

ABSTRACT

Title of dissertation: A Search for the Double-Beta Decay
of ^{136}Xe to an Excited State of ^{136}Ba
with EXO-200

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This thesis presents a search for the two neutrino double beta decay ($\beta\beta 2\nu$) of ^{136}Xe to the 0_1^+ excited state of ^{136}Ba using data from the EXO-200 detector collected between 2011 and 2012. The $\beta\beta 2\nu$ decay to the excited state is a process that have been observed for other double beta decay nuclei. An observation of this decay would shed some light on the validities of the various nuclear physics models. Located at the Waste Isolation Pilot Plant (WIPP) near Carlsbad, NM, EXO-200 is a liquid xenon time projection chamber filled with 200 kg of 80.6% isotopically enriched ^{136}Xe . The liquid xenon serves both as the decay source and the detection medium. Maximum likelihood fits of the sum energy spectra based on Monte Carlo simulations are used to constrain the number of $\beta\beta 2\nu$ decay to the 0_1^+ excited state of ^{136}Ba . A half-life lower limit on this decay of $1.2 \cdot 10^{23}$ year at 90% C.L is set, still a couple orders of magnitude from our expected theoretical rate of $2.5 \cdot 10^{25}$ year from the applying the calculated phase space factor and the nuclear matrix element suppressions on the measured $\beta\beta 2\nu$ decay to the ground state. A developing analysis using a new energy variable designed specifically for the search of the decay to the excited state is also discussed.

A Search for the Double-Beta Decay of ^{136}Xe to an Excited State of
 ^{136}Ba with EXO-200

by

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Dedication

To my family, particularly my mother.

Acknowledgments

What a *long* and winding journey this has been! I certainly would not be able to get to this point without the great fortune of getting a variety of help from a great number of people along the way.

First and foremost, I like to thank my advisor, Carter Hall, for the opportunity to work on such an interesting experiment as EXO, particularly with the wildly diverse tasks this project had me do in the last 6 years. I also would not be at this stage without his guidance and support. I also like to thank all the members on my committee for taking the time to review my thesis and finding the time for my defense.

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Even though my suggestions (FLEXO for Full, Large EXO or the EXORCIST for EXO Radioimpurity-Clean Ionization and Scintillation detecting TPC, the latter of which is more suitable as the nickname for EXO-200) for the name of the next EXO experiment was not chosen, I wish luck to everybody who is involved with nEXO. I thank the potential future readers of this thesis, and I sincerely hope that you find some value in looking through this.

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List of Abbreviations

ADC	Analog-to-Digital Converters
APD	Avalanche Photodiode
C.L.	Confidence Level
DAQ	Data Acquisition
FEC	Front End Card
EC	Electron Capture
e.s.	Excited State
EXO	Enrich Xenon Observatory
g.s.	Ground State
LXe	Liquid Xenon
MC	Monte Carlo
NLL	Negative Log-Likelihood
NME	Nuclear Matrix Element
PCD	Pixilated Charged Deposit
PDF	Probability Density Function
PSF	Phase Space Factor
TPC	Time Projection Chamber
VUV	Vacuum-Ultraviolet
WIPP	Waste Isolation Pilot Plant
$\beta\beta 2\nu$	Two Neutrino Double Beta Decay
$\beta\beta 0\nu$	Neutrinoless Double Beta Decay

Chapter 1

Introduction

The search for neutrinoless double beta decay ($\beta\beta 0\nu$) has been the catalyst of a great number of experiments recently. For nine nuclei, the two neutrino form of the double beta decay ($\beta\beta 2\nu$) has been directly observed [4, 16]. An observation of $\beta\beta 0\nu$ would be direct evidence of lepton-number violating new physics, as well as proof for the existence of the neutrinos' Majorana nature. The Enriched Xenon Observatory (EXO) is a collaboration seeking the $\beta\beta 0\nu$ decay of ^{136}Xe . EXO-200 is the current experiment from the collaboration, running with ~ 200 kg of liquid xenon (LXe) in a single phase detector at the Waste Isolation Pilot Plant near Carlsbad, NM. The EXO-200 detector is a time projection chamber (TPC), made from carefully selected low background materials, that measures both the ionization and scintillation of the energy depositions. ^{136}Xe is both the source of the decays as well as the detector medium.

While the focus of the experiment is to search for the $\beta\beta 0\nu$ decay of ^{136}Xe to the ground state of ^{136}Ba , EXO-200 is also the first experiment to observe the $\beta\beta 2\nu$ decay of ^{136}Xe to the ground state of ^{136}Ba [16]. Another interesting type of ^{136}Xe decay is the transition to the first 0_1^+ excited state of ^{136}Ba . The $\beta\beta 2\nu$ mode of this decay is a process that EXO-200 may be capable of discovering.

This thesis will go over, in Chapter 2, the general physics and motivations

of double beta decay experiments, from the neutrinoless case to the decays to the excited state. Concluding that chapter is a review of the various xenon double beta decay experiments. In Chapter 3, the EXO-200 detector design is described in detail. The reconstruction of the detector signals is next discussed in Chapter 4. Since Monte Carlo (MC) simulations are an important part of the analysis, the next two chapters are devoted to it. Chapter 5 details the $\beta\beta$ generators to simulate the physics signals. Chapter 6 covers the MC of the modeled backgrounds, ending with how the probability density functions (PDFs) used in the final fits were generated. The calibration hardware system and the data corrections derived from the calibration runs are next explained in Chapter 7. The final fitting results are presented in Chapter 8. In Chapter 9, progress on a more sophisticated analysis is detailed. Results, including the current best limit on the decay of $\beta\beta 2\nu$ of ^{136}Xe to the first 0_1^+ excited state, are summarized in Chapter 10. The Appendix describes a source of single Barium ions using ^{137}Cs atoms from $^{137}\text{CsCl}$ salts.

Chapter 2

Massive Neutrinos and Double Beta Decay Processes of Xenon

Neutrinos have an interesting and unique history in particle physics, but the discovery of a nonzero neutrino mass in the last 15 years has started a new chapter in their story. Massive neutrinos have profound consequences in particle physics, as well as impacting astrophysics and cosmology. By studying the neutrino sector, we stand at the gateway to physics beyond the Standard Model. In this chapter, the basic physics and implications of a massive neutrino are described. The various double beta decay processes of xenon nuclei are discussed, concluding with a brief historical survey of double beta decay searches using xenon.

2.1 Neutrino Mass

From the convincing results of the neutrino oscillation experiments, neutrinos are determined to be massive [17, 18, 19]. The Standard Model of particle physics assumes that neutrinos are massless. To include massive neutrinos, extra parameters with values determined experimentally must be added into the Standard Model. The flavor oscillations of solar, atmospheric, reactor and accelerator neutrinos imply the existence of three massive neutrino eigenstates m_1 , m_2 , m_3 , distinct from the three flavor eigenstates ν_e , ν_μ , and ν_τ .

Each flavor eigenstate can be related to a mass eigenstate by a complex-valued

mixing matrix, U_{fj} :

$$\nu_f = \sum_{j=1}^3 U_{fj} \nu_j, \quad (2.1)$$

where f indicates one of the flavor states and j represents the three mass eigenstates.

Known as the Pontecorvo-Maki-Nakagawa-Sakata (PMNS) matrix, the matrix U_{fj} may be written as:

$$U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & c_{23} & s_{23} \\ 0 & -s_{23} & c_{23} \end{pmatrix} \begin{pmatrix} c_{13} & 0 & s_{13}e^{-i\delta} \\ 0 & 1 & 0 \\ -s_{13} & 0 & c_{13} \end{pmatrix} \begin{pmatrix} c_{12} & s_{12} & 0 \\ -s_{12} & c_{12} & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} e^{i\alpha/2} & 0 & 0 \\ 0 & e^{i\beta/2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (2.2)$$

where $c_{ij} = \cos(\theta_{ij})$ and $s_{ij} = \sin(\theta_{ij})$. The first three matrices describe the mixing of a pair of mass eigenstates. The fourth matrix contains two phases which are only present if the neutrino is a *Majorana* particle (discussed in much more detail in section 2.2). Overall, the PMNS matrix contains six parameters: the mixing angles θ_{12} , θ_{23} , and θ_{13} ; a CP-violating phase δ ; and two Majorana phases α and β .

The measured parameters of the PMNS matrix include the two squared mass difference terms from solar and atmospheric neutrino oscillation experiments. The squared mass differences of the different neutrino eigenstates are found to be $\Delta m_{21}^2 = (7.41_{-0.19}^{+0.21}) \cdot 10^{-5}$ eV from “solar” neutrinos and $\Delta m_{32}^2 = (2.32_{-0.08}^{+0.12}) \cdot 10^{-3}$ eV from “atmospheric” neutrinos [17, 18, 19]. From these experiments, θ_{12} and θ_{32} values are also measured. Recent results for $\sin^2 2\theta_{13}$ from Daya Bay of $0.092 \pm 0.016(\text{stat}) \pm 0.005(\text{syst})$ [20] and RENO of $0.113 \pm 0.013(\text{stat}) \pm 0.014(\text{syst})$ [21] have confirmed a nonzero value for θ_{13} that is also consistent with the results of

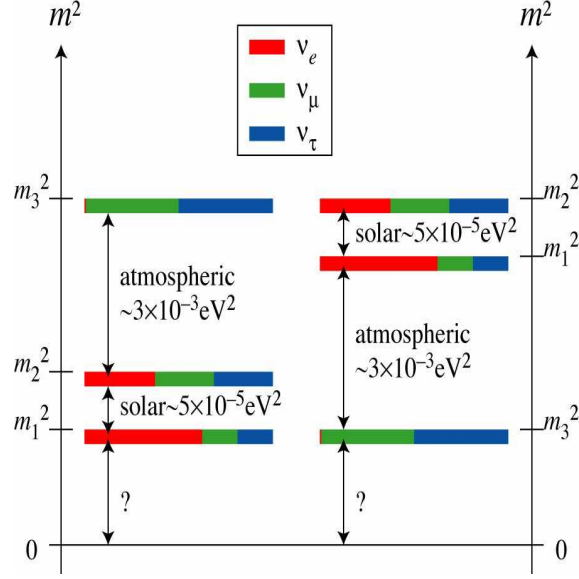


Figure 2.1: The normal (left) and inverted (right) mass hierarchy of neutrino mass, based upon the ordering of the mass differences from the neutrino oscillation experiments.

T2K [22] and Double Chooz [23].

2.1.1 Mass Hierarchy

The oscillation experiments are only sensitive to the differences in the squares of the neutrino masses, not the absolute neutrino mass scale. Different mass hierarchical models are plausible. Figure 2.1 shows the hierarchical models for the normal case ($m_1 \sim m_2 \ll m_3$) and the inverted case ($m_1 \ll m_2 \sim m_3$). Another possibility is the degenerate case ($m_1 \sim m_2 \sim m_3$).

2.1.2 Constraints on the Absolute Neutrino Mass

Even with these mass hierarchy considerations, only a lower limit on the absolute value of the neutrino mass scale can be made from the largest mass difference

($m > 0.04$ eV) [24]. To find an upper limit on the neutrino mass, one would need to measure a characteristic that depends directly on the absolute neutrino mass, such as the rate of the $\beta\beta 0\nu$ decay.

Two other approaches to arrive at a neutrino mass upper limit are the careful measurement of the end point energy of the single β decay spectrum, where the nonzero neutrino mass has a tiny effect on the kinematics, and the indirect constraint from cosmological bounds. The KATRIN experiment [25] is planning to study the β decay of tritium with a neutrino mass sensitivity down to 0.2 eV. The current limit of this kind from the Mainz and the Troitsk experiments [26, 27] is 2.3 eV at 95% confidence level. From cosmology, the massive neutrino would impact baryon acoustic oscillations, cosmic microwave background radiation, weak gravitational lensing of galaxies, and supernovae properties. The latest results from Planck's precise measurement of the Cosmic Microwave Background and Baryon Acoustic Oscillations [28] set a limit of $\sum_{i=1}^3 m_i < 0.23$ eV at the 95% confidence level.

2.2 Majorana Neutrino

Massive fermions in the Standard Model are represented by four-component spinors, Ψ . Ψ can be split into left- and right- handed components, Ψ_L and Ψ_R , where Ψ_L and Ψ_R are eigenfunctions of the γ^5 operator, also known as the chirality

matrix. The spinors must satisfy the Dirac equation:

$$\begin{aligned} i(\hat{\sigma}^\mu \partial_\mu) \Psi_R - m_D \Psi_L &= 0, \\ i(\sigma^\mu \partial_\mu) \Psi_L - m_D \Psi_R &= 0, \end{aligned} \tag{2.3}$$

where m_D is the Dirac mass and σ^μ are the Pauli matrices.

Ettore Majorana discovered in 1937 that for an electrically neutral particle, such as the neutrino, the four-component spinor could be expressed in terms of a single independent two-component spinor, ψ [29]. Written in this way, the right- and left- handed fields, ψ_R and ψ_L , both independently obey the Majorana equation:

$$\begin{aligned} i(\hat{\sigma}^\mu \partial_\mu) \psi_R - m_R \epsilon \psi_R^* &= 0, \\ i(\sigma^\mu \partial_\mu) \psi_L - m_L \epsilon \psi_L^* &= 0, \end{aligned} \tag{2.4}$$

where $\epsilon = i\sigma_y$ and m_R and m_L are the right- and left- handed masses. The full four-component spinor is now an eigenstate of the CP transformation. Due to this property, the particle and anti-particle are identical. A particle that is identical to its anti-particle is called a *Majorana* particle.

