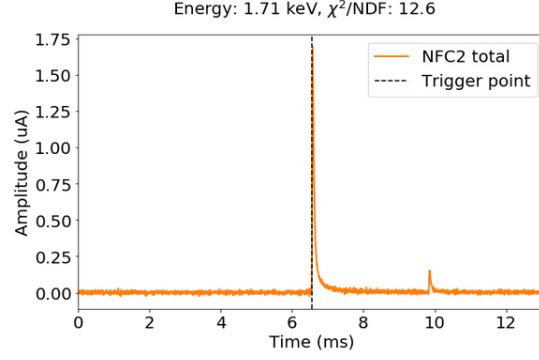


Figure 6.4: An event from the second cluster that includes an extra pulse in addition to the triggered pulse. Courtesy of Sudipta Das.

6.3 Cross-talk amplitude and surface trapping

The calibration with optical photons is susceptible to two recognized issues: cross-talk noise and surface trapping. The cross-talk noise refers to interference generated in the detector readout when the **LED** is triggered. Surface trapping refers to energy depositions by a subset of photons that do not get amplified through the **NTL** gain. The leading hypothesis for surface trapping suggests that e^-h^+ pairs recombine immediately without drifting in the external electric field [28]. This is based on the idea that e^-h^+ pairs may have initial momenta opposite to the direction of the force due to the crystal bias.

These effects appear in the position of the zeroth e^-h^+ peak when it is profiled as a function of the average number of photons hitting the detector, λ . This relation for the NFC1 detector is shown in Fig. 6.5. Cross-talk amplitude does not rely on λ , and it is given by the intercept of the linear fit. In comparison, surface trapping grows linearly with λ . In other words, surface trapping causes a constant fraction of the incident photons to get trapped. In the absence of aforementioned effects the zeroth peak should be centered at zero.

Assuming a constant probability of surface trapping for individual photons results in a uniform shift in the positions of all e^-h^+ peaks. That means, the magnitude of the shift follows the same statistical distribution for each peak. Let λ represent the mean number of photons hitting the detector, and N the total number of photons in a pulse. Define $N_{e^-h^+}$ as the number of untrapped photons, N_{st} as the number of trapped ones, and f_{st} as the probability of surface trapping for individual photons. Given these parameters, the probability of obtaining N_{st} surface-trapped photons, given $N_{e^-h^+}$ untrapped ones, is given by [77]:

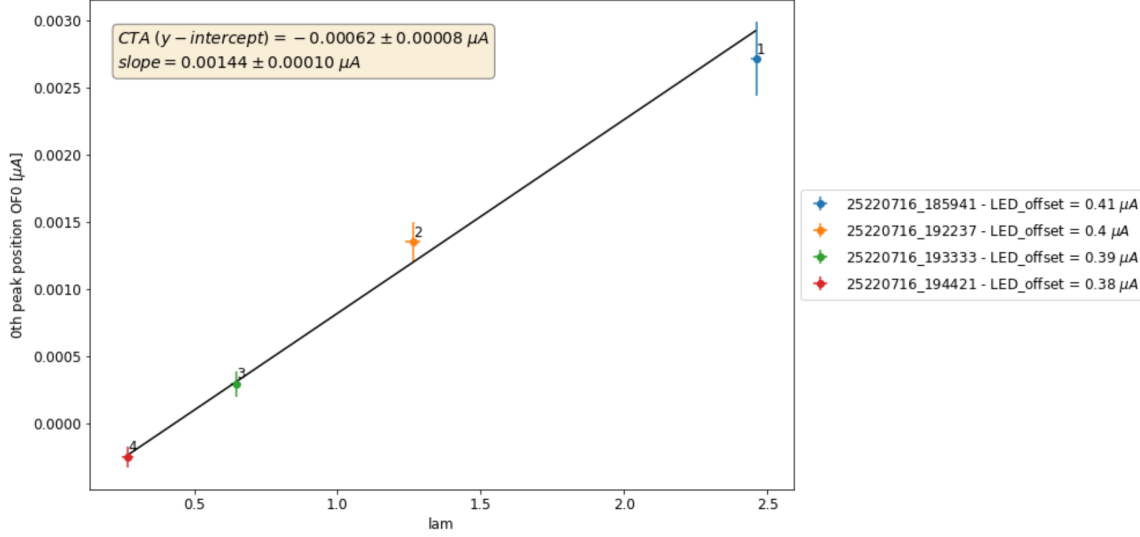


Figure 6.5: The positions of the zeroth **LED** peak as a function of average number of photons hitting the detector. The numbers in the legend shows the data sets used in this plot. Courtesy of Sudipta Das.

$$\begin{aligned}
P(N_{st} | N_{e^{-}h^{+}}) &= \frac{P(N_{st} \cap N_{e^{-}h^{+}})}{P(N_{e^{-}h^{+}})}, \\
&= \frac{\text{Poisson}(N; \lambda) \cdot \text{Binomial}(N_{st}; N, f_{st})}{\text{Poisson}(N_{e^{-}h^{+}}; \lambda(1 - f_{st}))}, \\
&= \text{Poisson}(N_{st}; \lambda f_{st}).
\end{aligned} \tag{6.3}$$

This relation may seem counter-intuitive. For instance, it suggests that the number of surface-trapped photons does not increase for higher $e^{-}h^{+}$ peaks. We validated this relation by examining the surface trapping coefficient (represented by the slope in Fig. 6.5) for higher $e^{-}h^{+}$ peaks. That is done by measuring the slope of changes in the position of higher $e^{-}h^{+}$ peaks rather than the zeroth one. This validation is shown in Fig. 6.6 where the x-axis represents the $e^{-}h^{+}$ peak number.

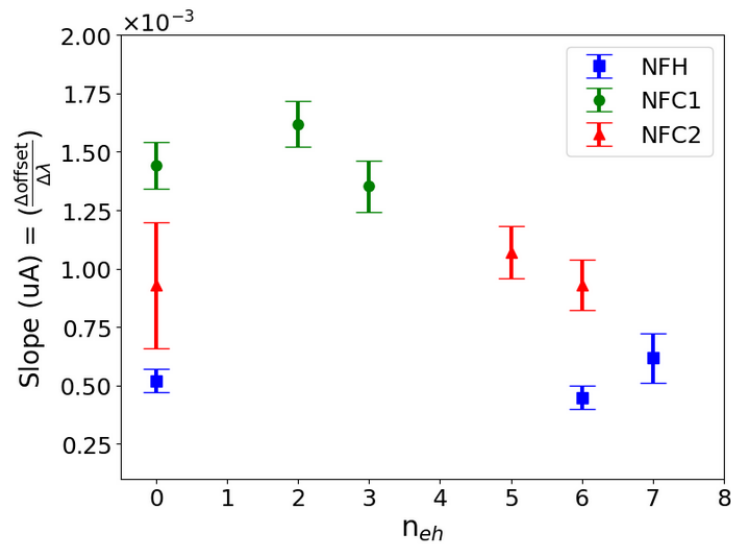


Figure 6.6: This plot shows the slope of the change in the positions of e^-h^+ peaks as the average number of photons hitting the detector varies. It represents the same measurement as in Fig. 6.5, but across different detectors and using multiple e^-h^+ peaks. Due to time constraints, the experiment was unable to collect additional data sets for this figure. Courtesy of Sudipta Das.

The **LED** calibration requires correcting the surface-trapping offset in the position of the e^-h^+ peaks. To remove this offset, we need to measure λ . An effective λ value, which represents the average number of boosted e^-h^+ pairs rather than incident photons, can be determined from the population of events under e^-h^+ peaks. Before applying the surface-trapping offset correction, we used the effective λ to estimate the surface-trapping probability across the **HVeV** detectors. We expected the probability to be consistent across all detectors, assuming the underlying physics is governed by the crystal material and the applied bias, which were identical for all **HVeV** detectors.

We assume that surface trapping and cross-talk collectively shift the e^-h^+ peaks without altering the distance between them. This assumption holds true for both the actual energy of the peaks and their values in the spectrum of the energy estimator for a linear calibration function. We used the gap size between low-energy e^-h^+ peaks (linear calibration) to find an initial calibration for the energy estimator. Using this calibration and the effective λ values, the surface trapping offsets (as shown in Fig. 6.6) was converted into missing energy values. The missing energy, when divided by the mean photon energy, gives the average number of surface-trapped photons. We found these values to be consistent across the **HVeV** detectors.

6.3.1 Measuring the effective λ

An effective λ can be extracted by fitting a Poisson distribution to the spectrum of **LED** events, as shown for detector NFC2 in Fig. 6.7. The observed spectrum does not reflect the primary λ because a fraction of the photons are removed from the peaks due to surface trapping. To illustrate, consider an edge case where the surface trapping probability is 100%. In that case, all photons will go into the zeroth peak. Keep in mind that the measurements in Fig. [6.5,6.6] report the effective λ .

6.3.2 Surface trapping probability

The surface trapping and cross-talk are assumed not to change the relative distance between e^-h^+ peaks. Therefore, the difference in mean value of the energy estimator between two consecutive peaks should be proportional to 152 eV, 150 eV due to the **NTL** gain in a voltage bias of 150 V, and 2 eV due to the extra energy of a single photon. The **OF** energy estimators provides a better energy resolution compared to the pulse integral. Therefore, we used the **OF** to find the energy equivalent of the surface trapping offset. The missing energy resulted from trapped photons can be

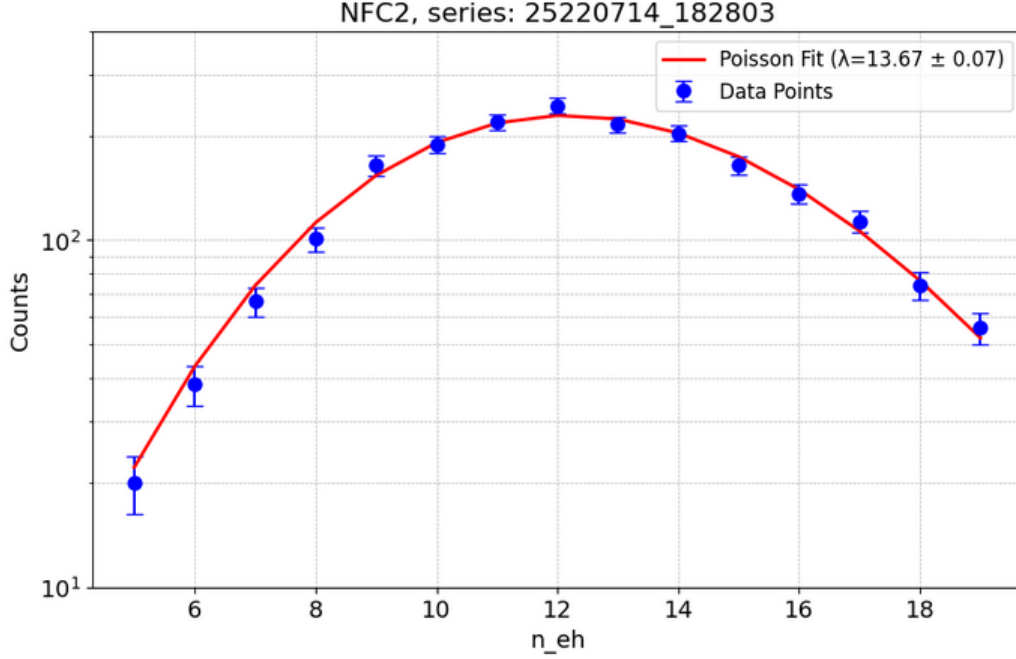


Figure 6.7: Fit of a Poisson function to an **LED** data set from NFC2 detector. Courtesy of Sudipta Das.

found following

$$\begin{aligned}
 E_{\text{offset}} &= \frac{E_{\text{photon}} + e \cdot V_{\text{bias}} \text{ (eV)}}{(\text{1st peak} - \text{zeroth offset}) \text{ (}\mu\text{A)}} \times \text{Surface trap offset (}\mu\text{A)}, \\
 &= \frac{152 \text{ eV}}{(\text{1st peak} - \text{zeroth offset}) \text{ (}\mu\text{A)}} \times \text{Surface trap offset (}\mu\text{A)}.
 \end{aligned} \tag{6.4}$$

Given the missing energy and the average energy per photon, we can determine the probability (f_{st}) of individual photons getting trapped by

$$f_{st} = \frac{\lambda_{\text{missing}}}{\lambda_{\text{missing}} + \lambda}, \tag{6.5}$$

where λ_{missing} is equal to $E_{\text{offset}}/2$. A summary of the f_{st} measurements is presented in Table 6.1. For the detector NFC1, the value is approximately 5% lower than the surface trapping probability measured with the same detector setup at a 100 V crystal bias [28]. Despite, that, an older measurement with NFC1 reported a consistent surface trapping probability [56, 28]. More investigation is needed to understand the physics, and the difference in the measurements.

Detector & Series	λ	Avg. trapped photon count ($E_{\text{offset}}/2$)	f_{st}
NFH 25220719_152937	14.85 ± 0.05	$\frac{15.51 \text{ eV}}{2 \text{ eV}} \approx 7.775 \pm 0.73$	0.34 ± 0.03
NFC1 25220716_165820	9.66 ± 0.05	$\frac{10.61 \text{ eV}}{2 \text{ eV}} \approx 5.305 \pm 0.37$	0.35 ± 0.03
NFC2 25220714_182803	13.67 ± 0.07	$\frac{13.13 \text{ eV}}{2 \text{ eV}} \approx 6.57 \pm 1.90$	0.33 ± 0.09

Table 6.1: Summary of the surface trapping measurements. Courtesy of Sudipta Das.

6.4 LED calibration at 150 V

We first subtracted the cross-talk amplitude (shown for NFC1 as the intercept in Fig. 6.5) from the energy estimator, then found the equivalent energy of e^-h^+ peaks using

$$E_n = n \cdot (E_{\text{photon}} + e \cdot V_{\text{bias}}) + E_{\text{offset}}, \quad (6.6)$$

where E_{offset} shows the surface trapping offset in units of eV. A second order polynomial without a the constant term was then used to extract the calibration function. For instance, the calibration function for detector NFC2 is shown in Fig. 6.8.

The uncertainties considered to extract the calibration functions include:

1. The uncertainty of the E_{offset} that is propagated to E_n . Note that the uncertainties from the bias voltage and E_{photon} are assumed to be negligible.
2. The fit uncertainty to locate e^-h^+ peaks in the spectrum of energy estimator. Each peak is located with a fit model that was consisting of a Gaussian and a linear function. The uncertainty in the mean value of the Gaussian function was taken as the uncertainty in the location of the peak.
3. The uncertainty in the cross talk subtraction from the energy estimator.

We considered the uncertainties associated with the energy estimator (items 2 and 3) to be uncorrelated, and combined them in quadrature.

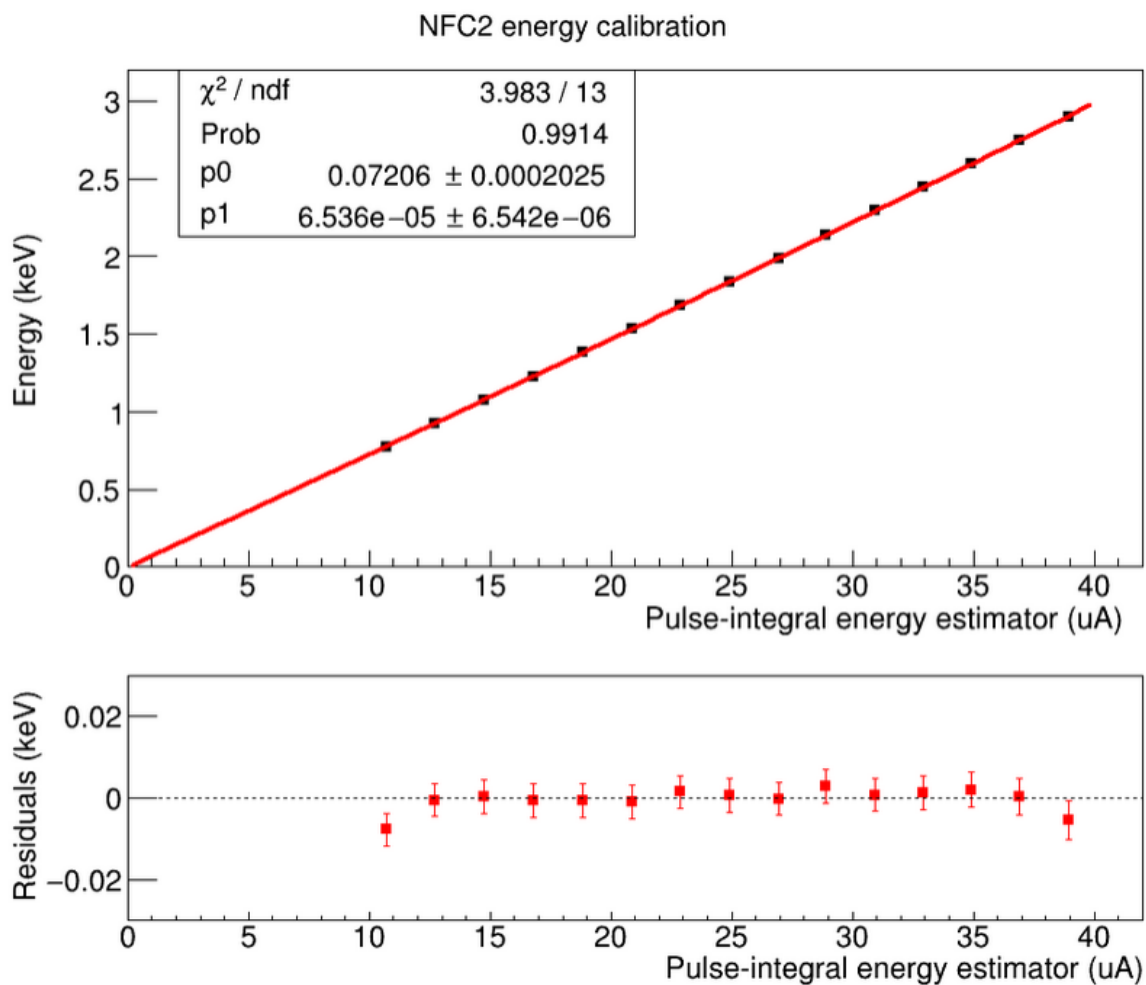


Figure 6.8: A second order polynomial fit to calibration points for detector NFC2. The polynomial provides the calibration function. The constant term in the polynomial is set to zero, p_0 is coefficient for the linear term, and p_1 is the coefficient for the quadratic term. Courtesy of Sudipta Das.

6.5 Effect of detector setup on the calibration

Changes to the detector setup for the LED calibration affected the detector response. In this section, we correct these changes to ensure that the LED calibration at 150 V is comparable to the Compton calibration at 0 V. Also, we propagate additional uncertainties from the corrections.

To align the detector responses between the Compton detector setup (NEXUS Run 13, or NR13) and the LED detector setup (NEXUS Run 14, or NR14), we need to identify matching energy signatures. The LED data from NR14 provides the e^-h^+ peaks. During NR13, background data was collected at a 100 V crystal bias over an extended time period. This background data only produces the first e^-h^+ peak, which results from leakage current— e^-h^+ pairs that are spontaneously liberated within the crystal under an external electric field. This energy signature was used to match the detector responses between NR13 and NR14.

First, we compared the detector response at 100 V and 150 V for the LED data, which provided a scaling factor to relate the positions of the e^-h^+ peaks at different biases. We scaled the position of the first e^-h^+ peak in the NR13 data, originally taken at 100 V, to estimate its position at 150 V. The scaled NR13 peak was then compared to the corresponding peak from NR14. We repeated this process, varying the current across the TES in NR14 to determine the systematic uncertainty in the matching. The final step is illustrated schematically in Fig. 6.9, where the detector working point 3 (WP3) during NR14 shows the closest match to the detector response observed in NR13.

Note that we refer to the process to match the detector response between NR13 and NR14 as "working point (WP) matching".

6.5.1 Detector response at 150 V and 100 V

We selected LED datasets from NR14 at bias values of 100 V and 150 V. For each dataset, the zeroth e^-h^+ peak offset is subtracted. We determined a constant scaling factor to align the e^-h^+ peaks between two datasets. This involved calculating individual scaling factors for the corresponding e^-h^+ peaks, and then fitting these factors with a constant line across all peaks. An example of this process for detector NFC2 is illustrated in Fig. 6.10.

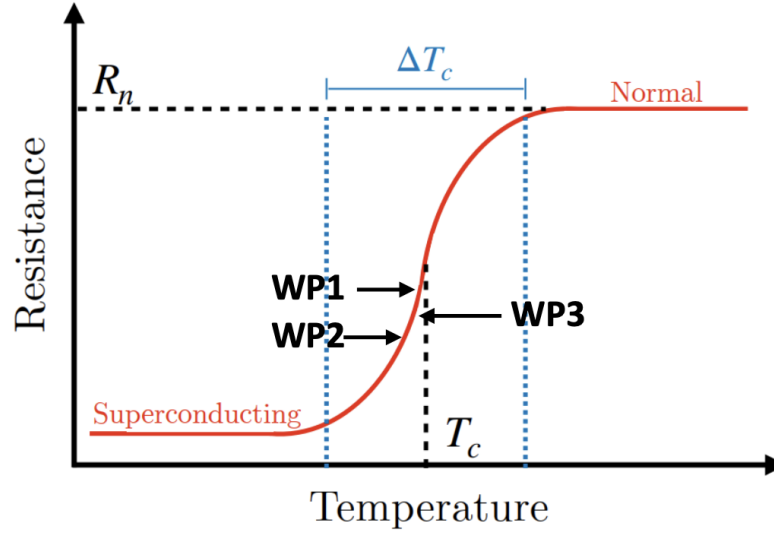


Figure 6.9: Illustration of the detector run conditions to collect LED data sets [32].

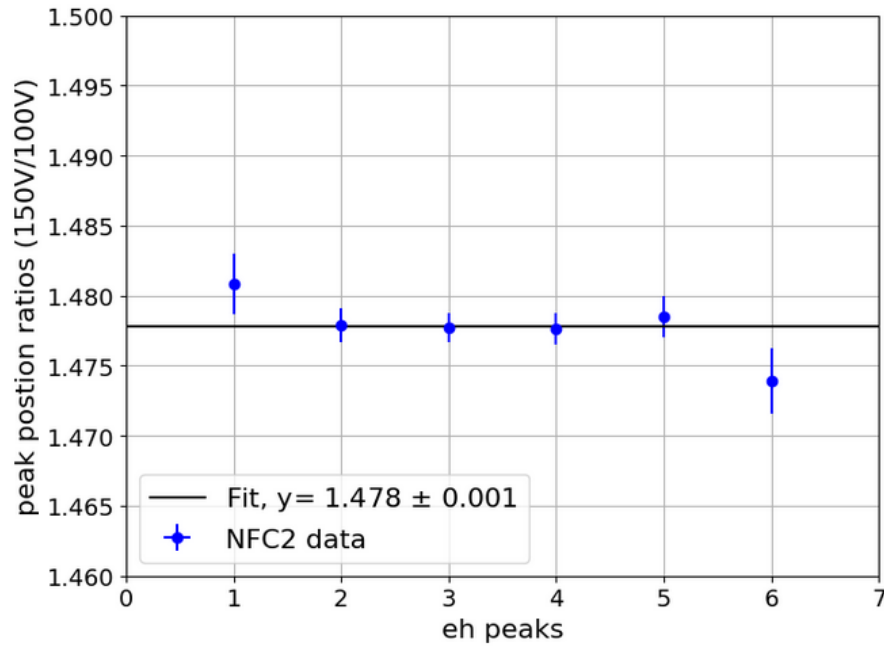


Figure 6.10: The plot shows the scaling factors that matches the corresponding e^-h^+ peaks across the 100 V and 150 V data sets. Points are then fitted with a constant line. Courtesy of Sudipta Das.