A neutral fermion can have both types of mass terms: Dirac and Majorana. The full Lagrangian mass term, $\mathcal{L}$, is then written as the sum

$$\begin{aligned} \mathcal{L} &= \mathcal{L}_D + \mathcal{L}_M \\ &= -m_D (\overline{\Psi}_L \Psi_R + H.c.) - \frac{m_L}{2} [(\overline{\Psi}_L^c) \Psi_L + H.c.] - \frac{m_R}{2} [(\overline{\Psi}_R^c) \Psi_R + H.c], \end{aligned} \tag{2.5}$$

where $\mathcal{L}_D$ and $\mathcal{L}_M$ are the Dirac and Majorana mass terms, respectively. This

Lagrangian can be rewritten as

$$\mathcal{L} = -\frac{1}{2}(\overline{n_L^c})\mathcal{M}n_L + H.c., \quad (2.6)$$

where a combined spinor, n_L is defined as

$$n_L = \begin{bmatrix} \Psi_L \\ (\Psi_R)^c \end{bmatrix}, \quad (2.7)$$

and the mass matrix, $\mathcal{M}$, is defined as

$$\mathcal{M} = \begin{pmatrix} m_L & m_D \\ m_D & m_R \end{pmatrix}. \quad (2.8)$$

Majorana neutrinos are favored by theorists due to their potential to explain the unusually small value of the neutrino masses compare to other Standard Model particles. The explanation is through a process known as the “see-saw” mechanism [30]. The see-saw mechanism arises if there is a hierarchy among the mass matrix elements in equation 2.8 such that $m_L \ll m_D \ll m_R$. In many theories, m_L is expected to be zero, while m_R is expected to be very large, on the order of the symmetry-breaking Grand Unified Theory (GUT) scale. The Dirac mass term, m_D , on the other hand, can be taken to be of the same order as the quark or charged lepton masses, since it should come from similar mechanism. Diagonalizing $\mathcal{M}$

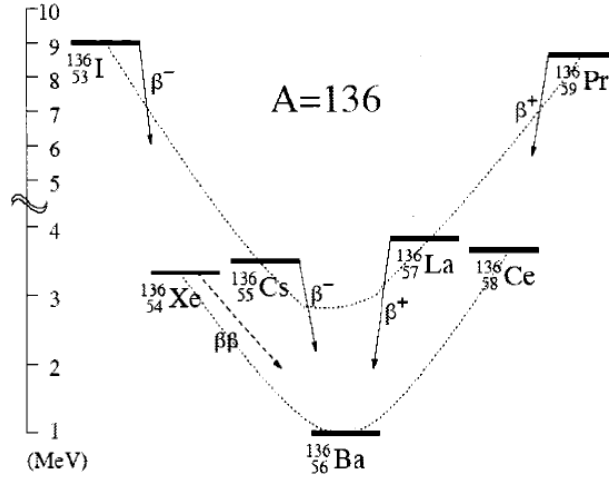


Figure 2.2: Nuclear binding energy levels for nuclei with $A=136$. Note that there are two separate parabolas: one for the “odd-odd” and the other for “even-even” nuclei. The single β decay for ^{136}Xe is forbidden.

would then result in two mass eigenvalues:

$$m_\nu \approx m_{\text{light}} \approx \frac{m_D^2}{m_R}, \quad (2.9)$$

and

$$m_{\text{heavy}} \approx m_R. \quad (2.10)$$

The result of the see-saw mechanism is that we have one extremely light neutrino, which is consistent with experimental results, and one extremely heavy neutrino, which has yet to be observed.

2.3 Double Beta Decay

Double beta decay is a second order semileptonic process in which a nucleus with charge Z and mass A decays into a nucleus with charge $Z-2$ (or $Z+2$ for the

case of $\beta^+\beta^+$ decay) and mass A . The standard two neutrino channel ($\beta\beta 2\nu$), first considered by Goeppert-Mayer in 1935 [31], is allowed by the Standard Model. The neutrinoless channel ($\beta\beta 0\nu$) would constitute new physics beyond the Standard Model. Schematic Feynman diagrams of these two processes are shown in Figure 2.3.

Since the expected half-life for this process is much smaller than that of regular beta decay, experiments looking for double beta decay choose nuclei where the single beta decay is not energetically allowed. In these nuclei, the initial nucleus must be less bound than the final one, but more bound than the intermediate nucleus. Such is the case for some even-even (even number of protons and even number of neutrons) nuclei such as ^{136}Xe , whose nuclear binding energy level is shown in Figure 2.2, where the β decay to ^{136}Cs is forbidden compared to $\beta\beta$ to ^{136}Ba . All ground states of even-even nuclei have spin and parity 0^+ , so a $0^+ \rightarrow 0^+$ transition is expected for most double beta decays, although the $0^+ \rightarrow 2^+$ transition is also possible in certain cases, even though it is highly suppressed relative to the 0^+ transition [32]. The various modes of $\beta\beta$ decays are potentially distinguishable by the shape of the sum electron energy spectra, as shown in Figure 2.4. Since neutrinos (and also Majorons) are neutral particles that will likely elude the detector, the actual energy depositions detected will be only the total energies of the two electrons.

For all modes of the double beta decays, whether it is $\beta\beta 2\nu$ (section 2.3.1), $\beta\beta 0\nu$ (section 2.3.2), or Majoron (section 2.3.3.1), one can separate in the rate formula, the nuclear matrix element term (all nuclear structure dependent effects) and the phase space term. The phase space term can be calculated with high

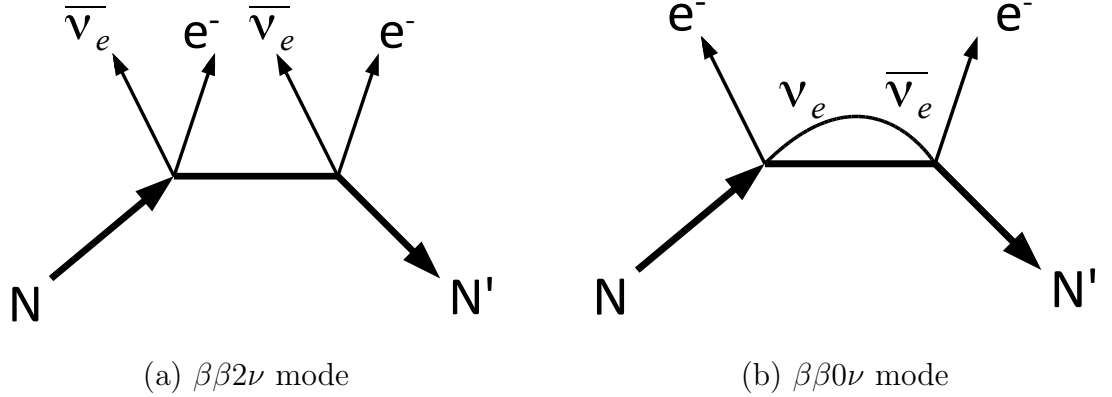


Figure 2.3: Schematic diagrams for the $\beta\beta 2\nu$ mode (a) and the $\beta\beta 0\nu$ mode (b) of the ^{136}Xe double beta decay.

accuracy. The nuclear matrix element depends on the nuclear model used for the calculations. For the $\beta\beta 2\nu$ case, the factors entering the $\beta\beta 2\nu$ matrix elements are related to other nuclear phenomena, and thus testable [4].

For xenon, two other isotopes are double beta decay candidates: ^{134}Xe and ^{124}Xe . The lower Q-value of 847 keV for ^{134}Xe severely restricts the experimental outlook to see this above the $\beta\beta 2\nu$ decay of ^{136}Xe . ^{124}Xe has a more unique signature because it would produce $\beta^+\beta^+$ (to be discussed in 2.3.3.2), but it is extremely rare in nature, consisting of only 0.10% of all natural xenon. Being the lightest isotope of xenon, ^{124}Xe has a negligible presence in the centrifugally enriched xenon used in EXO-200.

2.3.1 $\beta\beta 2\nu$ mode

The two neutrino double beta decay,

$$(Z, A) \rightarrow (Z + 2, A) + e_1^- + e_2^- + \bar{\nu}_{e1} + \bar{\nu}_{e2}, \quad (2.11)$$

is a second order process allowed by the Standard Model, as shown in Figure 2.3a. Both electric charge and lepton number are conserved. The first recorded inferred double beta decay observation occurred in 1949 in a geochemical experiment with ^{130}Te by Inghram and Reynolds [33]. Following that, 2ν double beta decays have been directly observed for ^{48}Ca , ^{76}Ge , ^{82}Se , ^{96}Zr , ^{100}Mo , ^{116}Cd , ^{130}Te , ^{136}Xe , and ^{150}Nd , while indirectly observed in another geochemical experiment for ^{238}U . The electron sum energy of this process (Figure 2.4), is that of a 4 body process (2 neutrinos and 2 electrons, with the nucleus essentially at rest). The end point of the spectrum, the maximum possible total energy for the two electrons, is determined by the Q-value (the energy difference of the parent and the daughter nucleus) of the decay.

The $\beta\beta 2\nu$ half-life is

$$[T_{1/2}^{2\nu}]^{-1} = G^{2\nu}(E_0, Z) \left| M_{GT}^{2\nu} - \frac{g_V^2}{g_A^2} M_F^{2\nu} \right|^2, \quad (2.12)$$

where the $M^{2\nu}$'s are the nuclear transition matrix elements (Gamow-Teller (GT) and Fermi (F) terms), $G^{2\nu}$ is the phase space integral that depends on the Q-value (E_0) and the atomic number of the daughter nucleus (Z), and g_V and g_A are the vector and axial-vector weak interaction coupling constants, respectively. For all $0^+ \rightarrow 0^+$ transition, including to the 0^+ excited state, the half-life can be written in this form. Between the decays to the ground state and to the excited state, the actual values of the nuclear matrix elements are expected to be different.

For $\beta\beta 2\nu$, the $M_F^{2\nu}$ term is suppressed because the Fermi operator does not

connect states of different isospin. Most models do contain a small isospin violation, so $M_F^{2\nu}$ is nonzero. Since $M_F^{2\nu}$ is much smaller than $M_{GT}^{2\nu}$, $M_F^{2\nu}$ is often neglected in calculations [32].

2.3.2 $\beta\beta 0\nu$ mode

The neutrinoless double beta decay,

$$(Z, A) \rightarrow (Z + 2, A) + e_1^- + e_2^-, \quad (2.13)$$

is a non-Standard Model process that violates lepton number conservation by two units, since two electrons or positrons are produced without antineutrino or neutrino. Neutrinoless double beta decay has not yet been conclusively observed for any nuclei. It is a process that requires that neutrinos are both massive and that they are their own anti-particle (Majorana in nature). If the neutrino does have a Majorana mass term, so that the Lagrangian looks like equation 2.5, then a $\beta\beta 0\nu$ decay is possible.

The neutrinoless double beta decay half-life is

$$[T_{1/2}^{0\nu}]^{-1} = G^{0\nu}(E_0, Z) \left| M_{GT}^{0\nu} - \frac{g_V^2}{g_A^2} M_F^{0\nu} \right|^2 \langle m_\nu \rangle^2, \quad (2.14)$$

where the $M^{0\nu}$'s are the nuclear transition matrix elements: Gamow-Teller (GT) and Fermi (F) terms, $G^{0\nu}$ is the phase space integral, and $\langle m_\nu \rangle$ is the effective neutrino mass defined as

$$\langle m_\nu \rangle^2 = \left| \sum_i^N (|U_{fi}|^2 e^{\alpha_i} m_i) \right|^2, \quad (2.15)$$

with U_{fi} representing the PMNS mixing matrix of the corresponding neutrino mass eigenstates m_i , and α_i are the Majorana phases which are unknown. The current best constraint on the $\beta\beta 0\nu$ half-life for all nuclei is $\sim 10^{25}$ year.

For the neutrinoless double beta decay to occur, a right-handed antineutrino must become a left-handed neutrino to be absorbed, as indicated in Figure 2.3b. Therefore, if neutrinoless double beta decay is observed, then the neutrino is a Majorana particle.

Since there are no other particles produced than the two electrons, the electron energy of $\beta\beta 0\nu$ would sum to the Q-value. In Figure 2.4, the total electron energy for $\beta\beta 0\nu$ is just a narrow line in the spectrum. In practice, however, a realistic energy resolution of the detector would turn the delta function at the Q-value into a gaussian distribution around the Q-value. Consequently, energy resolution is paramount in the neutrinoless double beta decay experiments in order to distinguish between $\beta\beta 0\nu$, $\beta\beta 2\nu$, and possible Majoron modes.

2.3.3 Other $\beta\beta$ decay modes

2.3.3.1 Majoron mode

Another class of double beta decays involves the emission of the Majoron, χ ,

$$(Z, A) \rightarrow (Z + 2, A) + e_1^- + e_2^- + \chi. \quad (2.16)$$

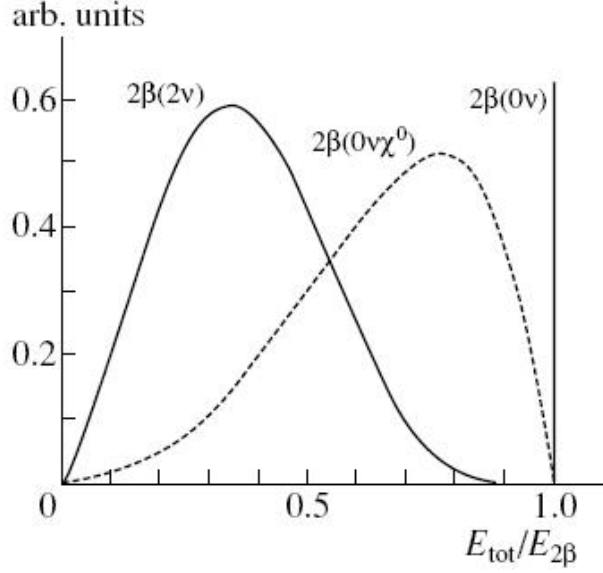


Figure 2.4: Sum electron energy spectra for the three modes of double beta decays: $\beta\beta 2\nu$, $\beta\beta 0\nu$, and the neutrinoless Majoron. Each is normalized arbitrarily and independently from the others. Figure is taken from [2].

The Majoron is a theorized massless Goldstone boson that arises from a global spontaneous breakdown of the B-L symmetry, where B and L are baryon and lepton numbers, respectively. Different Majoron models exist based on its transformation properties under weak isospin [34]. The Majoron is similar to a neutrino in that both will elude detection by a standard double beta decay experiment. The Majoron changes the sum electron energy spectrum but in a different way from $\beta\beta 2\nu$, as indicated in Figure 2.4. Newer models of the “Majoron” encompass any massless and light bosons that are associated with neutrinos. In some of these models, the Majoron can carry a lepton charge and is not bound to be a Goldstone boson [2]. If they do exist, Majorons could affect the early evolution of the Universe or star formation.

2.3.3.2 $\beta^+\beta^+$ decays

Besides the cases where $(Z,A) \rightarrow (Z+2,A)$, analogous double beta decays where $(Z,A) \rightarrow (Z-2,A)$ are also possible. Six nuclei (including one xenon isotope, ^{124}Xe) are candidates for this decay. In these double β^+ decays, a pair of protons decay into a pair of neutrons producing a pair of positrons. The positrons deposit their kinetic energy in the xenon and annihilate quickly with nearby atomic electrons to create two pairs (one positron per pair) of back-to-back 511 keV photons, making it easier to detect than electrons. Despite this advantage, the $\beta^+\beta^+$ decays are suppressed compared to the $\beta^-\beta^-$ decays due to the Coulomb barrier for positrons and a substantially lower kinetic energy realized in such transitions [2]. The lower decay rate due to the Coulomb interaction is found in the Fermi function, as described in section 2.3.5.