The summary of scaling factors for different detectors is shown in Table 6.2. These numbers are close to the expectation from the **N****T****L** gain that is given by

$$\text{Ratio} \approx \frac{E_{\text{primary}}(1 + 150/3.7)}{E_{\text{primary}}(1 + 100/3.7)} \approx 1.48. \quad (6.7)$$

Detector	Relative HV gain
NFH	1.49 ± 0.003
NFC1	1.479 ± 0.001
NFC2	1.478 ± 0.001

Table 6.2: Detector response relative scale factor (100 V $\rightarrow$ 150 V). The response of the detector (quantified by the **O****F** energy estimator) at 100 V multiplied by the scale factor gives the expected response value at 150 V for the same amount of initial energy deposition. Courtesy of Sudipta Das.

Using the scaling factors from Table 6.2, we compare the detector responses between NR13 and NR14. We selected the first **e**⁻**h**⁺ peak from the 100 V background data in NR13 (**e**⁻**h**⁺_{Bg}¹) and scaled it for each detector using the corresponding values in Table 6.2 to estimate the expected detector response at 150 V. The estimated 150 V response is then corrected with an additional scaling factor (WP correction factor) to match the first **e**⁻**h**⁺ peak of the 150 V data from NR14 (**e**⁻**h**⁺_{led}¹). This new scaling factor is defined as

$$\text{WP correction factor} = \frac{\mathbf{e}^{-}\mathbf{h}^{+}_{\text{Bg}}^1 \cdot \text{Relative HV gain}}{\mathbf{e}^{-}\mathbf{h}^{+}_{\text{led}}^1}. \quad (6.8)$$

A summary of the new scaling factors (corrections) is provided in Table. 6.3.

Detector	e ⁻ h ⁺ _{led} ¹ (uA)	e ⁻ h ⁺ _{Bg} ¹ (uA)	WP correction factor
NFH	0.076 ± 0.000	0.052 ± 0.000	1.026 ± 0.003
NFC1	0.199 ± 0.001	0.150 ± 0.000	1.028 ± 0.001
NFC2	0.147 ± 0.000	0.092 ± 0.000	0.930 ± 0.001

Table 6.3: First **e**⁻**h**⁺ peak position with the LED and Compton detector setups (tagged with Bg) at crystal biases of 150 V and 100 V, respectively. Courtesy of Sudipta Das.

The (**e**⁻**h**⁺_{Bg}¹) peak is not caused by optical photons; to the best understanding, it results from charge leakage through the crystal bulk. Therefore, this peak does not require corrections for surface trapping or cross-talk noise. The charge leakage peak

is not used to compare the **LED** and Compton calibration setups primarily due to the event rate; the **LED** data sets are too short to observe the leakage peak.

Given the WP correction factors, we recalibrated the **LED** data following a similar workflow as discussed for Fig. 6.8. In addition to the previously described uncertainties, the uncertainty in the WP correction was also included. A comparison of the calibration points before and after the WP correction for detector NFC2 is shown in Fig. 6.11 on the right panel.

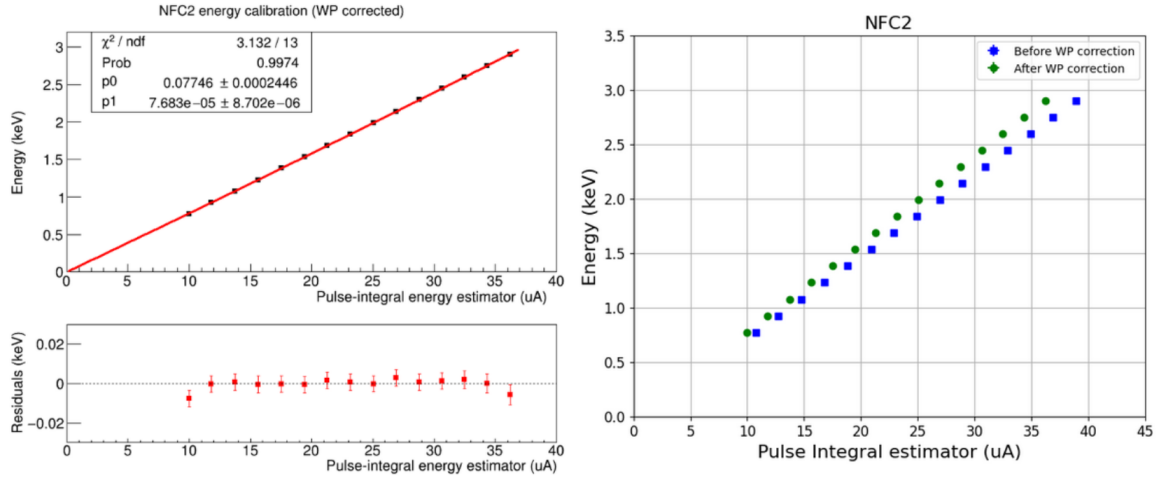


Figure 6.11: Left: A second order polynomial fit to calibration points for detector NFC2 after the WP correction. The polynomial provides the calibration function. The constant term in the polynomial is set to zero, $p0$ is coefficient for the linear term, and $p1$ is the coefficient for the quadratic term. Right: A comparison of the **LED** calibration points for detector NFC2 before and after the WP correction. Courtesy of Sudipta Das.

The new calibration function for the 150 V data sets can now be compared with the 0 V calibration function discussed in the previous chapter. We hope that the steps outlined have sufficiently mitigated the effects of the setup change on the detector response.

6.6 LED calibration function uncertainties

The calibration function is influenced by four sources of uncertainty:

1. Statistical uncertainty arising from fitting the calibration function to the data.
2. Systematic uncertainty associated with the choice of calibration function.

3. Systematic uncertainty from using the **OF** energy estimator instead of the Integral energy estimator to match $e^-h^+_{\text{Bg}}$ and $e^-h^+_{\text{led}}$.
4. Systematic uncertainty resulting from the WP correction.

We will discuss these uncertainties in the following subsections.

6.6.1 Calibration function statistical uncertainty

The calibration function is given by

$$\text{Energy} = p_0 \times \text{Integral} + p_1 \times \text{Integral}^2, \quad (6.9)$$

where the energy estimator is denoted by Integral, and p_0 and p_1 are the unknown parameters determined by the fits shown in Fig. 6.11.

The uncertainty is calculated by

$$\sigma_{\text{energy}}^2 = \begin{bmatrix} \text{Integral} & \text{Integral}^2 \end{bmatrix} \begin{bmatrix} \sigma_{p_0}^2 & \text{Cov}(p_0, p_1) \\ \text{Cov}(p_0, p_1) & \sigma_{p_1}^2 \end{bmatrix} \begin{bmatrix} \text{Integral} \\ \text{Integral}^2 \end{bmatrix}, \quad (6.10)$$

where it simplifies to

$$\sigma_{\text{energy}} = \sqrt{\sigma_{p_1}^2 \times \text{Integral}^4 + \sigma_{p_0}^2 \times \text{Integral}^2 + 2 \times \text{Integral}^3 \times \text{Cov}(p_0, p_1)}. \quad (6.11)$$

6.6.2 Calibration function systematic uncertainty

The deviation of the e^-h^+ peaks from the energy calibration function, given by Eqn. 6.9, introduces a systematic uncertainty in the energy calibration. The maximum observed deviation in energy, as shown by the residual plot in the left panel of Fig. 6.11, is used as a conservative estimate of the systematic uncertainty associated with the calibration function.

6.6.3 WP correction with OF instead of Integral

At low energies, in the hundreds of eV range, the **OF** energy estimator provides better energy resolution. Therefore, we selected the **OF** to match the detector response in Subsection 6.5.1. In the keV range, the Integral energy estimator was used to derive the **LED** calibration function. Applying the WP correction factor obtained from the **OF** to the Integral spectrum introduces a systematic uncertainty.

We performed two similar corrections using **LED** data sets at different working points, as shown in Fig. 6.10. These corrections were first applied between WP1 and WP3, and then between WP2 and WP3. The Integral and **OF** energy estimators were matched separately. For each detector, the uncertainty in matching the spectra is taken as the maximum difference between the **OF** and Integral ratios obtained from the fit at different WPs. For example, this systematic uncertainty for detector NFC2 is shown in Fig. 6.12. The upper row shows the scaling ratio for the **OF**, while the bottom row displays the same for the Integral. The right column presents the scaling factor from WP1 to WP3, and the left column from WP2 to WP3.

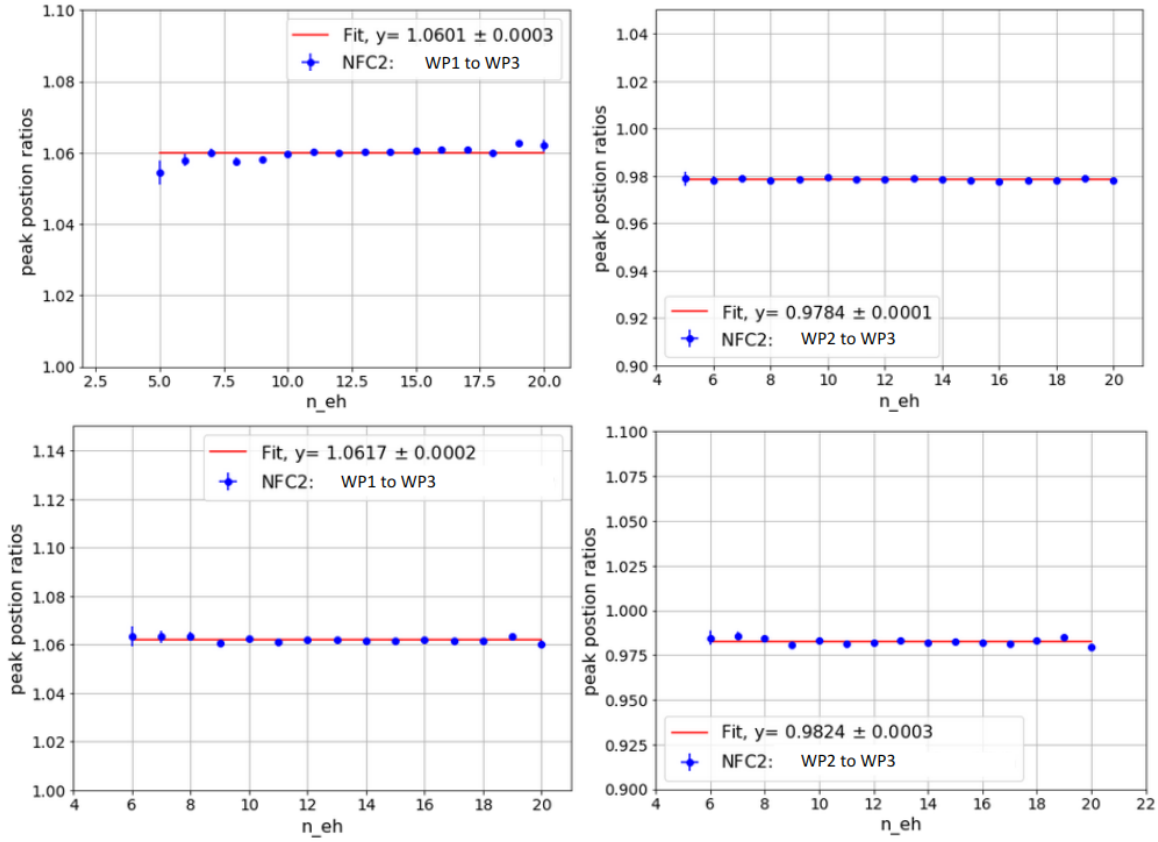


Figure 6.12: Linear working point correction factors for the **OF** and Integral energy estimators that are used to convert the detector response across different working points in **LED** data sets. Courtesy of Sudipta Das.