2.3.3.3 EC captures

A competing process for double β^+ decay is the electron capture (EC) decay, which is energetically favored over β^+ decays [2]. In the case of EC, however, the rest mass of the initial-state atomic electron contributes to the available energy of the decay, whereas for β^+ decay, the rest mass of the final-state positron subtracts from the decay energy. This means that $\beta^+\beta^+$ modes have Q-values which are smaller than the competing EC decays by two electron masses. Furthermore, since the electron mass contributes energy in the case of EC, the final-state nucleus may be larger than the initial-state nucleus by up to one electron mass. This means that

many decays which are kinematically forbidden for β^+ decays are allowed as EC decays.

2.3.4 $\beta\beta$ decay rates

For a $\beta\beta 0\nu$ process, the differential beta decay spectrum has the form of

$$d\Gamma(\beta\beta 0\nu) \sim F(E_1, Z)F(E_2, Z)p_1p_2E_1E_2, \quad (2.17)$$

where p_1 , p_2 , E_1 , and E_2 are the momenta and energies of the final state electrons, and $F(E, Z)$ is the Fermi function.

For $\beta\beta 2\nu$, the rate as approximated by Boehm and Vogel [32] is

$$d\Gamma(\beta\beta 2\nu) \sim (E_0 - E_1 - E_2)^5 F(E_1, Z)F(E_2, Z)p_1p_2E_1E_2, \quad (2.18)$$

with the same parameterization and E_0 is the maximum energy difference (the Q-value plus twice the electron mass for the case of the β^+). Note that in this expression, the angular terms have already been integrated out in the sum spectrum. These rates are sometimes written in other forms, often using a closed form approximation of the Fermi function. We will show how the standard Fermi function approximation (Primakoff-Rosen) does not really apply for the ^{136}Xe decays in section 5.2.1.

2.3.5 Fermi Function

In beta decay theory, the Fermi function describes the effect of the Coulomb interaction between the final-state beta particle and the final-state nucleus. In β^- decay, the beta experiences a force of attraction to the positively charged nucleus. This attraction has the effect of distorting the beta spectrum towards lower energies. In β^+ decay, the positive charges repel one another, and the spectrum is biased towards higher energies.

In addition to changing the spectrum, the Coulomb interaction also has a large effect on the total decay rate, because the amplitude for the decay depends on the overlap of the wavefunctions of the final state particles. The electron wavefunction is larger near the nucleus compared to the positron wavefunction. Consequently, the β^- decay is favored over the β^+ decay, when all other factors are equal. The parameterization of the Fermi function used in the EXO simulation's phase space calculations to generate $\beta\beta$ events is discussed in more detail in section 5.2.1.

2.3.6 Nuclear Matrix Elements

Nuclear matrix elements (NME) typically consist of a wavefunction describing the 0^+ ground state of the even-even parent nucleus, a wavefunction describing the final state of the even-even daughter nucleus, and an operator connecting those states. Historically, the two main methods for calculating the matrix elements of $\beta\beta$ decays are the Interacting Shell Model (ISM) and the Quasiparticle Random Phase Approximation (QRPA). These two methods are rather complementary to

each other. The QRPA uses a large number of single particle states, but in a limited number of configurations; the ISM treats only a small fraction of the single particle nucleon states, but includes all possible configurations of those states. The less computationally intensive nature of QRPA means that there are more QRPA calculations than ISM. In addition to QRPA and ISM, a few new methods have been developed in recent years. The Interacting Boson Model (IBM-2) treats the nucleus as a correlated $J^P = 0^+$ (S) and $J^P = 2^+$ (D) bosonic pair states of identical nucleons and use the bosonic neutron-proton quadrupole interaction to account for the deformation effect. One of the $\beta\beta$ calculations consulted, from Kotila and Iachello [35], is based upon IBM-2. The advantage of this method is that any nuclei of interest, whether it is $\beta^-\beta^-$ or $\beta^+\beta^+$ can be calculated with the same model. A more detailed review of the various NME can be found in [36] by Vogel, although when this review was written in 2012, IBM-2 was not capable of calculating $M^{2\nu}$.

2.3.7 Usefulness of $\beta\beta 2\nu$ Measurements

The detection of the $\beta\beta 2\nu$ process allows for a cross-check of the matrix element calculations and the models upon which they are based. Improvements in these 2ν calculations will also help with the 0ν decay predictions. While the actual matrix elements are not the same for the $\beta\beta 0\nu$, $\beta\beta 2\nu$, or either of the two to the excited state cases, the theories that correctly predict the measurable $\beta\beta 2\nu$ matrix elements are usually held in higher regard. Additionally, certain free parameters of the theories can be tuned by knowing the $\beta\beta 2\nu$ matrix element from experiment.

There have also been theoretical attempts to relate the NME's $M^{2\nu}$ and $M^{0\nu}$ directly, in particular because the two modes have the same initial and final states. For example, Simkovic et al. [37] tried to relate the dominant Gamow-Teller part, $M_{GT}^{0\nu}$, of $M^{0\nu}$ to the matrix element, $M^{2\nu}$ of the $\beta\beta 2\nu$ in the closure approximation, $M_{cl}^{2\nu}$, and then to relate $M_{cl}^{2\nu}$ to the true value of $M^{2\nu}$. The result is a relation that involves a neutrino potential, $H(r, E)$, that is dependent on the distance, r , between the two neutrons in the nuclei that decay into the two protons.

2.4 $\beta\beta$ Decays to the Excited State

Typically, the search for double beta decay focuses on the transition to the ground state (g.s.). However, for the cases where an excited state (e.s.) of the daughter ion is energetically accessible, the decays to the excited state are also allowable. The decays to the excited states are interesting in that they give information about the decay schemes of nuclei, constrain aspects of the nuclear matrix elements, and limit exotic theories about alternate decay mechanisms of $\beta\beta$ decay candidates. By measuring the decays to the excited state, supplementary information about $\beta\beta$ decays can be obtained. The nuclear matrix elements of the transition to the ground state and to the excited state may have common uncertainties, which would cancel in the ratio of the two decay rates. More precise extraction of the effective neutrino mass from half-life measurements is possible with better knowledge of these nuclear matrix elements. In some extreme cases, the $\beta\beta 0\nu$ decay to the excited state may present an unique signature (with only a minimal suppression relative to the ground

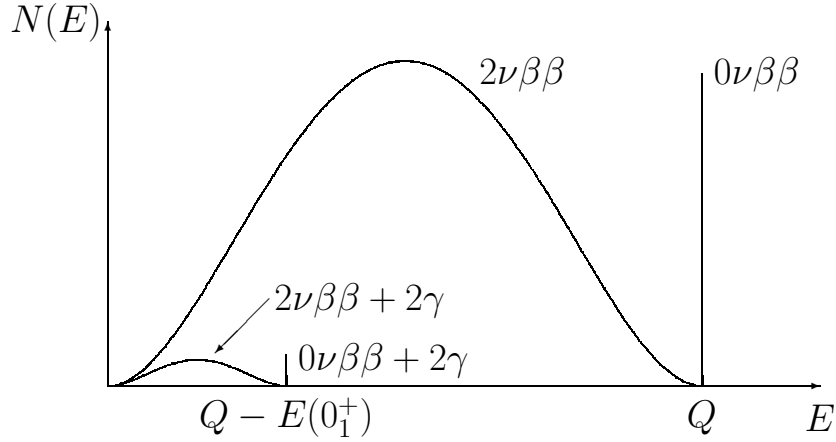


Figure 2.5: Sum electron energy spectra for the regular $\beta\beta 0\nu$ and $\beta\beta 2\nu$ and the $\beta\beta 0\nu$ and $\beta\beta 2\nu$ to the excited state. Note that for the decay to the excited state, the energies of the γ 's are not included here, even though they are expected to be measured by a detector. Figure is taken from [3].

state decay) that may make it easier to be detected than the regular $\beta\beta 0\nu$ decay [38].

Figure 2.5 compares the $\beta\beta$ spectra (including only the energies of the β 's) for the decay to the excited state and the decay to the ground state. Basically, the $\beta\beta$ energy is now much lower due to the smaller difference in energy level. However, two γ 's with very specific energy can be observed in coincidence (the half-lives of these excited states are typically very short), making for a rather unique signal.

The first investigation of double beta decay to excited states was performed by E. Fiorini in 1977 as a side study in a bigger $\beta\beta 0\nu$ to ground state experiment in ^{76}Ge [39]. The first dedicated search was the Milano experiment in 1982 [40], while the first positive signal was obtained in 1995 for the $\beta\beta 2\nu$ decay mode of ^{100}Mo to the excited state 0_1^+ of ^{100}Ru [41]. Decays to excited state have also been observed in ^{150}Nd in 2004 [42]. The decay of ^{100}Mo to the excited state was precisely

Table 2.1: Comparison of the measured half-lives to excited state (e.s.) vs. ground state (g.s.)

Nuclei	$E_{2\beta}$, keV	Experiment, $T_{1/2}$, yr (to g.s.)	Experiment, $T_{1/2}$, yr (to 0^+ e.s.)
^{150}Nd	2627.1	$6.8 \pm 0.8 \times 10^{18}$ [47]	$1.33^{+0.36}_{-0.23} \times 10^{20}$ [42]
^{100}Mo	1903.7	8.5×10^{18} [47]	$5.5^{+1.2}_{-0.8} \times 10^{20}$ [43]

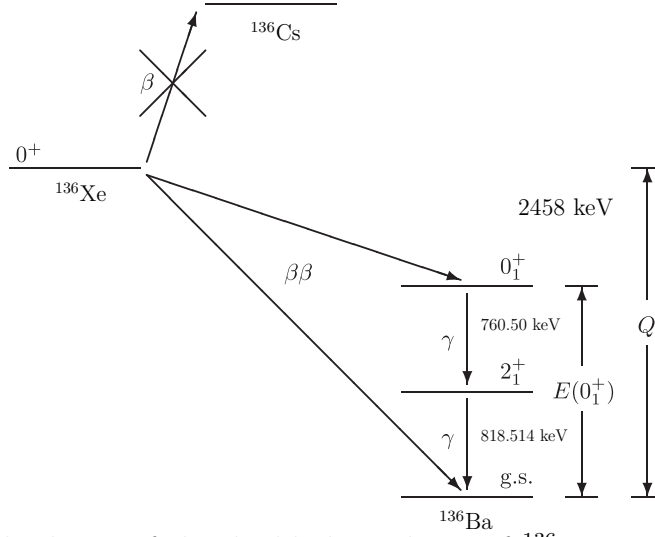


Figure 2.6: Level scheme of the double beta decay of ^{136}Xe . Decay to the excited state of 0_1^+ will result in the emission of two γ 's in its de-excitation to the ground state. The branching ratios of the γ de-excitations are nearly 100%. This figure is based upon a schematic of the ^{76}Ge decay to excited state in [3].

measured by the NEMO-3 experiment where all the β 's and γ 's tracks were observed [43]. All these observations are considered to be the $\beta\beta 2\nu$ case only. A comparison of the measured half-lives to the ground state and the excited state for ^{150}Nd and ^{100}Mo is shown in Table 2.1. Other isotopes for which the double beta decays to the excited state have been searched for include ^{82}Se , ^{76}Ge , ^{116}Cd [44], ^{110}Pd and ^{102}Pd (via β^+ or EC) by an experiment at HADES underground lab [45], and ^{130}Te by CUORICINO [46].

Figure 2.6 shows the energy level diagram for the decay to the excited state of

^{136}Xe in detail. Out of the usual 2458 keV transition to the ground state, only 879 keV goes to the $\beta\beta$ (and the neutrinos for the case of $\beta\beta 2\nu$) in the decay to the first excited 0_1^+ state. From this first 0_1^+ excited state of Ba-136, the nuclei de-excite to the ^{136}Ba ground state via the emission of two γ 's of energies 760.5 keV and 818.5 keV. The half-lives at these excited states are expected to be in the picosecond range or shorter.

Just like the regular $\beta\beta$ decays to the ground state, the decay to the excited state involves quite a few different possibilities. While the main focus of this thesis is the search for the $\beta\beta 2\nu$ decay to the first 0^+ excited state, the other decays are also interesting for various reasons.

The direct decay to the 2^+ state is highly suppressed due to phase space consideration. The phase space factor for $\beta\beta 2\nu$ to the 2^+ state contains a factor of $(E_1 - E_2)(p_1 - p_2)$, meaning that the two electrons must be antisymmetric in the electron and antineutrino energies, unlike the decay to the 0^+ where the spectrum has a maximum for $E_1 = E_2$ [32]. Nevertheless, there are certain isotopes (^{96}Zr , ^{100}Mo , and ^{130}Te) that are expected to have relatively reasonable half-lives in the 10^{22} to 10^{24} year range in the decay to the 2^+ state [38]. For right-handed currents, the transition to the first excited 2^+ state is interesting due to the vanishing of the mass term in the first order [34]. The $\beta\beta 0\nu$ decay to the 2^+ state is not sensitive to the neutrino mass contribution, however [38]. For ^{134}Xe , given the low Q-value, only the very unfavorable transition to 2^+ excited state of the daughter ^{134}Ba is lower in energy than the parent's ground state. Between the low likelihood of this transition and the low energy of the resultant particles, a search for the ^{134}Xe decay to the

excited state is not practical.

A slightly different process is the ECEC(0ν) transition, although it is not plausible in xenon due to the ^{124}Xe Q-value. In these electron capture case, the “decay” is more of a resonance transition to an excited state that is almost degenerate in energy (~ 1 keV difference). This decay also benefits from the unique signature from the de-excitation and emissions of a couple of γ ’s with very specific energies. While the β^+ decays are suppressed relatively to the regular β^- decays, a possible enhancement of about 10^6 means that this unique transition may be competitive with $\beta\beta 0\nu$ for sensitivity to the neutrino mass [38]. A half-life limit in the 10^{18} year range has been set for the ^{74}Se - ^{74}Ge transition [48].

2.4.1 Expected Decay Rate Suppression for ^{136}Xe to 1st 0_1^+ e.s.

For the $0^+ \rightarrow 0^+$ transitions, equations 2.12 and 2.14 show the relationship between the decay rate, inversely proportional to the half-life, in terms of the corresponding phase space factor and nuclear matrix elements. In the decay to the excited states, the same relationship applies although the PSF and NME should both be different. For the phase space factor (PSF), the $G(Q,Z)$ term is now different given the smaller Q-value to the excited state. The nuclear matrix element (NME) is also expected to be different for the decay to the excited state, with different $M_{GT}^{2\nu}$ and $M_F^{2\nu}$ terms, although the constants g_V and g_A are the same. While the $\beta\beta 0\nu$ decay rate does depends on the effective mass, that term is cancelled out in the ratio of the decay rates to the excited and to the ground states. So for both $\beta\beta 2\nu$ and $\beta\beta 0\nu$,

the expected excited state decay rate can be obtained from the ground state decay rate by just knowing the phase space factors and NME's of both decays.