The difference between scaling factors in the left column is greater and that is chosen as a conservative systematic uncertainty:

$$\frac{0.9824}{0.9784} \approx 1.004 \quad (6.12)$$

A summary of the values for this systematic uncertainty is shown in Table. 6.4.

Detector	Systematic uncertainty
NFH	$\sim 0.93 \%$
NFC1	$\sim 1.75 \%$
NFC2	$\sim 0.40 \%$

Table 6.4: Systematic uncertainties of the **LED** calibration correction with Integral versus OF. Courtesy of Sudipta Das.

6.6.4 Working point correction with a linear function

The correction factors listed in Table 6.3 are determined by matching the first e^-h^+ peaks across data sets. Here, we evaluate the uncertainty introduced by choosing other peaks for the matching; particularly, those at higher energies where the detector response shows a slight non-linearity as a function of the energy estimator (as indicated by factor p1 in Fig. 6.11). The following steps represents the workflow:

1. Select an e^-h^+ peak and match data sets with a linear scaling factor.
2. Apply the calibration function to all data sets.
3. For each peak find the residual in the energy of the peak between WP1 and WP2 with WP3 (WP3 is the nominal working point according to Fig. 6.10). This steps is demonstrated in Fig. 6.13.
4. For each peak choose the greater residual as the calibration uncertainty.
5. Repeat the matching for all peaks. The greater residuals are demonstrated in Fig. 6.14 where each line corresponds to using a different e^-h^+ peak to match the data sets.
6. Choose the greatest residual as a conservative uncertainty for the detector calibration. This is shown by the shaded interval in Fig. 6.14.

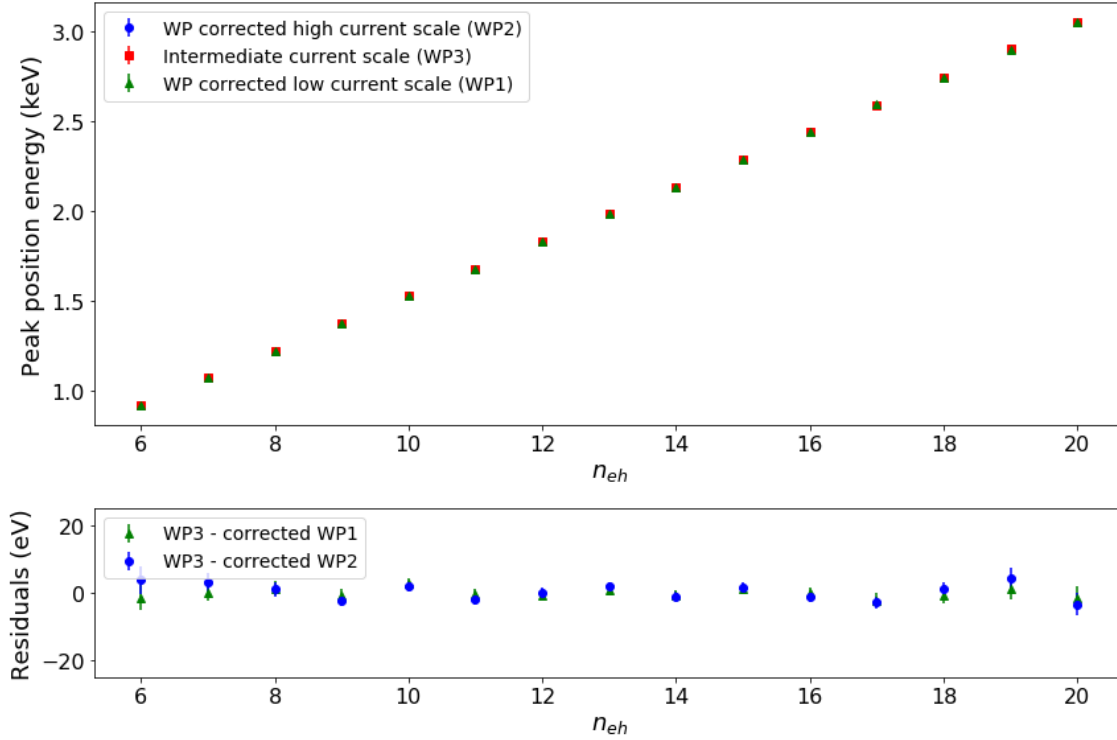


Figure 6.13: Energy residual extraction for matching with a selected e^-h^+ peak: The upper panel shows the calibrated positions of e^-h^+ peak after. The bottom panel displays the residuals with respect to WP3. The larger residual for each peak is selected as the peak residual associated with this correction. Courtesy of Sudipta Das.

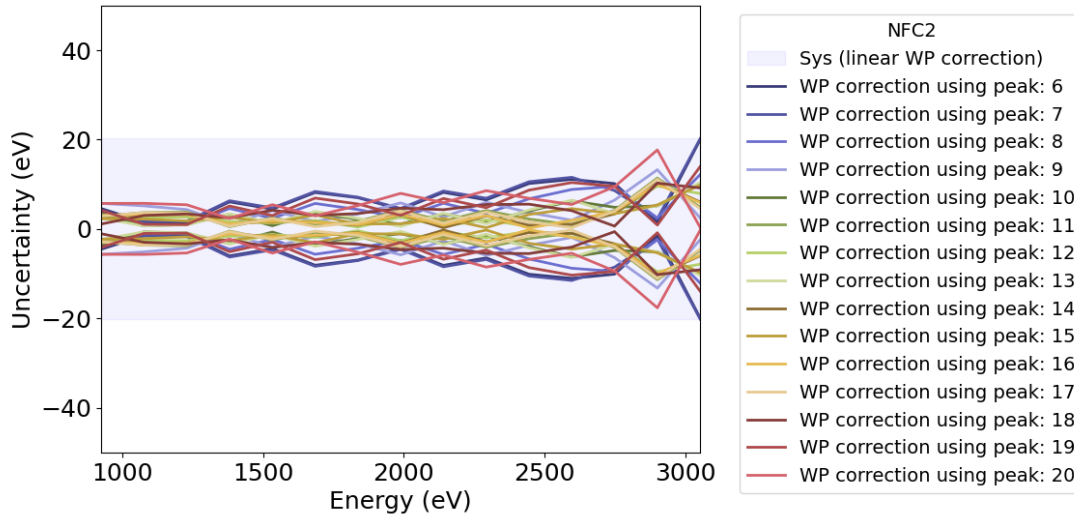


Figure 6.14: Determination of conservative uncertainty: The figure shows the comparison of uncertainties for each peak, selecting the highest uncertainty as a conservative estimate for all peaks. Courtesy of Sudipta Das.

6.6.5 Total uncertainty

We combined the uncertainties introduced in previous section in quadrature. The final results for different detectors is shown in Fig. 6.15.

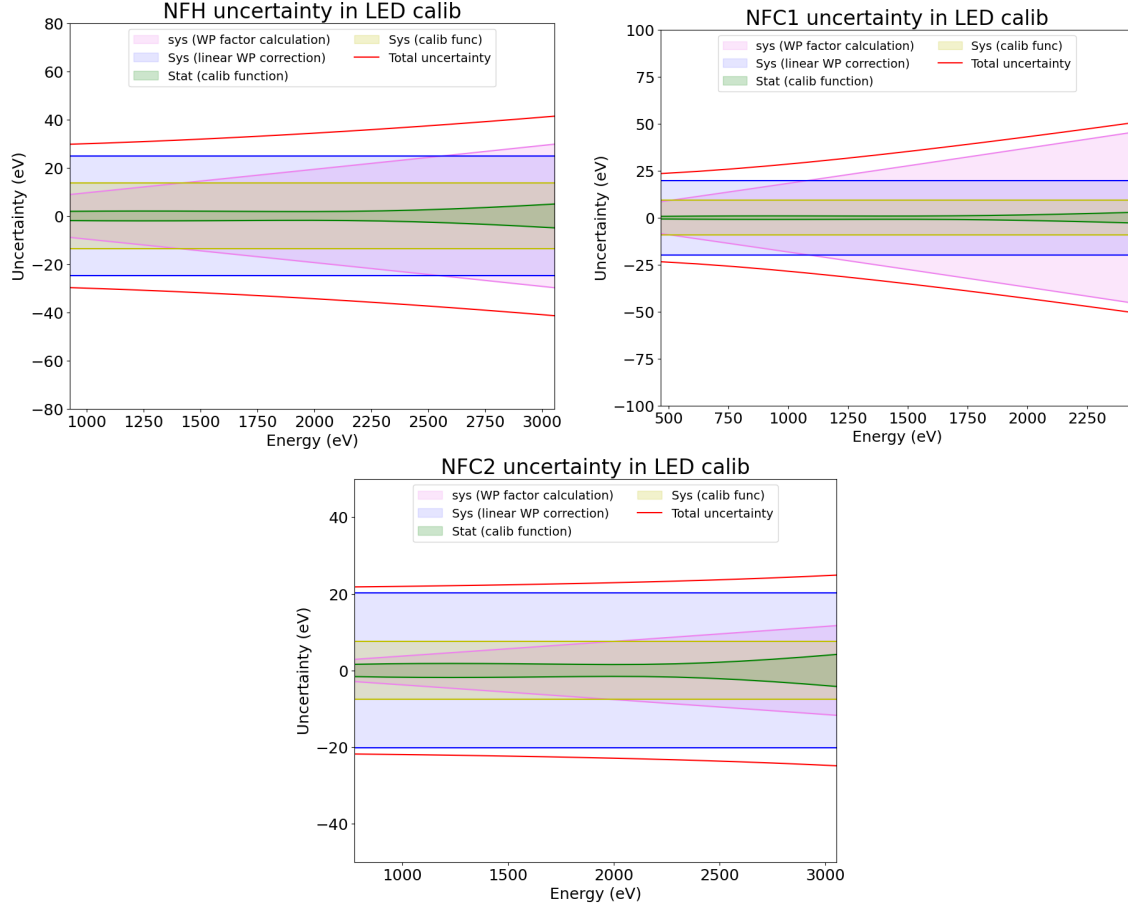


Figure 6.15: The total LED calibration uncertainty across different detectors. Courtesy of Sudipta Das.

6.7 Comparing calibrations at 150 V and 0 V

The calibration of the detectors at 0 V and 150 V is shown in Fig. 5.32 and Fig. 6.11, respectively. In this section, we compare the detector responses to the same total phonon energy at these two bias voltages. For this comparison, we introduce a scale parameter. This parameter fits the LED calibration curve (without any floating parameters, as it is fitted to the LED data points) to the 0 V Compton data points. The challenge in this processes is to propagate the uncertainty of the LED calibration

to this scale parameter. Note that the uncertainty in the 0 V Compton data points already gets included in the fit of the scale parameter.

We first adjusted the uncertainty of the **LED** data points (Fig. 6.11-left) according to total energy uncertainty that is shown in Fig. 6.15. This is done by keeping the nominal calibration points, but increasing the uncertainty ranges. We then redo the **LED** (Eqn. 6.9) calibration function fits to update the uncertainty of p_0 and p_1 . The fit provides a covariance matrix for p_0 and p_1 , which we used to generate a Bi-Gaussian distribution for these coefficients. The Bi-Gaussian distribution for detector NFC2 is shown in Fig. 6.16.

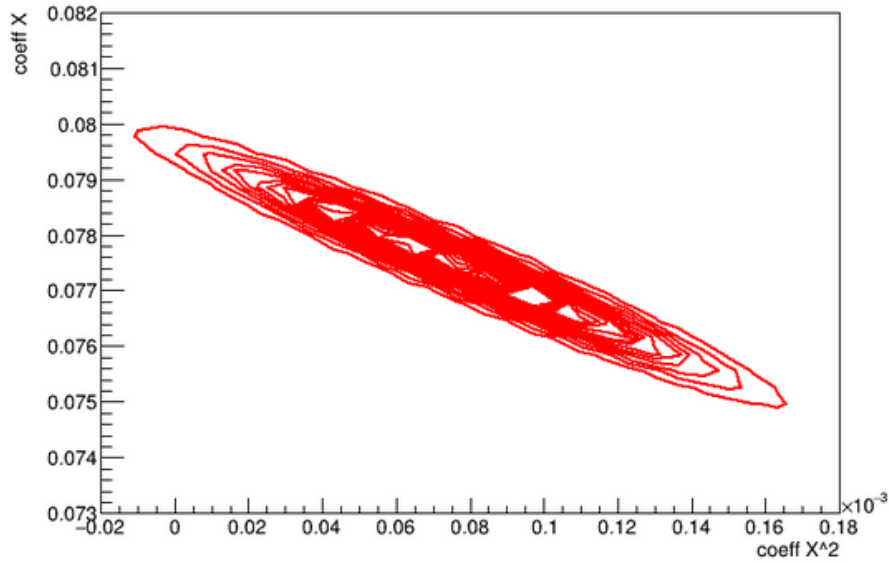


Figure 6.16: The Bi-Gaussian distribution of the coefficients for the **LED** calibration function for detector NFC2. The x-axis represents p_1 , and the y-axis represents p_0 , as defined in Fig. 6.11-left. The oscillations in lines are visualization artifacts.

To propagate the uncertainty of the **LED** calibration function, we generated a population of **LED** curves using the Bi-Gaussian distribution for p_0 and p_1 . Each curve was fitted to the 0 V Compton points with a floating scaling factor. The fit of the primary **LED** calibration curve to the 0 V Compton data determines the nominal value of this scaling factor and its statistical uncertainty. The systematic uncertainty of the scaling factor is derived by fitting the population of **LED** curves to the Compton data. These fits produced a population for the scaling parameter, which we modeled with Gaussian functions for individual detectors. The width of these Gaussian functions was taken as the systematic uncertainty. The population of scaling parameters for detector NFC2 is shown in Fig. 6.17.

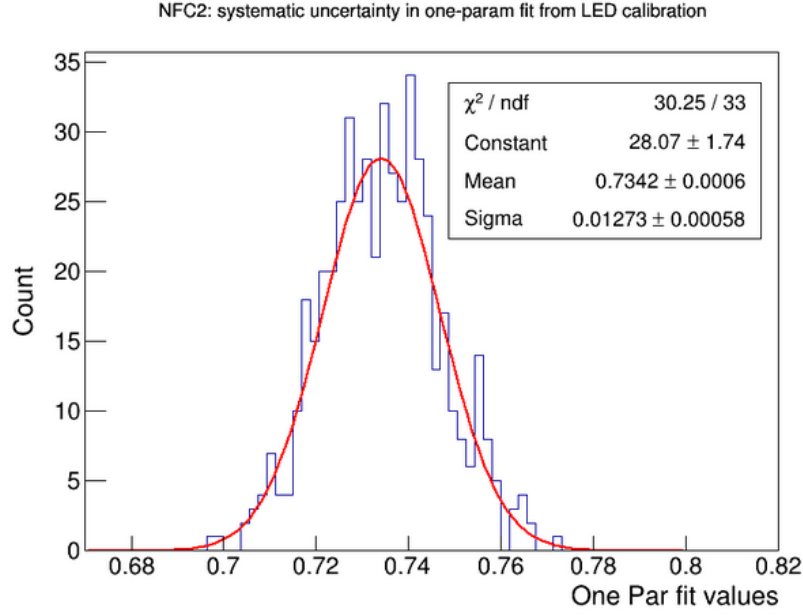


Figure 6.17: The scaling factor population for detector NFC2 from fits of the **LED** calibration curves to the 0 V calibration points. Courtesy of Sudipta Das.

Finally, the total uncertainty is calculated by combining the systematic and statistical uncertainties in quadrature for the scaling factor. A summary of the results for various detectors is shown in the bottom-right panel of Fig. 6.18. The other panels display the 150 V and 0 V calibration functions, where the x-axis represents the energy estimator and the y-axis represents the energy.

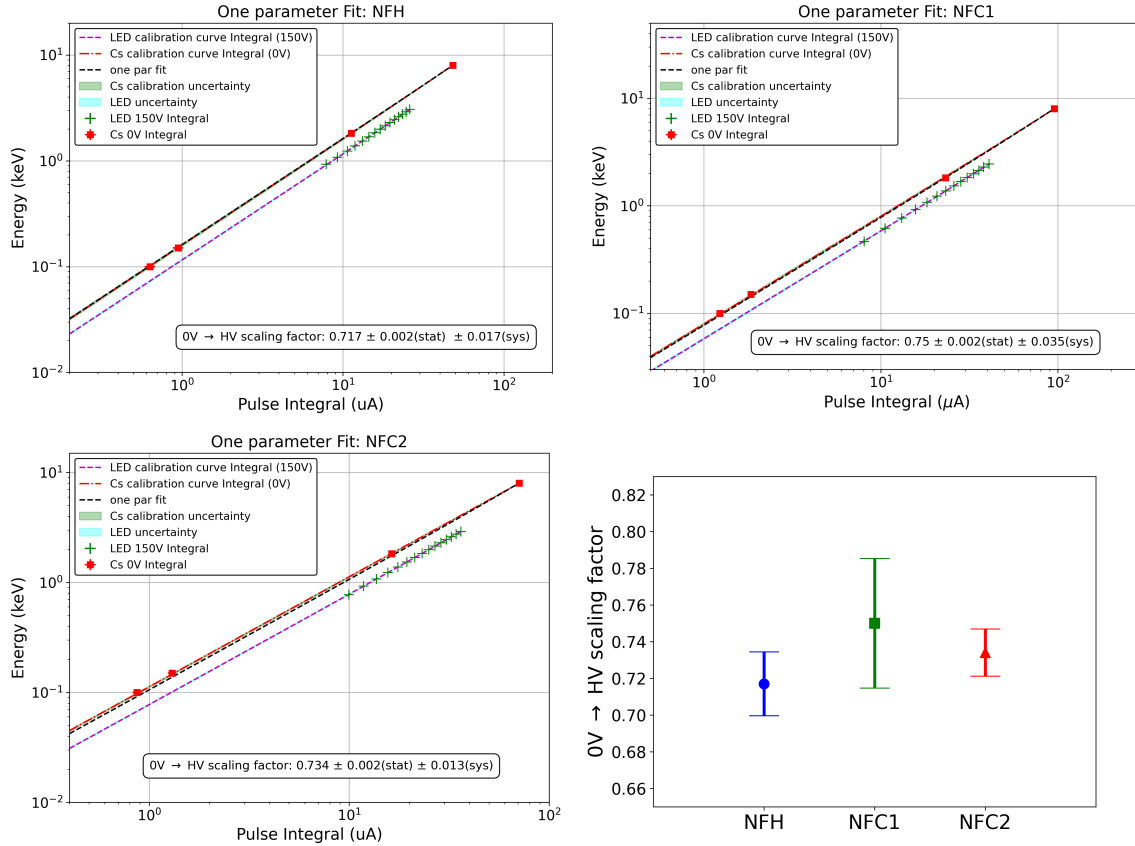


Figure 6.18: The **LED** (150 V) and Compton calibration (0 V) functions across different detectors. In all detectors, the upper curve represents the Compton calibration, while the lower curve represents the LED calibration. For a given amount of energy (y-axis values), the detectors exhibit a stronger response at 150 V, as indicated on the x-axis. The relative fraction of this response difference is shown in the bottom left panel. Courtesy of Sudipta Das.

6.8 Summary

The main observations in this chapter are the surface trapping values, and the detector response difference between the 0 V and 150 V calibrations for the same expected amount of final phonon energy.

Previous surface trapping measurements with **HVeV** detectors, along with the values from this study, are summarized in Table 6.5. We measured surface trapping at 150 V, while the 100 V measurements for detectors NFC2 and NFH were taken from a SuperCDMS internal document [78]. The values for detector NFC1 are taken from [56, 28]. All measurements are consistent, except for the **HVeV**-R4 measurements in NFC1.

The introduction of Section 6.3 describes a hypothesis for the surface trapping. If this effect arises from the recombination of e^-h^+ pairs with an initial momentum opposite to the direction of the force exerted by the crystal voltage, then altering the incident angle of the photons could change the fractions in Table 6.5. Future studies are needed to gain a deeper understanding of surface trapping.

Detector	Run	Bias Voltage (V)	Surface trapping
NFC1	HVeV-R2	100	37 ± 1
	HVeV-R4	100, 150	$41 \pm 2, 35 \pm 3$
NFC2	HVeV-R4	100, 150	$35 \pm 1, 33 \pm 9$
NFH	HVeV-R4	100, 150	$35 \pm 5, 34 \pm 3$

Table 6.5: Summary of surface trapping measurements with **HVeV** detectors.

The dominant uncertainty in the detector response difference measurement arises from the systematic uncertainty of the LED calibration, particularly due to the change of the detector setup between the Compton and LED data sets. Across all detectors, the response at 0 V is approximately 25% weaker compared to the 150 V response. A similar difference was previously reported in [25]. In the previous work, the difference was reported to be approximately 11% without discussing the uncertainties. In this study, we measured the effect to be approximately 25%, with uncertainties of only a few percent, consistent across different **HVeV** detectors. The previous study proposed three possible explanations:

1. A difference in detector response to **NTL** phonons at high-voltage and prompt phonons at 0 V.
2. Effects related to the depth of the energy depositions.

3. Local saturation of the TES sensors, as the photons in the previous measurement were directed toward the QET side of the detector.

In our setup, we did not illuminate the QET side of HVeV detectors. Therefore, we can reject the third possibility. The first possibility is also unlikely. Various factors affecting phonon collection efficiencies were discussed in Section 2.1. The efficiency of breaking Cooper pairs [79, 80, 29] could have explained this discrepancy if the average energy of NTL phonons was close to the minimum energy required to break Cooper pairs (approximately 0.3 meV). The average energy of NTL phonons at the voltage used in this measurement (and in [25]) is significantly higher than 0.3 meV as discussed in [81].

An alternative hypothesis to explain the measurement is the possibility of incomplete e^-h^+ recombination at 0 V. This hypothesis suggests that a fraction of the scattering energy that produces ionization may not fully convert into phonons. A definitive conclusion requires further investigation.

Chapter 7

Conclusion

The summary sections of the previous chapters offer a comprehensive review of the topics discussed throughout this thesis.

This chapter presents a general overview of the achievements of this work. It also highlights key points for calibrating the SuperCDMS SNOLAB detectors using the Compton scattering calibration scheme.