Specifically for this analysis, the expected rate for the $\beta\beta 2\nu$ decay of ^{136}Xe to the first excited state is calculated from the known measured $\beta\beta 2\nu$ rate to the ground state and theoretical values for the phase space factor and nuclear matrix elements. From equation 2.12, the half-life of the $\beta\beta 2\nu$ decay is related to the phase space factor (PSF) times the square of the nuclear matrix element (NME). By using the same nuclear physics model that can calculate the PSF's and NME's for the $\beta\beta 2\nu$ decays to both the ground state and the 0_1^+ excited state, a decay rate suppression (or half-life extension) for the excited state may be theorized. By applying this expected rate suppression on the known rate of the ground state decay, an expected decay rate to the excited state can be obtained.

The expected phase space factor suppression can be trusted with some level of confidence. For the ^{136}Xe $\beta\beta 2\nu$ decays, Petr Vogel calculated the ratio of the phase space factor (using the Schenter-Vogel fermi function approximation and the Wilkinson correction for nuclei size, discussed in more depth in Chapter 5) to be $\Gamma_{g.s.} / \Gamma_{0_1^+} = 1.200 \times 10^{-18} \text{ (MeV}^2/\text{year)} / 3.065 \times 10^{-22} \text{ (MeV}^2/\text{year)} = 3956$ [49]. The smaller phase space for the decay to the excited state is due to the relatively smaller Q-value of the $\beta\beta$ transition. For every 4000 $\beta\beta 2\nu$ to the ground state events that we observe, we would expect to observe one $\beta\beta 2\nu$ event to the excited state by considering phase space factor alone. Using the phase space factors from Kotila and Iachello [11], we compared the two different phase space terms: $G_{\beta\beta 2\nu}^{gs} = 1433 \cdot 10^{-21} \text{ y}^{-1}$ and $G_{\beta\beta 2\nu}^{0_1^+} = 0.3622 \cdot 10^{-21} \text{ y}^{-1}$ and got the same suppression ratio

of 3956. For the $\beta\beta 0\nu$ case, the suppression factor to the excited state is a smaller 21.6 (Vogel) or 23.8 (Kotila/Iachello).

In some literature [3], a more crude model of the phase space factor is mentioned where the phase space factor $G(Q) = Q^n$ where $n = 5$ for $\beta\beta 0\nu$ and $n = 11$ for $\beta\beta 2\nu$. This model is based upon using the non-relativistic Primakoff-Rosen approximation for the Fermi function term that goes into the the phase space factor calculations. In Chapter 5, we will show how this model is inaccurate for the relativistic case that is a heavy daughter nucleus; in the non-relativistic Primakoff-Rosen approximation, the phase space factor does not depends on Z , the atomic mass of the daughter nucleus. By this model, the suppression of the decay to the excited state due to Q -value consideration is bigger by about an order of magnitude.

Previous searches for decays to the excited state, such as the original search of ^{100}Mo in 1995 [41], had assumed that the $M^{2\nu}$ to the excited state is the same as that to the ground state. Modern theoretical calculations expect the suppression factor to be affected by the nuclear matrix terms. While the values for the nuclear matrix elements are debatable based upon which nuclear theory one favors, an additional suppression factor of about 3 is obtained from the values of Kotila and Iachello [35] for the $\beta\beta 2\nu$, calculated using the microscopic interacting boson model (IBM-2). For the decay to the excited state, both the Gamow-Teller and Fermi nuclear matrix element terms are about 1.7 time smaller than their counterparts in the decay to the ground state. Since the rate is related to the square of the nuclear matrix element, the actual factor of importance is the square of 1.7 which is about 3. In this particular calculations, both the Gamow-Teller and Fermi terms are non-zero,

Table 2.2: Theoretical phase space factor (PSF) and nuclear matrix elements (NME's) suppressions for the ^{136}Xe $\beta\beta 2\nu$ decay to the first 0_1^+ excited state (e.s.) vs. the decay to the ground state (g.s.). Note that there is only one suppression factor from the two NME terms.

	to g.s.	to 0_1^+ e.s.	g.s./e.s. ratio	suppression factor on e.s. $[T_{1/2}^{2\nu}]^{-1}$
PSF	10^{-21} y^{-1}	10^{-21} y^{-1}		$\propto G_{2\nu}^{(0)}$
$G_{2\nu}^{(0)}$	1433 [11]	0.3622 [11]	3956	3956
NME				$\propto (M^{2\nu})^2$
$M_{GT}^{2\nu}$	2.76 [35]	1.63 [35]	1.67	2.9
$M_F^{2\nu}$	-1.44 [35]	-0.83 [35]	1.73	3.0

even though the Fermi term of the nuclear matrix element for $\beta\beta 2\nu$ is sometimes set to zero in calculations with the absence of isospin violation.

Table 2.2 shows the expected suppressions from both the phase space factor and the nuclear matrix element values obtained by the model of Kotila and Iachello [11, 35]. Because the NME consists of two terms that are not necessarily linear, it was fortunate in this situation that the suppression factors for both NME terms are about the same. Between the phase space (3956) and NME considerations (3.0), for $\beta\beta 2\nu$ of ^{136}Xe , the decay to the first 0_1^+ excited state is expected to be ~ 12000 times slower than the observed decay of $\beta\beta 2\nu$ to the ground state. Given that the observed $\beta\beta 2\nu$ rate to the ground state is $2.11 \cdot 10^{21} \text{ year}$, the expected half life for the decay to the first 0_1^+ excited state is $2.5 \cdot 10^{25} \text{ year}$. Nevertheless, the decay to the 0_1^+ state is associated with the emission of two γ 's in quick succession, creating a rather unique signature for the decay to the excited state. This thesis will focus on the search of the $\beta\beta 2\nu$ decay to the 0_1^+ state in Xe-136 in the EXO-200 experiment.

While the discussion here is to use theory to get an expectation on the decay rate to the excited state, the reverse will be true when a decay to the excited state is measured. Given the better reliability in the phase space calculations, a measured rate would be used mostly to constrain theories concerning the NME calculations. For example, the decay rates to the ground and the excited states of ^{100}Mo were used by Griffiths and Vogel [50] to compare the nuclear matrix elements, particularly the Gamow-Teller transition in a relatively heavy nucleus. The hope is that, nuclear matrix elements for a single nucleus to the excited and ground states would have common uncertainties that would cancel in the ratio of the two rates [3]. Improvement in the knowledge of the nuclear matrix elements is expected to lead to a more precise extraction of the effective neutrino mass, despite how the nuclear matrix elements knowledge would likely come from the $\beta\beta 2\nu$ case while it is the $\beta\beta 0\nu$ nuclear matrix elements that are directly related to the neutrino mass.

Looking again at Table 2.1 for the comparison of the measured half-lives to the ground state and to the excited state for ^{150}Nd and ^{100}Mo , the measured suppressions factors of the decay to the excited state were 19.5 and 64.7, respectively. Going back to the same Kotila and Iachello model [11, 35], the theoretical suppressions of the excited state rates are 240 and 3100 (see Table 2.3 for the full breakdown), about an order of magnitude greater than the actual values. It should be noted that the Fermi term of the NME is taken to be zero in these cases, so the NME suppression comes solely from the Gamow-Teller term. While it would not be prudent to say that this model systematically overestimate the suppression, perhaps the actual half-life for the decay of ^{136}Xe to the first 0_1^+ excited state could be an order of magnitude

Table 2.3: Theoretical phase space factor (PSF) and nuclear matrix elements (NME's) suppressions for the ^{100}Mo and the ^{150}Nd $\beta\beta 2\nu$ decay to the first 0_1^+ excited state (e.s.) vs. the decay to the ground state (g.s.). The $M_F^{2\nu}$ is basically taken to be zero for both isotopes in both cases. These numbers are compared to the measured values in the text.

^{100}Mo				
	to g.s.	to 0_1^+ e.s.	g.s./e.s. ratio	suppression factor on e.s. $[T_{1/2}^{2\nu}]^{-1}$
PSF	10^{-21} y^{-1}	10^{-21} y^{-1}		$\propto G_{2\nu}^{(0)}$
$G_{2\nu}^{(0)}$	3308 [11]	60.55 [11]	54.6	54.6
NME				$\propto (M^{2\nu})^2$
$M_{GT}^{2\nu}$	2.94 [35]	0.39 [35]	7.53	56.8
$M_F^{2\nu}$	0.02 [35]	0.00 [35]	n/a	n/a
Total				3100
^{150}Nd				
	to g.s.	to 0_1^+ e.s.	g.s./e.s. ratio	suppression factor on e.s. $[T_{1/2}^{2\nu}]^{-1}$
PSF	10^{-21} y^{-1}	10^{-21} y^{-1}		$\propto G_{2\nu}^{(0)}$
$G_{2\nu}^{(0)}$	36430 [11]	4329 [11]	8.4	8.4
NME				$\propto (M^{2\nu})^2$
$M_{GT}^{2\nu}$	1.54 [35]	0.29 [35]	5.31	28.2
$M_F^{2\nu}$	0.03 [35]	0.00 [35]	n/a	n/a
Total				240

smaller than our estimation of $2.5 \cdot 10^{25}$ year.

2.5 Experimental Searches for Double Beta Decay

Potential double beta decay nuclei with a Q-value of a few MeV are good candidates for $\beta\beta 0\nu$ decay searches. The natural abundance of that isotope and the feasibility of enrichment are also key considerations. The list of candidate for which $\beta\beta$ decay experiments have been designed include ^{48}Ca , ^{76}Ge , ^{82}Se , ^{100}Mo , ^{116}Cd , ^{128}Te , ^{130}Te , ^{136}Xe , and ^{150}Nd . Table 2.4 lists the current best experimental limit for each of these isotopes and a brief description of the experimental technique.

The $\beta\beta 0\nu$ experiments have used quite a variety of different detector technologies. Typically, these detectors measure the energy deposited by the emitted electrons in the form of ionization, scintillation, heat, or a combination of the above. While single mode detectors that measure only one kind of energy deposition often have the better energy resolutions, the measurement of a combination of two modes can often help discriminate between the different particle types, which is pivotal for background rejection.

2.5.1 Experimental Consideration for $\beta\beta 0\nu$ Search

Low background experimental techniques have advanced greatly over the last sixty years, leading to the discoveries of $\beta\beta 2\nu$ decays of various nuclei. The search for $\beta\beta 0\nu$ is much harder, however, in part due to the more suppressed rate.

For an experiment with mass M that runs for time t, the $\beta\beta 0\nu$ half-life limit

Table 2.4: Half-life lower limits for $\beta\beta 0\nu$ to the ground state in various isotopes.

$\beta\beta 0\nu$ 90% C.L.		Technique	Experiment
Isotope	Limit (yr)		
^{48}Ca	5.8×10^{22}	CaF ₂ scintillating crystal	ELEGANT VI Collaboration
^{76}Ge	1.9×10^{25}	High Purity Ge detector	Heidelberg-Moscow Experiment
^{82}Se	3.6×10^{23}	Thin-foil tracking calorimeter	NEMO-3 Collaboration
^{96}Zr	9.2×10^{21}	Thin-foil tracking calorimeter	NEMO-3 Collaboration
^{100}Mo	1.1×10^{24}	Thin-foil tracking calorimeter	NEMO-3 Collaboration
^{116}Cd	1.7×10^{23}	$^{116}\text{CdWO}_4$ crystal scintillators	Solotvina Experiment
^{130}Te	3.0×10^{24}	TeO ₂ bolometers	COURICINO Collaboration
^{136}Xe	5.7×10^{24}	Xenon doped scintillator	KamLAND-ZEN Collaboration
^{150}Nd	1.8×10^{22}	Thin-foil tracking calorimeter	NEMO-3 Collaboration

can be estimated in the background-limited case to be

$$T_{1/2}^{0\nu} \propto \sqrt{\frac{M \times t}{B \times \Delta E}} \quad (2.19)$$

where B is the background (typically in counts/year/kg/keV) and ΔE is the energy resolution. Sensitivity to the neutrino mass is inversely proportional to the half-life. A larger source mass, a longer data taking time, a low background, and an extremely good energy resolution are ways to increase an experiment's sensitivity to neutrino mass. In the zero background cases, the half-life limit is proportional to $M \times t$.

$\beta\beta 2\nu$ is potentially the ultimate background in the search for $\beta\beta 0\nu$, even if all other backgrounds are eliminated. Since the search for the $\beta\beta 0\nu$ signal is basically the hunt for a peak at the end of a continuum, good energy resolution at the end point energy is of paramount importance to distinguish any $\beta\beta 0\nu$ events from $\beta\beta 2\nu$ events in the tail. Figure 2.7 illustrates a $\beta\beta 0\nu$ spectrum with a realistic energy resolution along with the $\beta\beta 2\nu$ spectrum.

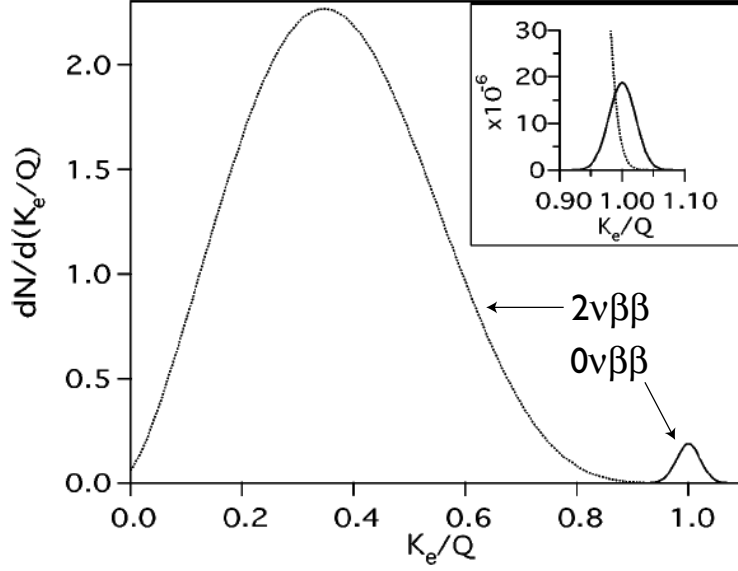


Figure 2.7: Spectra showing the $\beta\beta 0\nu$ and $\beta\beta 2\nu$ spectra with realistic energy resolution (5%). The identification of the $\beta\beta 0\nu$ line depends on great energy resolution. The $\beta\beta 2\nu$ spectrum is normalized to 1 (dotted curve) and $\beta\beta 0\nu$ decays (solid curve) is normalized to 10^{-2} (10^{-6} in the figure inset). This figure is taken from [4].