I conducted FEFF simulations and used SuperCDMS Geant4 simulations (Fig. 3.15) to construct a likelihood function that locates L-steps in the experiment data. The L-steps combined with higher energy signatures were used to calibrate the SuperCDMS HVeV detectors with 0 V crystal bias. This calibration approach should also be applicable at higher crystal biases, where the phonon signal is boosted through the NTL gain. The method developed in this thesis fulfills the technologically-driven calibration requirement for the SuperCDMS SNOLAB silicon detectors.

Locating the L-steps in the data has proven to be a challenging aspect of the Compton calibration scheme. Accordingly, I estimated that approximately 20,000 Compton scattering events below 500 eV are required to achieve a statistical uncertainty of about 1 eV in the position of the L-steps (Fig. 5.12). At this level, the systematic uncertainty in the L-step fits would be comparable to or dominate the statistical uncertainty (Table 5.2). My analysis is for the SuperCDMS HVeV detectors; however the numbers should shed light on the requirements for the SuperCDMS SNOLAB detectors.

I further developed a scheme to determine the theoretically achievable event rate in our detectors (Eqn. 5.19 and Figs. [5.40, 5.41]). This modeling aims to facilitate the planning of future calibration runs for the SuperCDMS detectors. The discussed machinery is particularly helpful in scenarios when an excessive pileup rate of events is a concern. That is relevant to the calibration data collection runs including the

Compton calibration efforts.

In my study, the gammas interacting with the detectors predominantly undergo Compton scattering (Fig. 3.15). Consequently, other scattering channels were not included in the likelihood model for the L-steps. The SuperCDMS SNOLAB detectors are larger and separated from the gamma source by additional material layers compared to my calibration setup. Additionally, the gamma source for the SuperCDMS SNOLAB detectors is planned to be ^{133}Ba , which emits primary gammas at 356 keV with a reduced mean free path compared to the 662 keV gammas from the ^{137}Cs source used in this study. Therefore, Geant4 simulations for the SNOLAB geometry may indicate that scattering processes other than Compton scattering are important. If so, adjustments to the L-step modeling described in this thesis would be necessary, as the FEFF simulations account only for Compton scattering.

The difference in geometry and detector size of the SNOLAB detectors necessitates a closer examination of the cut efficiencies. In this study, I argued that the applied cuts do not introduce an energy-dependent efficiency. However, the combination of a coincidence cut and multi-scattered Compton events could yield an efficiency that varies with energy.

The SNOLAB detectors are silicon and germanium cylinders with a diameter of 100 mm and a height of 33 mm, arranged in four towers with direct lines of sight. For Compton scatters at incident gamma energies of approximately 500 keV, the mean free path is approximately 5 cm in Si and Ge. That suggests a high probability of coincidence Compton scatters across multiple detectors. Consequently, it is essential to understand the energy distribution of multi-scattered events for the SNOLAB detectors if a coincidence cut will be applied to the data prior to Compton calibration.

Appendix A

Modeling Compton Scattering

According to the Geant4 documentation, none of the electromagnetic physics lists have been validated for energy depositions at the 100 eV energy scale. Therefore, it is essential to understand the underlying physics of Geant4 simulations to ensure the accuracy of the simulated spectrum.

The goal of this subsection is to gain more insight into the physics of light interacting with matter. We closely follow the description laid out in [82] and confine this summary to a non-relativistic limit. This is justified as the average speed of the fastest electrons in silicon is an order of magnitude smaller than the speed of light. This can be approximated by $Z\alpha c \approx 1/10c$ where Z is the atomic number of silicon, and alpha is the fine-structure constant ($1/137$).

The simplified Hamiltonian for a system of electrons in an electromagnetic field is given by two terms, H_0 for the non-interacting part, and H_{int} leading to interaction between photons and electrons,

$$\begin{aligned} H &= H_0 + H_{int} \\ &= \sum_j \left[\left(\frac{1}{2m} p_j^2 + \sum_{j'} V(r_{jj'}) \right) + \left(\frac{e^2}{2mc^2} A^2(r_j) - \frac{e}{mc} A(r_j) \cdot p_j \right) \right], \end{aligned} \quad (\text{A.1})$$

where A and V are the vector and scalar potential fields. Electrons are described by their momentum p_j and position r_j , where index j goes over the electrons in the system. Here we ignored the spin-dependent terms that cause interactions smaller by a factor of $\frac{\hbar}{mc^2}$. In H_{int} , the A^2 term corresponds to an interaction with two photons, whereas the $p \cdot A$ term only has one photon. To the second-order, the cross section of photons scattering off atomic electrons is described by the Kramers-Heisenberg

formula. It consists of three terms shown in Fig. A.1.

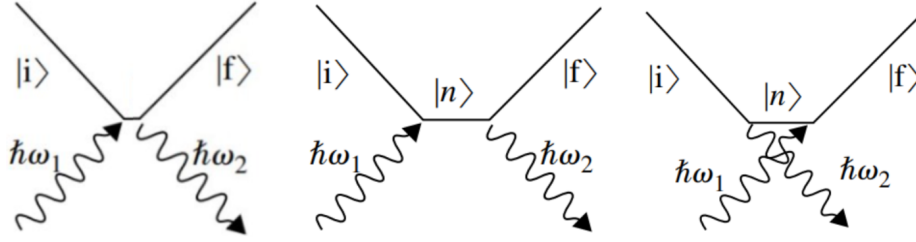


Figure A.1: Interaction of light with electrons.

The Kramers-Heisenberg formula provides the probability of incoming photons scattering into a differential solid angle and final energy window. This relationship, also known as the **double-differential scattering cross section (DDSCS)**, is given by

$$\begin{aligned}
 \left(\frac{d^2\sigma}{d\Omega_2 dw_2} \right)_{|i\rangle \rightarrow |f\rangle} &= \left(\frac{e^2}{mc^2} \right)^2 \left(\frac{w_2}{w_1} \right) \left| \langle f | \sum_j e^{iq \cdot r_j} | i \rangle (e_1 \cdot e_2^*) \right. \\
 &\quad + \left(\frac{\hbar^2}{m} \right) \sum_n \sum_{jj'} \left[\frac{\langle f | (e_2^* \cdot p_j / \hbar) e^{-ik_2 \cdot r_j} | n \rangle \langle n | (e_1 \cdot p_{j'} / \hbar) e^{ik_1 \cdot r_{j'}} | i \rangle}{E_i - E_n + \hbar w_1 - i\Gamma_n/2} \right. \\
 &\quad \left. + \frac{\langle f | (e_1 \cdot p_j / \hbar) e^{ik_1 \cdot r_j} | n \rangle \langle n | (e_2^* \cdot p_{j'} / \hbar) e^{-ik_2 \cdot r_{j'}} | i \rangle}{E_i - E_n - \hbar w_2} \right] \Big|^2 \\
 &\quad \times \delta(E_f - E_i - \hbar w),
 \end{aligned} \tag{A.2}$$

where $|i\rangle$, $|f\rangle$, and $|n\rangle$ are the initial, final, and intermediate states of the electron with respective energies E_i , E_f , and E_n . Additionally, k_1 , w_1 , and e_1 (k_2 , w_2 , and e_2) are the wavevector, frequency, and polarization unit vector of the incident(scattered) photon with the transferred energy and momentum given by $q = k_1 - k_2$, and $w = w_1 - w_2$. Finally, the summation over j and j' goes over the electrons in the target.

The first term of the **DDSCS** is the dominant term when the incident photon energies are much above binding energies of electrons. This term is a component of the **Non-Resonant Inelastic X-ray Scattering (NRIXS)** according to condensed matter literature. When the photon energy is comparable to the binding energy of electrons, the second term in the equation, **Resonant Inelastic X-ray Scattering (RIXS)**, becomes strong due to the resonance in the denominator, which corresponds to the half-life of the excited atomic state.

The detectors used for the calibration study are placed inside a tightly sealed

copper housing. The copper housing eliminates the majority of low-energy photons moving toward the detectors. Consequently, we will focus on the **NRIXS** term, reducing the **DDSCS** to

$$\frac{d^2\sigma}{d\Omega_2 dw_2} = r_0^2 \left(\frac{w_2}{w_1} \right) |e_1 \cdot e_2^*|^2 \sum_f \left| \langle f | \sum_j e^{iq \cdot r_j} | i \rangle \right|^2 \delta(E_f - E_i - \hbar w), \quad (\text{A.3})$$

where we used $r_0 \equiv e^2/mc^2$ to represent the classical electron radius. The cross section now highlights two distinct aspects. First, the Thomson scattering,

$$\left(\frac{d\sigma}{d\Omega_2} \right)_{Th} \equiv r_0^2 \left(\frac{w_2}{w_1} \right) |e_1 \cdot e_2^*|^2, \quad (\text{A.4})$$

describing the interaction between the photon and a single electron. Then, the component specific to the target, namely the **Dynamical structure factor (DSF)**

$$s(q, w) \equiv \sum_f \left| \langle f | \sum_j e^{iq \cdot r_j} | i \rangle \right|^2 \delta(E_f - E_i - \hbar w). \quad (\text{A.5})$$

As the name implies, **DSF** is related the dynamics of electrons within a target material through scattering processes. Intuitively, at scattering energies significantly exceeding the electron binding energies, the potential experienced by the target electron due to other interactions within the material should remain constant overtime. This is because the time scale of the scattering event is much shorter than the time scale of any response by the target material. Consequently, detailed knowledge of the potentials imposed on the electron should not be necessary to calculate the cross section in high-energy transfers.

The theoretical framework for this approximation, known as the impulse approximation, was first described in [83], and later refined to include relativistic corrections in [84]. This approximation significantly simplifies the calculation of the cross section and has been the foundation for many Monte Carlo Compton scattering models, including those used in Geant4, such as the Monash model [46]. In the next subsection, we will follow a simplified derivation leading to the impulse approximation.

A.1 High-energy transfer limit

For simplicity, we consider only a single electron and continue in natural units ($\hbar, c=1$). We can expand the delta function using the spectral representation to get

$$\delta(E_i - E_f - w) \equiv \frac{1}{2\pi} \int dt e^{-it(E_f - E_i - w)} dt. \quad (\text{A.6})$$

Then we substitute that in Eqn. A.5 to get

$$\begin{aligned} s(q, w) &= \frac{1}{2\pi} \int dt e^{iwt} \sum_f \langle i | e^{-iE_f t} e^{-iq \cdot r} e^{iE_i t} | f \rangle \langle f | e^{iq \cdot r} | i \rangle \\ &= \frac{1}{2\pi} \int dt e^{iwt} \langle i | e^{-iHt} e^{-iq \cdot r} e^{iHt} e^{iq \cdot r} | i \rangle, \end{aligned} \quad (\text{A.7})$$

where in the second line we use the completeness relation for $\sum_f |f\rangle \langle f| = \mathbb{1}$ and express the energy eigenvalues in terms of the original Hamiltonian.