2.5.2 Non-xenon Double Beta Decay Experiments

2.5.2.1 Germanium Detectors

^{76}Ge , with a Q-value of 2039 keV, was among the first choices for a $\beta\beta$ decay experiment due to the excellent energy resolution of Ge semiconductors. Typically, a Ge semiconductor is accurate within 3-4 keV at 2 MeV. The p-type point contact (PPC) germanium detectors used by the Majorana collaboration claims a 0.2 % FWHM energy resolution at the Q-value [51]. Along with ^{136}Xe , ^{76}Ge is at the forefront of setting the current best limit on the effective neutrino mass.

2.5.2.2 Heidelberg-Moscow Experiment

The Heidelberg-Moscow experiment was a 11 kg of 86% enriched Ge detector that ran in the Gran Sasso Laboratory. After setting the then best limit on effective neutrino mass at 0.35 keV after 53.9 kg · year of data taking, a subset of that collaboration made a controversial claim of a $\beta\beta 0\nu$ observation [5, 52]. Figure 2.8 shows the energy spectrum near the Q-value, from [5]. This controversial analysis also saw an additional unidentified peak with great statistical significance. They also never studied the effect of changing the analysis energy window. The claim, in the 2006 updated analysis [52], is for a half-life of $(2.23^{+0.44}_{-0.31}) \cdot 10^{25}$ years with a significance of $> 6\sigma$. The equivalent effective neutrino mass obtained from this “measurement” has been disfavored by $\beta\beta 0\nu$ experiments with other isotopes, mainly ^{136}Xe [14, 53].

2.5.3 Xenon Double Beta Decays

2.5.3.1 ^{136}Xe and ^{134}Xe

^{136}Xe , with a Q-value of 2457.83 keV [54], is a double beta decay candidate with a large enough Q-value ($Q > 2$ MeV) to be experimentally observable. ^{134}Xe is another potential double beta decay candidate, but its lower Q-value of 830.1 keV makes its decay harder to be detected experimentally. Using a centrifuge, ^{136}Xe , the heaviest xenon isotope, can be separated from natural xenon. In general, these enriched xenon would also contain a high concentration of ^{134}Xe due to its mass. While it is possible to look for $\beta\beta$ decays in both of these xenon isotopes, most past and current experiments including EXO-200 focus on just ^{136}Xe because of its

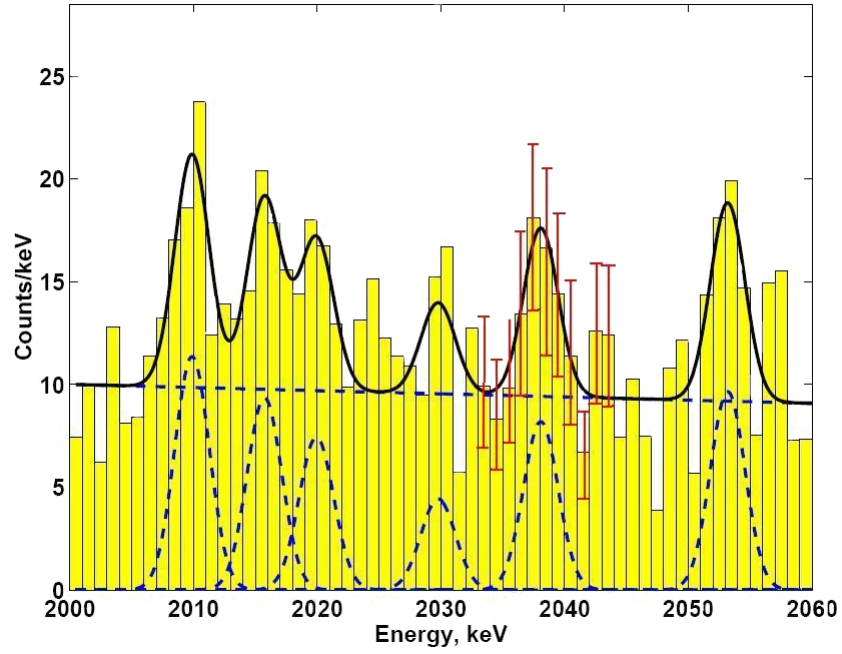


Figure 2.8: Energy spectrum from one analysis of the Heidelberg-Moscow experiment result [5] with a fit to a linear background plus six Gaussian, including four known lines from ^{214}Bi at 2011, 2017, 2022, and 2053 keV, $\beta\beta 0\nu$ at 2039 keV, and an unidentified line near 2030 keV.

advantage in the Q-value.

In 2011, EXO-200 became the first experiment to observe the $\beta\beta 2\nu$ decay to the ground state for ^{136}Xe [55]. That measurement had since been confirmed by the KamLAND-Zen experiment [56]. Only limit on the half-life has been set for the $\beta\beta 2\nu$ of ^{134}Xe .

2.5.3.2 ^{124}Xe

Despite a natural abundance of merely 0.09%, ^{124}Xe is of special interest due to its potential to undergo a double positron decay into ^{124}Te . Because of it being the lightest xenon isotope, ^{124}Xe represents a negligible amount of the centrifugally enriched xenon, like that used in EXO-200. Like ordinary β^- decays, multiple modes of the $\beta^+\beta^+$ decay are also possible, the familiar $\beta\beta 0\nu$ and $\beta\beta 2\nu$ cases as well as many EC channels. Here is a full list of potential ^{124}Xe decays:

$$^{124}\text{Xe} \rightarrow ^{124}\text{Te}\beta^+\beta^+, \quad (2.20)$$

$$^{124}\text{Xe} \rightarrow ^{124}\text{Te}\beta^+\beta^+\nu\nu, \quad (2.21)$$

$$^{124}\text{Xe}(EC) \rightarrow ^{124}\text{Te}\beta^+(K), \quad (2.22)$$

$$^{124}\text{Xe}(ECEC) \rightarrow ^{124}\text{Te}(KK), \quad (2.23)$$

$$^{124}\text{Xe}(EC) \rightarrow ^{124}\text{Te}\beta^+\nu\nu(K), \quad (2.24)$$

$$^{124}\text{Xe}(ECEC) \rightarrow ^{124}\text{Te}\nu\nu(KK). \quad (2.25)$$

In a detector, the very unique $^{124}\text{Xe } \beta^+\beta^+0\nu$ signature consists of an energy deposit of 822 keV at the center with the two positrons turning into four 511 keV annihilation gammas for a total of 2866 keV of total energy deposition. Geometrically, the five ionization clusters would be coplanar, as the photons are likely to create Compton electrons (or photo-absorptions) within 15 cm of the center cluster in liquid xenon. Imitation of such a specific events by natural backgrounds has negligible probability, even if the detector is located in an above-ground laboratory [57]. A new limit should be easily set by any sizable xenon experiment running with natural (unenriched) xenon.

Even if a limit can be easily set for the $\beta\beta0\nu$ channel, ^{124}Xe decay is not expected to produce a competitive limit on the mass of the neutrino due to the low Q-value. On the other hand, if $\beta\beta0\nu$ is one day observed in one of the more conventional isotopes like ^{136}Xe , a comparison with the neutrinoless mode of ^{124}Xe may provide information regarding the mechanism of the decay (neutrino mass vs. right-handed currents for example) [2].

2.5.3.3 Barium Tagging

Xenon double beta decays into barium. The EXO collaboration is working on developing the technology to tag the daughter barium ion to rule out natural radioactive background that deposit energy within the narrow $\beta\beta0\nu$ energy window. A successful barium tagging mechanism would require the ability to locate and extract the lone barium ion in a sea of xenon (gas or liquid) and to transfer the ion

into a typical atomic physics ion trap where laser spectroscopy can be performed to positively identify the barium ion. An effort toward developing a single ion Barium source for the testing and practice of the various tagging techniques is documented in Appendix A. If barium tagging is achieved, then the only background for the $\beta\beta 0\nu$ decay would be the $\beta\beta 2\nu$ decays at the tail of its energy spectrum whose energy has been smeared out due to the detector's nonzero energy resolution.

2.5.4 A Brief History of Xenon double beta decay searches

2.5.4.1 Baksan 1989

Installed at the Baksan neutrino observatory, at a depth of 850m water equivalent, this gridded ionization chamber experiment in 1989 [58] was one of the first xenon double beta decay experiment to set limits for all three possible xenon double beta decay isotopes. The active volume of the ionization was 3.66 liter at a pressure of 25 kgf/cm² or about 24.5 bar. Two separate turns of natural and enriched xenon were used to fill the chamber, with a small addition of 0.8% H₂ to achieve an energy resolution of about 3.8 % at an energy of 2.5 MeV. The measurement times were 243 hours for enriched xenon and 120 hours for natural xenon. At 68% C.L., the ¹³⁶Xe half life limits of 10²¹ year and 10¹⁹ year were measured for $\beta\beta 0\nu$ and $\beta\beta 2\nu$, respectively. For ¹³⁴Xe $\beta\beta 2\nu$ and ¹²⁴Xe $\beta\beta 0\nu$ and $\beta\beta 2\nu$, this experiment still has the current most sensitive half-life limits of 10¹⁶ year, 10¹⁷ year, and 10¹⁴ year, respectively [47]. The ¹³⁴Xe $\beta\beta 0\nu$ half-life limit of 10¹⁹ year was eventually passed by the DAMA experiment (see section 2.5.4.4).

2.5.4.2 Milano

The Milano experiment [59] was a multicell proportional counter experiment that ran at Gran Sasso with the results published in 1991 [60]. The detector consisted of 61 contiguous cells for a total volume of 140 liter (79 liter active volume), operating at the pressure of 9.5 bar. Three separate modes were conducted with 660 hours of natural xenon (8.86% ^{136}Xe), 6210 hours of enriched xenon (64% ^{136}Xe), and 5000 hours of xenon cleaned by ultracentrifugation to eliminate the Krypton background (10% ^{136}Xe). The experiment set a half-life limit of $2 \cdot 10^{22}$ year at 90% C.L. for $\beta\beta 2\nu$ and $6 \cdot 10^{19}$ year at 90% C.L. The authors concluded that the Gotthard gaseous TPC would be more sensitive than any proportional counter experiment. The Milano experiment also set a limit of $6.5 \cdot 10^{21}$ at 90% C.L. (and $1.1 \cdot 10^{22}$ yr at 68 % C.L.) for the ^{136}Xe decay to the first 2^+ excited state, where the sum electron energy is 1662 keV.

2.5.4.3 Gotthard

The Caltech-Neuchatel-PSI collaboration [61] built a xenon gas time projection chamber (TPC) filled with 62.5% ^{136}Xe of 180 liter at 5 atm (3.3 kg). The experiment was located at the Gotthard Underground Laboratory (3000 meters of water, equivalent) under the Swiss Alps. The simultaneous tracking and calorimetry capability of the TPC made this a significant improvement over previous xenon double beta decay experiments [62].

The first results were published in 1993. Upgrades to the readout planes and

the longer running time for $4.9 \text{ kg} \times \text{yr}$ resulted in the then most sensitive limit of $T_{1/2} > 4.4 \cdot 10^{23} \text{ yr}$ at 90% C.L. for $^{136}\text{Xe } \beta\beta 0\nu$ in 1998. Additionally, a $T_{1/2} > 0.72 \cdot 10^{22} \text{ yr}$ at 90% C.L. limit for the $\beta\beta 0\nu\chi$ was set by looking at the count rate in the energy range between 2150 and 2400 keV.

2.5.4.4 DAMA

Using 6.5 kg (about 2 liter volume) of liquid xenon pure scintillator, the DAMA collaboration [63] ran with a Kr-free xenon gas mixture with 17.1% ^{134}Xe and 68.8% ^{136}Xe for 8823.54 hours. The liquid xenon vessel was made with OFHC (oxygen-free high thermal conductivity) low radioactive copper and the scintillation light was collected by three photomultiplier tubes working in coincidence. The data collected corresponded to $1.1 \text{ kg} \times \text{year}$ for ^{134}Xe and $4.5 \text{ kg} \times \text{year}$ for ^{136}Xe . The experiment claimed a new $T_{1/2}$ limit for $\beta\beta 2\nu$ of ^{136}Xe (10^{22} yr) and $\beta\beta 0\nu$ of both ^{136}Xe ($1.2 \cdot 10^{24} \text{ yr}$) and ^{134}Xe ($5.8 \cdot 10^{22} \text{ yr}$), all limits at 90% C.L. DAMA's $\beta\beta 2\nu$ limit is in conflict with the EXO-200 $\beta\beta 2\nu$ half-life measurement [55].

2.5.4.5 Baksan 2005

Another xenon double beta decay search was conducted in Baksan Neutrino Observatory in 2005 [64], consisting of two high-pressure copper proportional counters (a fiducial volume of 9.16 liter at 14.8 atmosphere) at 4900 meter water equivalent of shielding. One counter was filled with enriched xenon while the other was filled with natural xenon with extracted light isotopes (9.2 % of ^{136}Xe). The com-

parison technique was used to minimize the problem of α backgrounds from Rn. With about 8000 hours of measurement time, the experiment found $T_{1/2}$ limits of $8.5 \cdot 10^{21}$ yr for $\beta\beta 2\nu$ of ^{136}Xe and $3.1 \cdot 10^{23}$ yr for $\beta\beta 0\nu$ of ^{136}Xe , at 90% C.L. An updated analysis in 2011 [65] with 17280 hours of measurement time, increases the $\beta\beta 0\nu$ of ^{136}Xe limit to $4.9 \cdot 10^{23}$ yr, at 90% C.L.

2.5.4.6 KamLAND-Zen

The KamLAND-Zen (KamLAND Zero-Neutrino DoubleBeta Decay) is a xenon double beta decay experiment that utilizes the KamLAND detector. The Kamioka Liquid Scintillator Antineutrino Detector (KamLAND) is an electron antineutrino observatory in Japan that measures the antineutrinos from the surrounding nuclear reactors, as well as observing the geologically produced antineutrinos from the Earth's crust and mantle. KamLAND-Zen is constructed out of 13 tons of Xe-loaded liquid scintillator (Xe-LS) in a 3.08 meter diameter transparent nylon-based inner balloon suspended inside the KamLAND detector. The inner balloon is inside an 13 meter diameter outer balloon, with 1 kilo-ton of liquid scintillator in between. Scintillation light is measured with 1325 17-inch and 554 20-inch photomultiplier tubes on the outside, which are mounted on a stainless steel tank. Outside of the stainless steel tank is a 3.2 kilo-ton water-Cherenkov detector for cosmic ray muon identification.

After the discovery of Xe-136 $\beta\beta 2\nu$ decay by EXO-200 [55], KamLAND-Zen was able to confirm the same $\beta\beta 2\nu$ rate and set the best limit for $\beta\beta 0\nu$ in Xe-136

[56]. KamLAND-Zen then set the current best limit, with 112.3 day of 125 kg of ^{136}Xe data, for the Majoron rate ($\beta\beta 0\nu\chi^0$) of $2.6 \cdot 10^{24}$ yr, at 90% C.L. [66]. After EXO-200 exceeded the KamLAND-Zen $\beta\beta 0\nu$ limit, KamLAND-Zen has an updated result [53]. They set a limit of $1.9 \cdot 10^{25}$ yr, at 90% C.L. Combining their own result with that from EXO-200 [14], KamLAND-Zen claims a combined result of $3.4 \cdot 10^{25}$ yr, at 90% C.L.

Chapter 3

The EXO-200 Detector

The EXO-200 detector is a single phase, liquid xenon time projection chamber (TPC). Xenon enriched to 80.6% in ^{136}Xe is both the source of the decay and the detection medium. The primary goal of the EXO-200 detector is to search for the $\beta\beta 0\nu$ decay of ^{136}Xe to the ground state.

The optimization of energy resolution and the minimization of radioactive background are the two main objectives that drove the EXO-200 detector design. The goal in the search for neutrinoless double beta decay is to measure the resultant energy deposition from the two betas as accurately as possible. Good energy resolution is crucial for discriminating the Standard Model allowed two neutrino double beta decays ($\beta\beta 2\nu$) from the neutrinoless decays ($\beta\beta 0\nu$). Suppression of the radioactive background, via both a very careful screening of construction material and shielding from cosmogenics, ensures that the desired neutrinoless double beta decay signal at 2458 keV is not obscured by the energy deposition of some other process.

Since radiation energy deposition inside liquid xenon results in both ionization and scintillation, the EXO-200 detector is designed for the simultaneous detection of ionization and scintillation. From the timing and the ionization charge collection location, a full three dimensional position plus time reconstruction of events is possible. By utilizing both energy deposition information from ionization and

scintillation, EXO-200 can exploit the anticorrelation characteristic of liquid xenon to further optimize energy resolution. Positional reconstruction of events, especially to distinguish events by size, also allows for some discrimination between β events from γ events.

This chapter will describe the EXO-200 detector. First, a brief discussion about the properties of liquid xenon (LXe), the detector medium, is presented. Next, the EXO-200 TPC design is depicted. Then, the support structures around the TPC to suppress backgrounds are described. The chapter ends with a discussion of the electronics.

3.1 Liquid Xenon Detector

Liquid xenon as a particle physics detector was first recognized by Alvarez's group at Berkeley in 1968 [67]. Since then, liquid xenon has now become a popular choice as a radiation detection medium in modern particle physics experiments. Like the rest of liquid noble gas detectors, liquid xenon responds to radiation with both ionization electrons and scintillation photons. Among liquid noble gases, liquid xenon has the highest stopping power for penetrating radiation due to its high atomic number (54) and density (~ 3 g/cm³). Liquid xenon also has the highest ionization and scintillation yield, the latter of which is comparable to that of NaI, but with a faster time response.

Both gaseous and liquid xenon detectors have been used in various experiments. Liquid xenon, while requiring cryogenic equipment to maintain the narrow

temperature range for the liquid phase (162K to 165K at one atmosphere), has the benefit of taking up less space than the same amount of xenon in gas form. A typical xenon detector will collect the deposited energy from both the ionization charge and the scintillation light. Measurements have shown an anti-correlation of ionization and scintillation in LXe. Thus, by summing the total signal, the fluctuations of two individual channels can be reduced to improve the energy resolution of the detector [68].

3.1.1 Ionization in LXe

In liquid xenon, the deposited energy mostly leads to the creation of electron-ion pairs. Since not all of the energy goes into the electron-ion pair, the W-value is defined as the average energy required to produce one electron-ion pair. Generally, the W-value depends weakly on radiation type and energy; therefore, it is often considered to be a constant. For xenon, the W-value is 22.0 eV in gas and about 15.6 eV in liquid [68]. The standard deviation, δ , in the fluctuation of electron-ion pairs produced by an ionizing particle depositing all of its energy in a stopping material is given by

$$\delta^2 = F \times N \tag{3.1}$$

where N is the mean number of electron-ion pairs and F , the Fano factor, is a constant less than 1 that depends on the material. For xenon, the calculated F is 0.15 in gas and 0.059 in liquid [68]. In theory, the potential energy resolution in liquid xenon could be quite good (comparable to Ge or Si detectors), but that has

yet to be achieved. In fact, experimental evidences have pointed to an unusually large Fano factor, >20 for liquid xenon [69], limiting the ultimate energy resolution achievable.

There are two regimes for the electron drift velocity in liquid xenon, depending on the electric field strength and roughly when the kinetic energy of electrons exceed kT (actual values depend on both the pressure and the temperature). At low field strength, the electron mobility is proportional to the field. The proportionality constant, known as the electron mobility μ , is about $2000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$. At high fields, however, the electron drift velocity saturates. For xenon, the electron drift velocity is much higher (by one to two orders of magnitude and decreasing with higher drift field) in liquid than in gas. A slight temperature dependence of 0.5% per $^{\circ}\text{C}$ exists for the drift velocity. A phenomenon known as electron-multiplication (or avalanche), an increase in gain which may hurt the energy resolution, occurs in liquid xenon for a very high electric field of greater than 10^6 V/cm .

To have a good measurement of the ionization yield inside the liquid xenon detector, the correct number of electron-ion pairs created needs to be known. A very high electric field is often applied in xenon detectors to minimize the recombination of electron-ion pairs. The presence of electronegative impurities can also decrease the measured ionization yield.

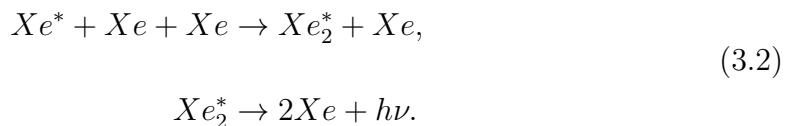
The success of a xenon detector requires the xenon to be free of electronegative impurities such as O_2 and H_2O . The impurities disrupt the transport of the ionization charge as well as the scintillation light. In many current and next-generation xenon detectors, the ionization charges are required to drift as much as 1 meter in

distance (~ 20 cm for EXO-200) before being collected by the sensing wires. This corresponds to a free electron lifetime of several hundred microseconds, or an oxygen contamination at the part-per-billion level. Electronegative impurities at the level of about 10^{-9} g/g (grams of impurity/grams of xenon) reduce the electron attenuation length to several tens of centimeters, depending on the electric field of the liquid xenon [70].

3.1.2 Scintillation in LXe

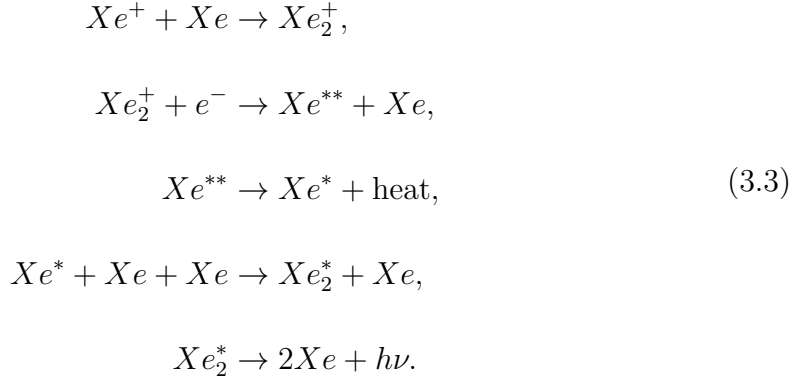
Liquid xenon scintillation has a wavelength of 178 nm which is in the “vacuum-ultraviolet” (VUV) region of the electromagnetic spectrum. In recent years, there has been much progress in developing detectors with high quantum efficiency at that wavelength, such as vacuum-ultraviolet sensitive photomultipliers (PMTs) and large area avalanche photodiodes (LAAPDs) [71].

Scintillations in liquid xenon, like other liquid noble gases, come from the decay of excited dimers to the ground state. There are two processes that produce VUV scintillation light in LXe. The first process of scintillation is exciton de-excitation:



The excited xenon atom (Xe^*) interacts with neutral xenon to form an excited dimer (Xe_2^*), which next decays with the emission scintillation light. The second process of scintillation is recombination. This process involves both the excited atoms (Xe^*)

and ions (Xe^+).



The ion (Xe^+) recombines with an electron to form a doubly excited atom, which then emits scintillation light via the same exciton de-excitations like the first process.

The equivalent of the W-value for scintillation is the W_{ph} -value, the average energy required for the production of a single photon. Because the scintillation yield depends on the linear energy transfer (LET), the density of electron-ion pair along the particle track, the W_{ph} -value is different for different particles. In liquid xenon, for α 's, W_{ph} is 17.9 eV and for β 's, W_{ph} is 21.6 eV [68]. Water vapor, from the outgassing of the liquid containment vessel and other components inside the liquid, is the most dangerous impurities for the absorption of VUV light in liquid xenon.

Scintillation light in pure LXe has two components, a short decay from the singlet state and a long decay from the triplet state of the excited dimer Xe_2^* . The intensity ratio of the two decays is related to the density of the deposited energy. Consequently, nuclear recoils have two components while scintillation from relativistic electrons has just one component. While it is not of much importance for double beta decay experiments, the ability to discriminate between nuclear and electron

recoils is very important for dark matter experiments, many of which use xenon. In LXe, however, the time separation of the two components is rather small (2.2 ns vs. 27 ns); thus, pulse shape discrimination in LXe is not used by current experiments [68].

3.2 Time Projection Chamber

The Time Projection Chamber (TPC) is installed inside a liquid xenon vessel volume of 58 liters. A cut-away view of the copper xenon vessel and the TPC is shown in Figure 3.1. Out of the total mass (~ 175 kg) of liquid xenon in EXO-200, 110 kg of liquid xenon is available in the active detector volume. The remaining xenon is either in the TPC legs or in the gas handling system. By being a TPC, the EXO-200 detector allows for the reconstruction of event position in 3 dimensions. The two, non-parallel, sets of wire planes give a position in the X-Y plane. By using the time difference between the prompt scintillation and the time that the charges are collected, the spatial position in the direction perpendicular to the plane of the wire grid can be determined.

The EXO-200 detector consists of two identical but distinct TPCs. Each half TPC is cylindrically shaped with a radius of 18.3 cm and a length of 19.8 cm. The cathode grids sits in the middle of the detector with each half having two identical wire planes serving as the induction wire grid (V-wires) and the charge collecting anode (U-wires) as well as an avalanche photodiode (APD) platter. Figure 3.2 is a photograph of one of the TPCs without the central cathode. The optical

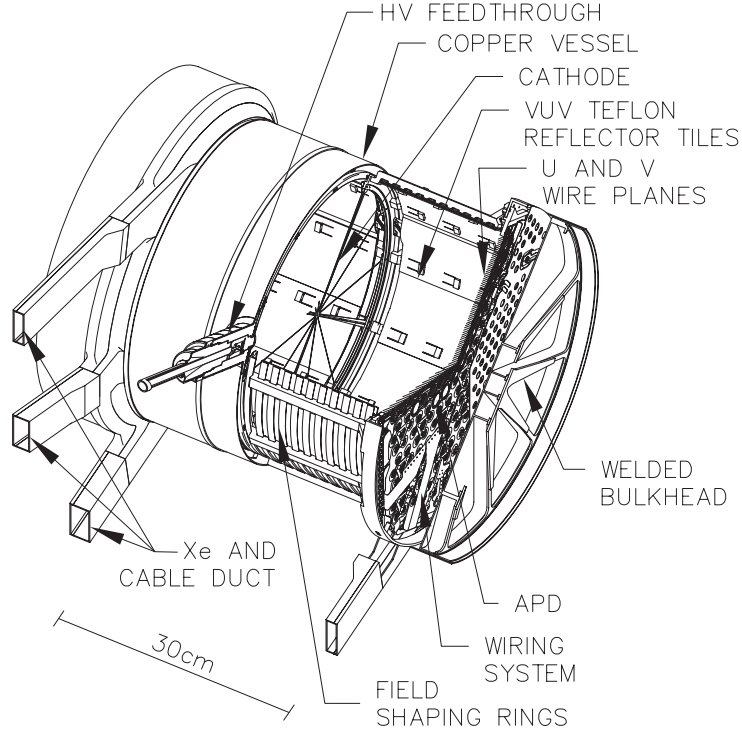


Figure 3.1: A cutaway view of the EXO-200 TPC and the copper xenon vessel, with the main components identified.

transparency of the cathode grid, along with the possibility for light to reflect off the teflon in the field shaping ring assembly and around the cathode, means that scintillation is almost always collected by both sets of APD platters. The central cathode is set to a negative high voltage of -8 kV for the data discussed in this thesis.

3.2.1 Ionization Detection in EXO-200

While a radiation deposition event in liquid xenon should produce both the negatively charged electrons and a much heavier positively charged ion, the ionization system of the EXO-200 detector is designed to detect just the electrons. The electrons are drifted inside a uniform electric field toward two sets of wire planes. All

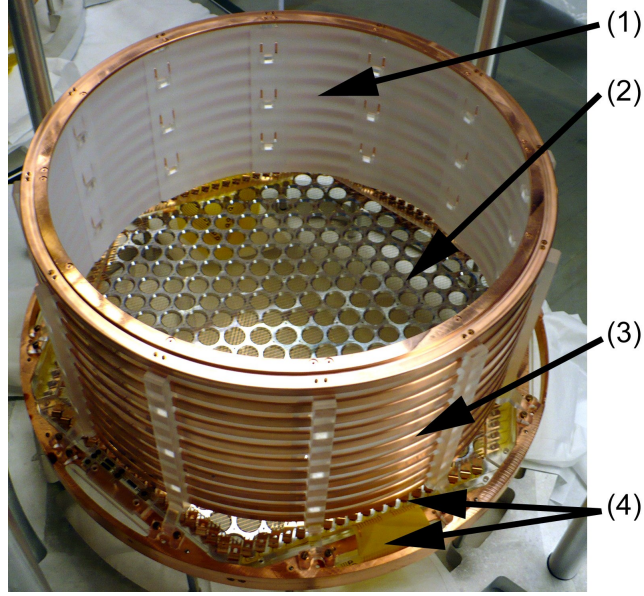


Figure 3.2: A view of one of the two EXO-200 TPC without cathode. Defining the active Xe volume, the PTFE tiles (1) on inside the field-shaping rings serve as reflectors of the scintillation light. Also visible are the aluminum-coated side of the LAAPD platter (2) without the APDs, the field cage (3), and the ionization wires and the flexible cables (4).

together, the entire charge collection system consists of the electrically opaque but optical transparent cathode wire plane in the center of the detector, the field shaping cage to provide the uniform electric field and effectively determine part of the active volume, and the two sets of identical wire planes that are 60° from each other. The first induction plane (V-wires) is biased to be electrically transparent, and the second plane (U-wires) is designed to be the charge collector. The non-parallel angular orientation of the two wire girds allows for a two-dimension reconstruction in the plane (X- and Y- in the coordinates used in this thesis) perpendicular to the drift length (in the direction Z).