The first line suggests that for a smooth integrand, the integral is determined within the interval where $t \ll w$ because it becomes oscillatory otherwise. This holds true when w is significantly larger than the characteristic energies of the target material, such as electron binding energies. Therefore, assuming $t \ll w$ and approximating the integral by expanding to the first order in t should provide a high degree of accuracy. This approximation can be applied to the expansion of the total Hamiltonian using the Baker-Campbell-Hausdorff formula which is given by

$$e^{iHt} \approx e^{iH_0 t} e^{iVt} \cancel{e^{-(1/2)[H_0, V]t^2} \dots} \quad (\text{A.8})$$

Knowing that potential V commutes with the position operator we rearrange Eqn. A.7 to get

$$\begin{aligned} s(q, w) &= \frac{1}{2\pi} \int dt e^{iwt} \langle i | e^{-iH_0 t} e^{-iq \cdot r} e^{iH_0 t} e^{iq \cdot r} | i \rangle \\ &= \frac{1}{2\pi} \int dt e^{iwt} \int d^3 p \langle i | p \rangle \langle p | e^{-iH_0 t} e^{-iq \cdot r} e^{iH_0 t} e^{iq \cdot r} | i \rangle \\ &= \frac{1}{2\pi} \int dt e^{iwt} \int d^3 p \langle i | p \rangle e^{-i(p^2/2m)t} e^{-iq \cdot r} e^{i((p+q)^2/2m)t} e^{iq \cdot r} \langle p | i \rangle \\ &= \int d^3 p \rho(p) \delta\left(\frac{q^2}{2m} + \frac{p \cdot q}{m} - w\right). \end{aligned} \quad (\text{A.9})$$

We inserted a complete set of momentum states in the second line, which are also the eigenstates of the free Hamiltonian H_0 . In the third line, we used the relation

$e^{iq \cdot r}|p\rangle = |p + q\rangle$. In the last line, we defined $\rho(p) = |\langle p|i\rangle|^2$ and reverted the integral over time to a delta function. This last line illustrates the conservation of energy for the photoelectron; if the initial momentum of the scattering electron is p , then for an energy (momentum) transfer $\omega(q)$, the relation should be

$$w = \frac{(p + q)^2}{2m} - \frac{p^2}{2m} = \frac{q^2}{2m} + \frac{p \cdot q}{m}. \quad (\text{A.10})$$

This relation indicates that the scattering energy depends on the projection of the electron's momentum onto the photon's trajectory and varies between $(q^2 - 2p \cdot q/2m) < \omega < (q^2 + 2p \cdot q/2m)$. Therefore, we observe the well-known broadening of the Compton scattering spectrum for a spectrum of photons hitting a calorimeter.

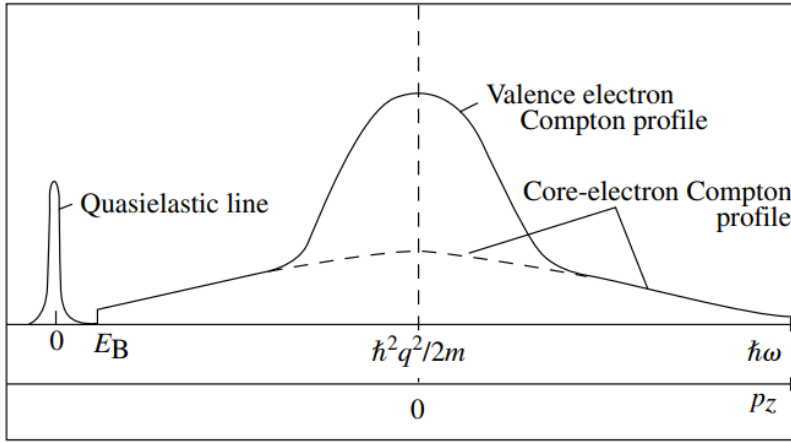


Figure A.2: Schematic of the Compton scattering spectrum. Compton broadening is shown for valence and core electrons. Core electrons have higher momentums on average which is the reason they show a wider spread [85].

According to Eq. A.9, it may seem that the potential does not play a role in the scattering; however, this is a misunderstanding, as emphasized by [83]. The potential actually determines the initial momentum distribution of the electrons. A more thorough discussion of the impulse approximation in the presence of multiple electrons follows the description above, with the additional constraint that the reciprocal momentum transfer q^{-1} must be much smaller than the average interparticle distances [85].

It is often preferred to rewrite the conservation of energy as $p_q \equiv \frac{(p \cdot q)}{|q|} = \omega m / |q| - |q|$ and substitute that in the Eqn. A.9 to get

$$\begin{aligned}
s(q, w) &= \frac{m}{q} \int d^3p \rho(p) \delta \left(\frac{p \cdot q}{|q|} - p_q \right), \\
&= \frac{m}{q} J(p_q),
\end{aligned} \tag{A.11}$$

where $J(P_q)$ is known as the **Compton Profile (CP)** which gives the average number of electrons with momentum-projection P_q . The total area of the **CP** represents the total number of electrons within the normalization volume of the quantum states. Conventionally, the unit cell of the crystals is used for that volume. From the definition of CP it follows that

$$\int J(p_q) dp_q = \int d^3p \rho(p) = N, \tag{A.12}$$

where N is the number of electrons in the normalizing volume. For most materials, the momentum distribution is mostly isotropic. So, CP integral in Eqn. A.11 reduces to

$$J(p_q) = 2\pi \int_{|p_q|}^{\text{inf}} p \rho(p) dp. \tag{A.13}$$

Therefore, the differential form becomes

$$\rho(p) = -\frac{1}{2\pi p} \frac{d}{dp_q} J(p_q) \Big|_{p_q=p}. \tag{A.14}$$

This suggests that, despite measuring only the projected momentum density through Compton scattering, we can indeed access the complete momentum distribution so long as it is isotropic. We used this equation for a correction that will be discussed for FEF simulations.

To summarize, **NRIXS** at high energy and momentum transfers (Compton scattering) effectively depends on the momentum distribution of individual electrons, rather than explicitly on the information about surrounding system. This outcome is expected because the time scale of the experiment is so brief, or the energy transfer (ω) is so significant, that the surrounding system does not have time to rearrange.

A.2 Low-energy transfer limit

At low energy transfer, the assumptions in Eqns. [A.8, A.9] become invalid, and the potential imposed on the electron cannot be neglected during the scattering process.

A method to calculate the cross section, incorporating the effects of various potentials on the electron, is introduced in [86, 87]. This method is implemented in an ab initio calculations package called FEFF. FEFF calculations adhere to Fermi's golden rule, employing the one-electron approximation as outlined in Eqn. A.5. The final states in Fermi's golden rule are the eigenvalues of the final-state Hamiltonian in the presence of a screened core-hole potential, i.e., the temporary hole formed during the scattering process when an electron is ejected from a core electronic shell. The potential terms in the Hamiltonian include $H'_{int} = V_{Coulomb} + \Sigma(E)$, where $V_{Coulomb}$ refers to the Coulomb potential due to neighboring atoms, and $\Sigma(E)$ is the self-energy potential (or dynamically screened exchange-correlation potential). The energy-dependent self-energy $\Sigma(E)$ factor, introduces two effects: (a) the imaginary part of self-energy describes inelastic energy losses causing the excited state (photoelectron) to have a finite lifetime, (b) the real part of the self-energy modifies the potential for the electron in the presence of the core-hole. To avoid explicit calculations of final states appearing in the golden rule, FEFF uses the one-particle Green's function (propagator) $G = 1/(E + H' + i\Gamma)$ in real space for the calculations, where Γ is the core-hole lifetime. We used FEFF to calculate the DSF over the entire range of viable momentum and energy transfers. Given the DSFs calculated individually for various electron shells(initial states), we used Eqn. A.3 to arrive at the cross section curves. For unpolarized incoming photons Eqn. A.3 reduces to

$$\left. \frac{d^2\sigma}{dw d\Omega} \right|_{nl} = r_0^2 \left(\frac{1 + \cos^2\theta}{2} \right) \left(1 - \frac{w}{w_1} \right) S_{nl}(q, w), \quad (\text{A.15})$$

where r_0 is the classical electron radius, θ is the scattering angle, w is the transferred energy, w_1 is the initial photon energy, and for completeness the quantum state of the electron shell is shown by nl . We then have to integrate over the scattering angle, and sum over the contribution of each electron shell to find the cross section as function of energy.

$$\begin{aligned} \frac{d\sigma}{dw} &= r_0^2 \int d\Omega \left(\frac{1 + \cos^2\theta}{2} \right) \left(1 - \frac{w}{w_1} \right) \sum_{nl} S_{nl}(q, w) \\ &= 2\pi \cdot r_0^2 \int -d(\cos\theta) \left(\frac{1 + \cos^2\theta}{2} \right) \left(1 - \frac{w}{w_1} \right) \sum_{nl} S_{nl}(q, w) \end{aligned} \quad (\text{A.16})$$

For the integral we need the relation between the scattering angle and the momentum transfer. The momentum conservation for the scattered photon provides the relation

$$\begin{aligned}
 q^2 &= k_1^2 + k_2^2 - 2k_1k_2\cos\theta \\
 &= w_1^2 + w_2^2 - 2w_1w_2\cos\theta \\
 \rightarrow \cos(\theta) &= \frac{w_1^2 + w_2^2 - q^2}{2w_1w_2} \\
 \rightarrow -d(\cos\theta) &= \frac{q dq}{w_1w_2}.
 \end{aligned} \tag{A.17}$$

Appendix B

Markov Chain Monte Carlo

A computational challenge in evaluating the posterior distribution, shown in Eqn. 5.3, lies in calculating the 'evidence' term in the denominator. The 'evidence' is defined as the integral of the posterior over the entire parameter space of the floating parameters:

$$\int d\theta L(\text{data}|\theta) \cdot \text{prior}(\theta), \quad (\text{B.1})$$

The integral serves to normalize the posterior distribution. Computing this high-dimensional integral by discretizing the parameter space quickly becomes infeasible. For example, if each dimension is discretized into 100 points and the parameter space has 5 dimensions, the total number of discrete points reaches 100^5 . This exponential growth in computational complexity, commonly referred to as the "curse of dimensionality", makes the computation impractical as the number of dimensions increases.

A well-established approach to approximating the posterior distribution involves generating samples from the numerator of Eqn. 5.3] while ignoring the evidence. Subsequently, the sample points can be accumulated in a high-dimensional histogram, and normalized to provide an approximate posterior distribution.

The **Markov chain Monte Carlo (MCMC)** algorithms are a class of methods designed to efficiently generate sample points (or states). These algorithms explore the parameter space by iteratively taking steps across the target function (moving between states) according to a proposal distribution for the steps. The algorithms then decide whether to accept or reject each state based on a probabilistic criterion. The sequence of states is typically referred to as a chain, and the head of the chain that moves between states and adopts new values is sometimes called a walker. Over time, the accepted states closely approximate the target function.

A basic **MCMC** algorithm is the Metropolis-Hastings algorithm [88, 89]. There

are more advanced algorithms including the affine-invariant samplers [90, 69] and Hamiltonian Monte Carlo [91, 92]. While all these algorithms are effective in sampling the target function, their efficiency varies depending on the number of parameters and the geometry of the function, with some methods outperforming others in specific scenarios.

The Metropolis-Hastings algorithm iterates through the following steps to generate samples from a target function $\pi(\theta)$ [69]:

1. Begin at an initial position θ_i in the parameter space, where θ represents the current state of a chain, and i denotes the iteration number.
2. Propose a new state θ' by taking a step in the parameter space according to a proposal distribution $g(\theta'|\theta_i)$. The proposal distribution is often chosen to be symmetric, such as a normal distribution, centered at the current position.
3. Accept or reject the proposed state θ' based on the acceptance probability:

$$P_{\text{accept}} = \min \left(1, \frac{\pi(\theta')}{\pi(\theta_i)} \frac{g(\theta_i|\theta')}{g(\theta'|\theta_i)} \right), \quad (\text{B.2})$$

where $\pi(\theta)$ is the target function we aim to sample. For example, with a symmetric proposal function g , steps toward greater values of the target function are always accepted, while downward steps are accepted with a probability less than 1.

4. If the proposed state θ' is accepted, set $\theta_{i+1} = \theta'$; otherwise, retain the current state by setting $\theta_{i+1} = \theta_i$.