Figure 3.3 illustrates the simulated result of how the electron cloud from a double beta decay event is collected by the two wire planes. The distances between

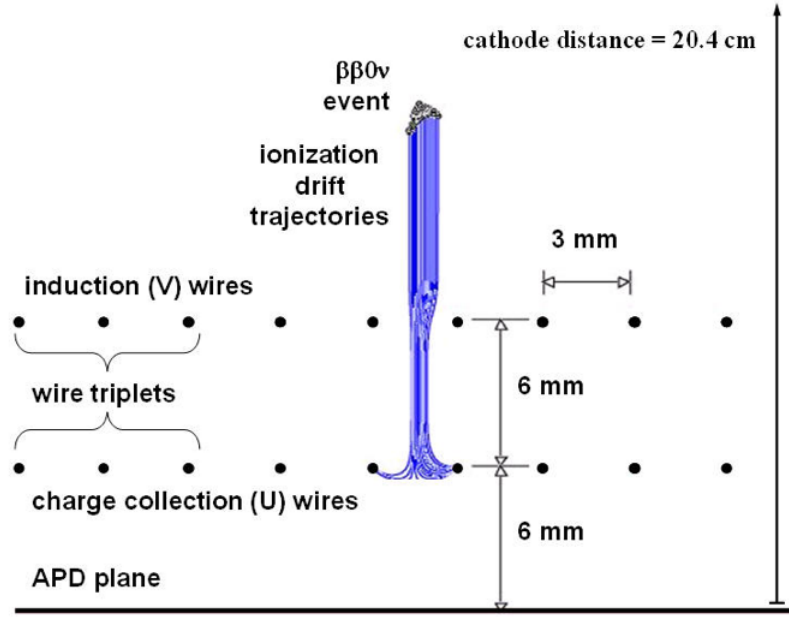


Figure 3.3: The dimension of the ionization measuring wire planes are indicated in this diagram. Electrons drift past the induction (V) wires to the charge collection (U) wires. The U- and V- wires are in reality at 60° angle from each other.

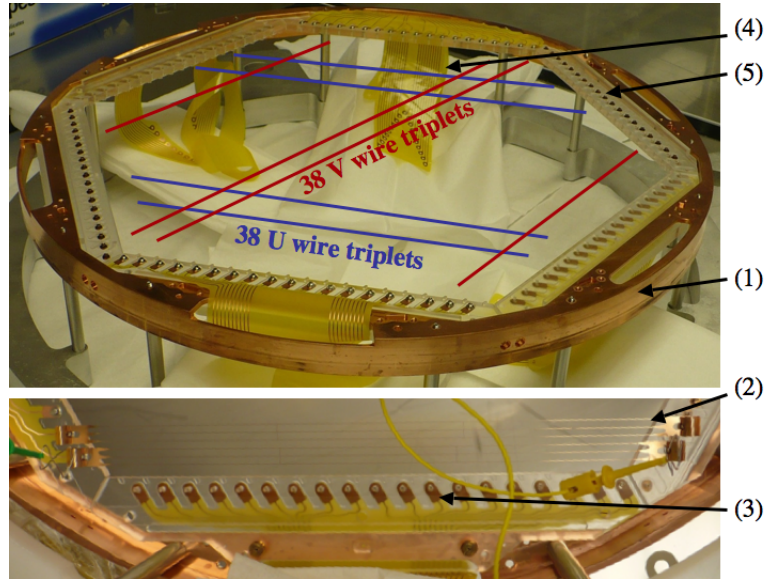


Figure 3.4: The copper support ring (1) holds the hexagonal patterned acrylic mount for the wire planes. U-wires are mounted on one side (2) while the V-wires (not shown) are mounted on the other side (3). Four flexible cables (4) make the electrical connections on one end of the wire triplets while the other end is anchored at (5).

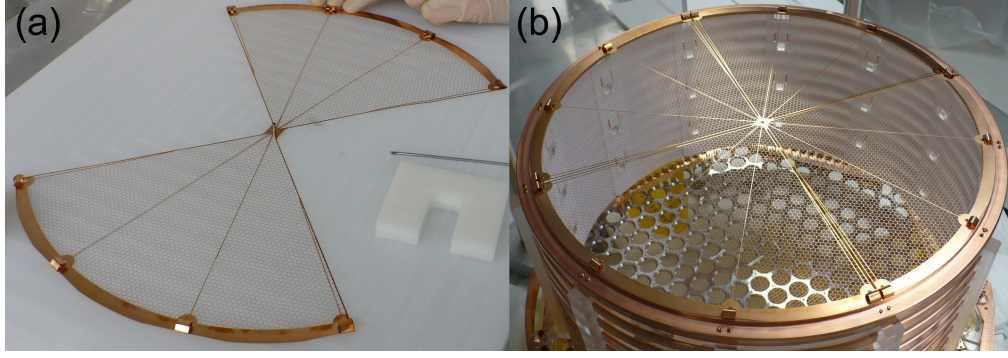


Figure 3.5: (a) One of the two photoetched phosphor bronze part of the cathode. (b) The completed cathode on the detector.

the various wires are also labelled. The two wire planes (U and V), each with 95.8% optical transparency, are in front of the APD platter that collects the scintillation signal. Each of the wire planes consists of 114 wires, forming 38 wire triplets for each plane (see Figure 3.4). In the direction of the length of the TPC, which we will call Z, the U- and V- wire planes and the APD platter are spaced 6 mm from each other. The wire pitch is 3 mm; however, the wires are electrically ganged into triplets for readout purposes, making the effective readout wire pitch to be 9 mm. The ganging reduces the amount of cabling material, which is a source of radioactive backgrounds. These dimensions were determined with the intention to maximize the amount of fiducial volume inside the detector while still maintaining the requisite relative voltage for the necessary electrical transparency. The cathode, consisting of two pieces of phosphor bronze wire meshes (see Figure 3.5a), and the two anode wire grids were manufactured by the photoetching of 0.13 mm thick plates of “full hard” CA-510 Grade A phosphor bronze, chosen for its reliability under thermal cycling and low radioactivity content. The thickness of each individual wire is 0.125 mm.

The timing difference between the scintillation light and the charge collection is used to determine the Z position of the original charge. For accurate position reconstruction, a uniform drift field between the cathode and the induction plane is required. Additionally, several detector properties of LXe, such as the ionization yield, the scintillation yield, and the effect of impurities on electron lifetime are all dependent on the electric field. Field uniformity is achieved by a field cage surrounding the drift volume, as shown in Figure 3.2.

The field cage for each TPC consists of ten coaxial copper rings uniformly spaced between the cathode and the anode. Resistors, each with $\sim 900 \text{ M}\Omega$, are connected between the rings to form a voltage divider. These resistors are each resistive paste deposited on a sapphire substrate with platinum-plated phosphor bronze spring contacts mounted on an acrylic block.

Electrostatic calculations via finite-element analysis by the MAXWELL program have been done to check the field uniformity. Variations of electric field are expected to be less than 1% over the full drift region except very close to the field shaping rings. The non-uniformity is expected to extend about 1 cm in radially from the field shaping rings in the bulk of the drift length but up to 2 cm near the cathode, with the non-uniformity extending in radially at about 2 cm.

3.2.1.1 Electrical Transparency

The induction V-wire planes need to be electrically transparent to the drifting charges, so that all the charges are collected at the U-wire planes. This electrical

transparency condition is given for the ideal case of infinitely long wires with circular cross section as

$$\frac{E_P}{E_Q} \geq \frac{1 + \rho}{1 - \rho}, \quad (3.4)$$

where E_P is the collection field (between the induction and collection planes) and E_Q is the drift field and

$$\rho = \frac{2\pi r}{d}, \quad (3.5)$$

with r being the wire radius and d the wire pitch. Using the previously stated value of 0.125 mm for the diameter($2r$) and 3 mm for d , we get a ρ of 0.131 for

$$\frac{E_P}{E_Q} \geq 1.30, \quad (3.6)$$

for full transparency. Since the actual geometry of the wires is not ideal, the electric field ratio is aimed to be set above a ratio of 2.0. Instead of having a circular profile, the wires of the wire grid are somewhat rectangular due to the photoetching process. Numerical calculation by MAXWELL confirmed this analytic calculation.

In practice, the voltage setting of the wire grids is the following: -8 kV on the cathode, -745 V on the v-wires, virtual ground on the u-wires, and $\sim$ -1400 V (-1420 V and -1390 V for TPC1 and TPC2, respectively) for the two APD planes.

3.2.2 Scintillation Detection in EXO-200

The scintillation light in LXe is in the vacuum ultraviolet (VUV) range and has a wavelength of 178 nm. It is detected in the EXO-200 detector by the large area avalanche photo-diodes (LAAPDs). The LAAPDs are silicon devices consisting of a p-n junction [72]. Light is absorbed on the active surface of the p-region to produce an electron; the electron is then driven by the applied electric field to a multiplication region. The LAAPDs are unencapsulated, since LXe acts as a good electrical insulator, to reduced their radioactive background. They have a circular active area (200 mm^2) with 16 mm diameter. The actual physical diameter can vary between 19.6 and 21.1 mm, and the thickness can vary between 1.32 and 1.35 mm. Each LAAPD has a mass of about 0.5 g and is mounted on a gold-plated copper platter (Figure 3.6). With one APD platter for each TPC, 234 devices in each platter are arranged in a hexagonal grid to allow for easy ganging into groups of seven (or less for some special gangs). In this physical arrangement, the photosensitive fraction of the plane is 48%. Due to the ganging, the 234 LAAPDs per platter require 37 electronic readout channels per side. The LAAPDs used by EXO-200 all have a quantum efficiency, a measure of how well the incident photons are absorbed to produce electrons, between 0.8 and 1.2.

The APD platters are held at $\sim -1400 \text{ V}$ potential (-1420 V on one, -1390 V on another), providing reverse bias to the LAAPDs. This potential also ensures that electrons will not drift past the collection U-wire plane. Since the LAAPDs are known to exhibit a substantial spread in the voltage required for a fixed response



Figure 3.6: Mounted LAAPDs (1) on a gold plated (for improved electrical contact) platter (2). In the inset, platinum plated photo etched phosphor bronze “spider” springs (3) anchor a gang of 7 LAAPDs to the platter while also electrically connecting the copper traces (4) to the flexible cable (5). Acrylic washers (6) prevent the electrical contact between the “spider” and the mounting screws.

[71], similarly behaving LAAPDs are ganged together so that separate trim voltage (between 10-60V) can be applied. Overall, a spread of 2.5% difference in LAAPD response is expected.

Since the cathode wire grid is 90% optically transparent and the VUV light can reflect within the detector due to the teflon tiles, the scintillation light from an event is generally observed by both sets of APD platters. Teflon (PTFE) is known to be good diffuse reflector of VUV light. The teflon reflectors, mounted between the field-shaping rings, are believed to have improved the light collection efficiency by 50-150%, depending on the location of the event in the detector [71].

3.2.3 Anticorrelation

An EXO prototype has shown that the energy resolution in liquid xenon detectors can be improved by measuring both the ionization and scintillation signals. While liquid xenon exhibits large event-to-event fluctuations in the amount of charge created, these fluctuations in ionization are strongly anti-correlated with the fluctuations in scintillation. Ionization only energy resolution is about 3.5 % at the desired Q-value of 2458 keV, but anticorrelation can improve the energy resolution at the Q-value down to 1.6 % [69]. Figure 3.7 is a 2D histogram of a Th-228 source calibration event where the ionization energy (x-axis) is plotted against scintillation energy (y-axis), both axis are in some arbitrary energy units. The anticorrelation effect manifests as the island with a clear negative slope.

3.2.4 Detector Regions

During operation, the liquid xenon in EXO-200 can be considered as either in the active xenon volume or the inactive xenon volume. The inactive xenon region consists of the entire internal xenon vessel volume, including some LXe in the TPC legs, that is outside the cylindrical active xenon region formed by the teflon reflectors (radius 183 mm) with the APD platters as the end caps. In addition to the TPC legs, where LXe enters and leaves the liquid xenon vessel, there is also LXe in the high voltage feedthrough. High energy γ 's from the possible excited state de-excitation that originate in the inactive xenon region may penetrate the teflon and deposit energy in the fiducial xenon region with some efficiency.

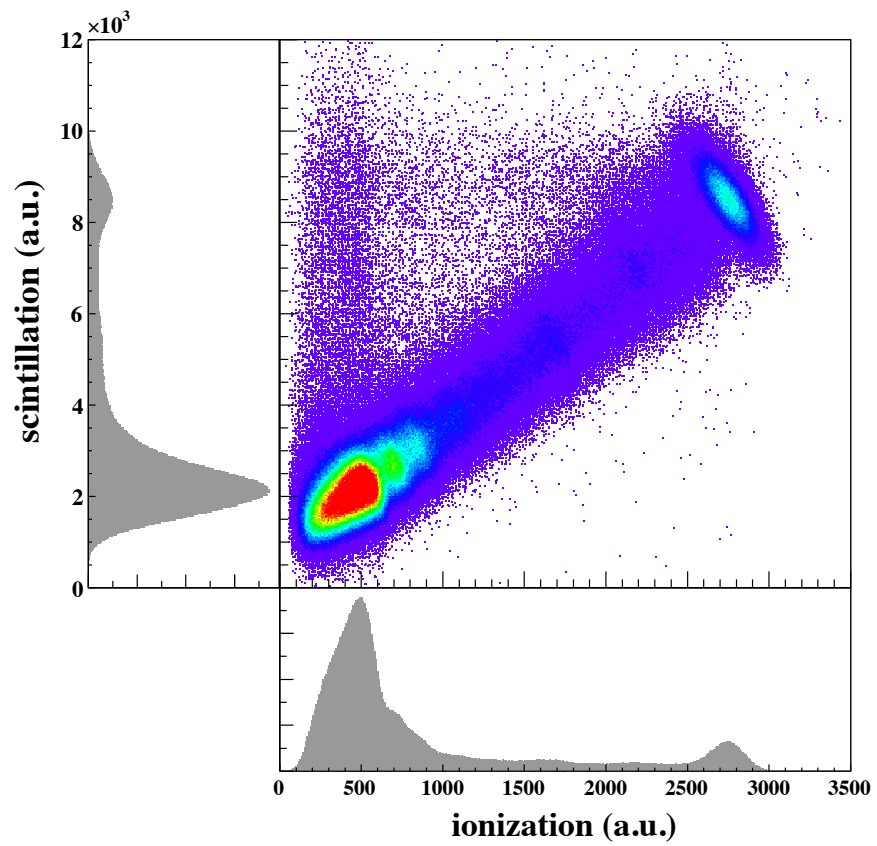


Figure 3.7: Ionization versus scintillation in an uncalibrated 2D histogram of an EXO-200 Th-228 source calibration data run. Projections onto the ionization and scintillation axes are also shown. Figure taken from [6].