A critical component of the Metropolis-Hastings algorithm is the tuning of the proposal function. If the step sizes are too large relative to the size of the high-density region of the target function, they are likely to be rejected frequently. Conversely, overly small steps may result in slow exploration of the target function, requiring considerable time to achieve adequate coverage. To address these issues, adaptive strategies can be employed. For example, parameters of the proposal function, such as the covariance matrix in a high-dimensional Gaussian distribution, can be adjusted during a burn-in phase before collecting samples.

More advanced algorithms, such as affine-invariant samplers and Hamiltonian Monte Carlo, can reduce or even eliminate the need for tuning based on the target function. For instance, affine-invariant samplers use a group of walkers to explore

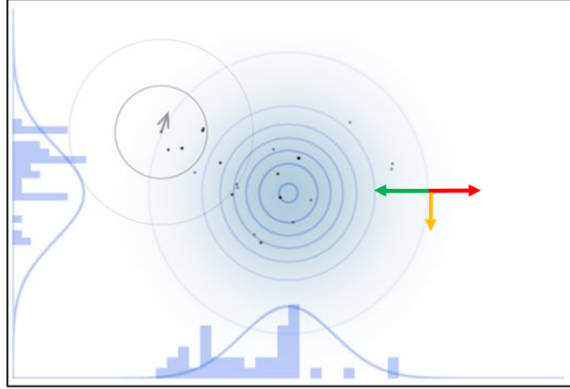


Figure B.1: A demonstration of the Metropolis-Hastings algorithm sampling from a two-dimensional normal distribution [93]. The one-dimensional histograms on the x-axis and y-axis illustrate the distribution of accepted states. The grey arrow with circles on the top-left represents the proposed step, and the proposal distribution which is a normal distribution centered around the current state. According to Eqn. B.2, steps toward greater values of the target function are always accepted (green arrow). However, steps in directions with lower target function values are accepted probabilistically, based on the relative heights of the target function at the proposed states compared to the current state. The yellow and red arrows represent medium and low probability moves.

the target function, proposing steps that are independent of the geometric shape of the target function, thus removing the need for tuning. Affine-invariant samplers are conceptually similar to the Nelder–Mead simplex algorithm [94], commonly used in optimization packages. An example of an affine-invariant sampler is the stretch move algorithm, detailed in [90], which requires at least two walkers. In this algorithm, the next step for each walker is determined by its relative position to another walker, rather than being sampled from a fixed proposal distribution. This process is illustrated in Fig. B.2.

The MCMC algorithms typically require a burn-in phase before they can generate samples that faithfully represent the target function. During this phase, the chain (or chains) must reach an equilibrium condition. This process can be illustrated using a discrete two-state system with multiple chains, as shown in Fig. B.3. In this figure, the red dots represent the initial state of the chains, while the values of 0.5 indicate an equal probability of either remaining in the current state or transitioning to the other state. This probability is similar to the proposal function on a continuous target function.

The system in Fig. B.3 undergoes several MCMC iterations before the red dots are adequately mixed between the states. Once equilibrium is achieved, the probability

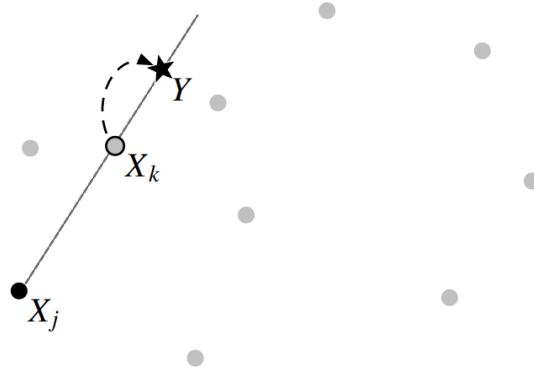


Figure B.2: Illustration of the stretch move where $X_k \rightarrow Y = X_j + Z(X_k - X_j)$. The dots represent the walkers distributed across the target function, with a minimum of two walkers necessary for the stretch move algorithm. X_j and X_k denote the two walkers chosen for the current move. For each move, the value of Z is drawn from a distribution that is independent of the geometry of the target function, as discussed in [90].

of finding the system in either the left or right states will be equal. In the early iterations, the red dots gradually move from the left state to the right state, thereby reducing the density on one side while increasing it on the other. Recording the states during these initial iterations would falsely suggest a higher probability to be in the left state due to the initial position of the chains prior to reaching the equilibrium.

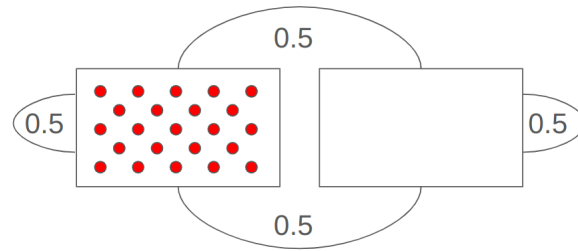


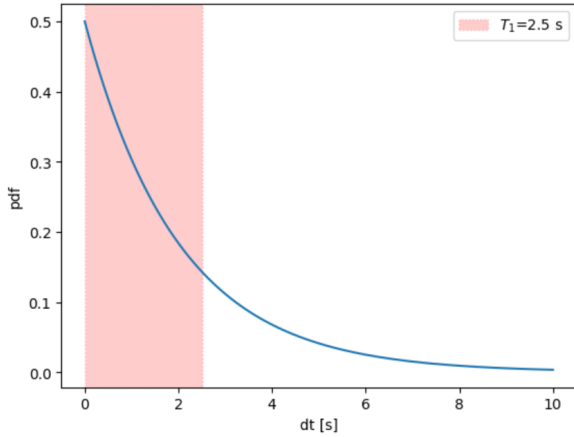
Figure B.3: Illustration of a two-state system with initial conditions and transition probabilities.

Convergence checks for equilibrium state of the chain (or chains) are generally heuristic. One of the most widely adopted methods is the Brooks-Gelman test [95, 70]. This test involves running multiple chains in parallel and comparing the variance of all sample points across the chains with the variance of sample points within individual chains to assess convergence.

Appendix C

No-pileup probability

We begin with a simplified case where the energy depositions are monoenergetic, with pulse lengths of T_1 . In this scenario, applying a cut of $\Delta T > T_1$, where ΔT is the minimum time gap between accepted events, removes overlapping events from the data. For a randomly selected event, the probability that the preceding event to occur at least by a time gap of T_1 earlier (i.e., no-pileup) is given by Eqn. C.1. This corresponds to the region of plot that is not shaded in Fig. C.1.



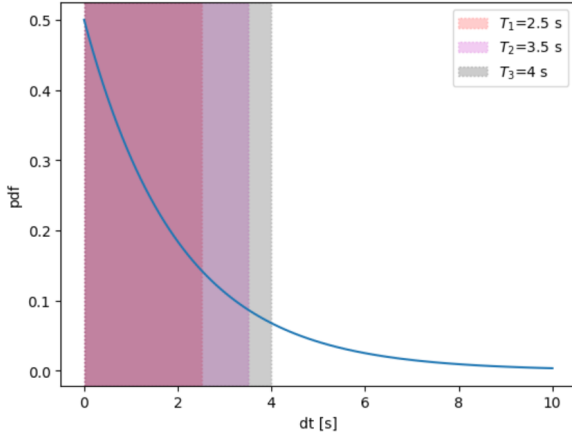
$$P(\Delta T > T_1) = \int_{T_1}^{\infty} \lambda e^{-\lambda t} dt \quad (\text{C.1})$$

Table C.1: Left: Events falling within the shaded area are rejected to eliminate pileups. Right: The probability of an event not occurring in the shaded area.

Next, we consider three groups of energy depositions corresponding to pulse length values denoted by $[T_1, T_2, T_3]$, ordered from shortest to longest. The ΔT distribution is divided into four intervals based on the pulse length values, as illustrated in Fig. C.2.

- $\Delta T > T_3$: No pileup occurs for a random event.

- $T_2 < \Delta T < T_3$: Pileup occurs for events with a prior pulse length of T_3 . Events with prior pulse lengths of T_1 and T_2 do not experience pileup.
- $T_1 < \Delta T < T_2$: Pileup occurs for events with prior pulse lengths of T_2 and T_3 . Events with a prior pulse length of T_1 do not experience pileup.
- $\Delta T < T_1$: All events experience pileup.



$$\begin{aligned}
 1. \quad & P(\Delta T > T_3) = \int_{T_3}^{\infty} \lambda e^{-\lambda t} dt, \\
 2. \quad & P(T_3 > \Delta T > T_2) = \int_{T_2}^{T_3} \lambda e^{-\lambda t} \frac{\lambda_2 + \lambda_1}{\lambda} dt, \\
 3. \quad & P(T_2 > \Delta T > T_1) = \int_{T_1}^{T_2} \lambda e^{-\lambda t} \frac{\lambda_1}{\lambda} dt, \\
 4. \quad & P(\Delta T < T_1) = 0.
 \end{aligned} \tag{C.2}$$

Table C.2: Left: Events falling within the shaded area are rejected to eliminate pileups. Right: Probabilities of events not occurring in the shaded regions.

We can find the total no-pileup probability for a randomly selected event by adding individual terms in Eqn. C.2 to be

$$\begin{aligned}
 P(\text{No pileup} \mid T_1, T_2, T_3) = & \int_{T_3}^{\infty} \lambda e^{-\lambda t} dt + \\
 & \int_{T_2}^{T_3} (\lambda_2 + \lambda_1) e^{-\lambda t} dt + \\
 & \int_{T_1}^{T_2} \lambda_1 e^{-\lambda t} dt.
 \end{aligned} \tag{C.3}$$

Reorganizing the terms and extending the sequence to accommodate 'm' individual

pulse lengths results in

$$\begin{aligned}
 P(\text{No pileup}) = & \int_{T_0}^{\infty} \lambda_0 e^{-\lambda t} dt + \\
 & \int_{T_1}^{\infty} \lambda_1 e^{-\lambda t} dt + \\
 & \vdots \\
 & \int_{T_m}^{\infty} \lambda_m e^{-\lambda t} dt.
 \end{aligned} \tag{C.4}$$

In a continuous limit, Eqn. C.4 turns into

$$\begin{aligned}
 P(\text{No pileup}) = & \int_{E_0}^{E_0+\delta} \int_{T_0}^{\infty} \phi(E) dE \lambda e^{-\lambda t} dt + \\
 & \int_{E_1}^{E_1+\delta} \int_{T_1}^{\infty} \phi(E) dE \lambda e^{-\lambda t} dt + \\
 & \vdots \\
 & \int_{E_m}^{E_m+\delta} \int_{T_m}^{\infty} \phi(E) dE \lambda e^{-\lambda t} dt,
 \end{aligned} \tag{C.5}$$

where $\phi(E)$ is the probability distribution function of events at different energies and λ is the total recoil rate. It is possible to write Eqn. C.5 as a double-integral of the form

$$\begin{aligned}
 P(\text{No pileup}) = & \lambda \int_{E_0}^{E_1} \phi(E) dE \int_{f(E)}^{\infty} e^{-\lambda t} dt \\
 = & \int_{E_0}^{E_1} \phi(E) e^{-\lambda f(E)} dE,
 \end{aligned} \tag{C.6}$$

where E_0 and E_1 represent the lower and upper bounds of the energy, respectively, and $f(E)$ is a function that provides the pulse length as a function of energy. We can use the same reasoning to determine the probability of a randomly selected event being pileup-free in the front. Since the no-pileup probability due from the back and in the front are independent, we can simply square Eqn. C.6 to obtain the total probability of no-pileup for a randomly selected event. Consequently, the no-pileup rate can be expressed as

$$R = \lambda \left[\int_{E_0}^{E_1} \phi(E) e^{-\lambda f(E)} dE \right]^2. \tag{C.7}$$

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