The active xenon region can be divided into the fiducial xenon and the dead layer, see Figure 3.8. The fiducial xenon is the xenon volume that corresponds to the actual number of xenon atoms that the experiment is monitoring. Full energy and position reconstruction is expected from the xenon in the fiducial region. The dead layer, on the other hand, is the rest of the volume inside the teflon reflectors that is not fully measured by the detector. Given the mounting of the wire grids, the edges of the grids include regions where only one set of the wires (U or V) exists. Electrostatically, the field lines around the edge also may not end on the grid. For the EXO-200 analysis, the determination of the actual dimension and shape of the fiducial volume is a major task and a source of error. Due to the geometry of the wire supports, the fiducial volume for the EXO-200 detector is a hexagonal prism, rather than a cylinder, with the center and the apothem of the hexagon (in the same plane as the U and V wires) being 163 mm.

3.3 Cryogenic Components

Figure 3.9 shows the full assembly of the EXO-200 detector. The TPC is inside the cylindrically shaped object labeled *LXe Vessel*. The liquid xenon vessel is inside a double walled cryostat. EXO-200 operates typically at a liquid xenon vapor pressure of ~ 1100 Torr at ~ 168 K. This section will discuss the components inside the cryostat.

All components used for the EXO-200 experiment were carefully screened for radioactive impurities. A detailed list of the materials considered can be found in

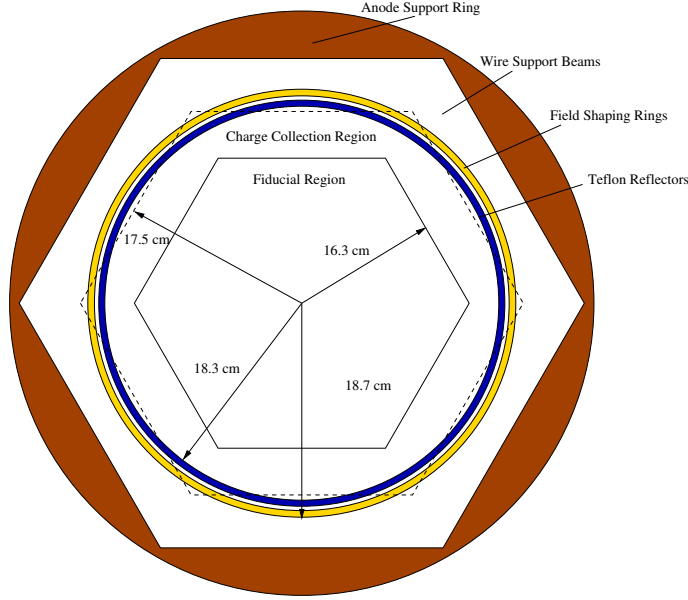


Figure 3.8: Schematic axial view of a half-TPC. The fiducial volume used for analysis is indicated by the small hexagon inside the circular field shaping rings (yellow) and teflon reflectors (blue). Figure taken from [1].

[73]. Various methods, such as neutron activation analysis (NAA), mass spectrometry (MS), and direct counting were used to measure the radioactive content of the considered materials.

Surface contaminants were minimized by assembling components inside a class 1000 clean room with a shallow (7 meters water equivalent) concrete overburden. Detector components were cleaned with acetone and ethanol to degrease the surface. The surfaces of detector components were then etched with acid, either nitric acid (HNO_3) or the stronger hydrochloric acid (HCl). The LAAPDs were left uncleaned from the manufacturer, although their radioactivities were measured. Once on-site (see section 3.4.1), the experiment is again assembled inside class 1000 clean rooms, located within the harsh environment of an active salt mine.

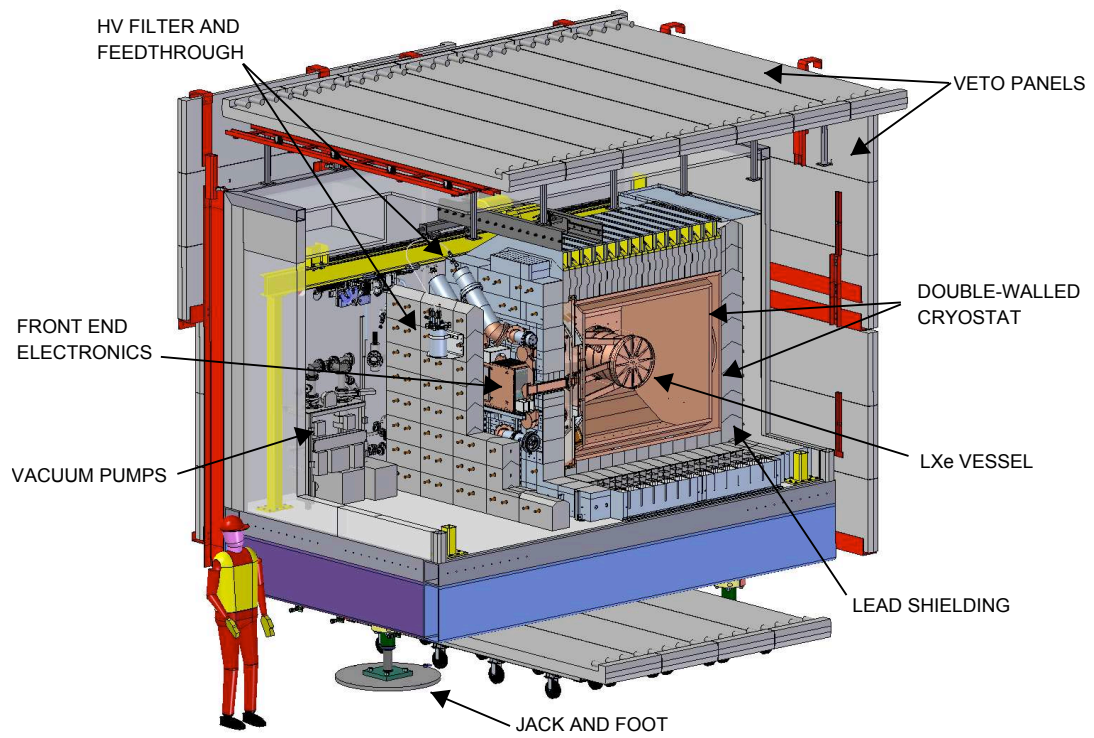


Figure 3.9: The entire detector assembly inside the class 1000 clean room (the muon veto panels are right on the outside of the cleanroom). The TPC is inside the LXe Vessel.

3.3.1 Liquid Xenon Vessel

The liquid xenon vessel (cutaway view in Figure 3.1) is made of copper only 1.37 mm thick. Metals naturally have some trace amount of U and Th impurities in them (discussed in more detail in section 6.2). The thinness of the copper vessel means that the difference in pressure inside and outside of the vessel cannot exceed 250 Torr. To provide both pressure equilibrium across the LXe vessel as well as thermal and cosmogenic shielding, a cryogenic heat transfer fluid (HFE-7000) surrounds the vessel.

3.3.2 Cryogenic System

EXO-200 uses a double walled copper cryostat to cool the LXe vessel. The liquid xenon vessel is inside the inner vessel of the cryostat. The rest of the cryostat inner vessel is filled with 4 tons of an ultra clean heat transfer fluid called HFE-7000, manufactured by DuPont corporation. Given the thinness of the copper liquid xenon vessel, the entire cryogenic control system for the experiment is designed to maintain a very small differential pressure between the liquid xenon and the HFE during all operations.

Two separate fridges (and their backups) are used in the experiment. One fridge feeds directly into the cryostat, keeping things cold at around 168 K. The other fridge cools the condenser which liquefies the xenon gas prior to the xenon entering the cryostat. Outside of the cryostat, the xenon system consists of a specially made xenon gas pump [74] that recirculates the xenon constantly during operations. The

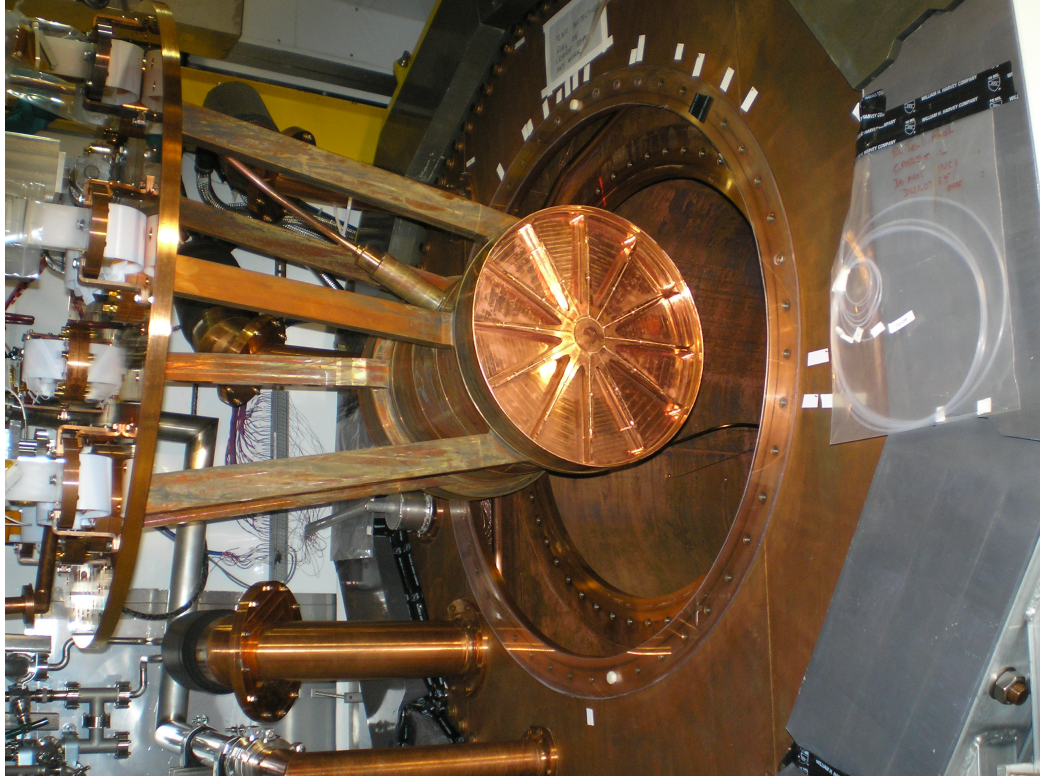


Figure 3.10: Installation of a sealed liquid xenon vessel into the cryostat. Opening of both inner and outer cryostats are visible.

pump pushes gaseous xenon through purifiers into the xenon condenser while also pulling xenon gas out of the LXe vessel return, where a xenon heater is present. As will be shown later in Figure 7.3, the electron lifetime (a measure of xenon purity) is highly correlated with the xenon flow rate.

3.3.3 Xenon Cleanliness

The xenon used for EXO-200 is enriched to 80.6% in Xe-136, with 19.1% being Xe-134. One advantage of xenon, as opposed to other potential double beta decay isotopes, is that the xenon can be continuously purified during the experiment. Any impurities that outgassed from the plumbing into the xenon can be taken out by

the purifiers.

In EXO-200, the xenon is passed through a hot zirconium getter (SAES Mono-Torr getter). These purifiers are very efficient in taking out electronegative impurities. However, these getters have little to no effect on other noble gases such as Helium, Krypton, Argon, Neon, and Radon. The purifiers are operated at 550°C rather than the default temperature of 400°C, because the one-pass efficiency for removing electronegative impurities, particularly nitrogen and methane, improves at the higher temperature [70]. An electron lifetime of at least 3 ms was obtained for the EXO-200 data analyzed in this thesis. This electron lifetime translates to only 4% of the charges being absorbed by electronegative impurities for the maximum drift length.

Using the mass spectrometer/liquid nitrogen cold trap technique, EXO-200 was able to measure the impurities content of the xenon [75]. For the enriched xenon, a sample was taken prior to filling the detector. A nitrogen concentration of $329 \pm 81 \times 10^{-9}$ g/g (Nitrogen/Xe) was measured. This concentration of nitrogen corresponds to 0.06 gram for all the xenon used, which could be taken out by the purifier without exhausting the zirconium getter cartridge. A limit on oxygen of less than 0.4×10^{-9} g/g was set. Additionally, a measurement of natural krypton concentration of $25.5 \pm 3 \times 10^{-12}$ was also obtained. Natural krypton contains ^{85}Kr which β -decays with a Q-value of 687.1 keV. The measured krypton concentration is similar to a very conservative goal for allowable krypton contamination.

3.3.4 HFE

Inside the cryostat but outside the liquid xenon vessel is the HFE-7000 (chemical formula of $\text{CF}_3\text{CF}_2\text{CF}_2\text{OCH}_3$), an ultra-clean heat transfer fluid to provide thermal uniformity on the enclosed liquid xenon vessel (which contains the TPC). HFE is found to be very radioimpurity-clean, as all relevant contaminants (K-40, U-238, and Th-232) for the entire 4 ton of HFE were all measured to be less than 20 mBq [73].

The shielding power of HFE is such that 50 cm thickness (the amount of HFE on all sides of the liquid xenon vessel) corresponds to about 3.3 attenuation lengths for a 2.615 MeV γ . Thus, the HFE provides some further shielding to the detector.

3.4 Cosmogenic Shielding

In addition to the components inside the cryostat being carefully screened for radioactive-impurities, background control also requires additional shielding while the experiment is running to avoid activations or direct interactions from the external radioactivities. Nested layers of passive shielding outside the cryostat further shield the TPC from external radiation. Layers of lead is found on all sides of the cryostat. Plastic scintillator muon veto panels then cover 4 sides of the experiment from the outside of the class 1000 clean rooms.

Cosmogenic activations of materials surrounding the detector (in the copper) and even inside the TPC itself are real concerns. For example, ^{136}Xe can capture a neutron and become ^{137}Xe . ^{137}Xe β -decays with a half-life of 3.8 minutes with an

end point energy of 4.2 MeV. ^{135}Xe and ^{137}Xe in the active xenon as well as the longer lived activated isotopes from the copper vessel (^{60}Co , ^{54}Mn , and ^{65}Zn) were considered in the background model (see section 6.2).

3.4.1 Installation

The EXO-200 experiment is installed at the Waste Isolation Pilot Plant (WIPP), located near Carlsbad, New Mexico, USA. While the facility serves as a disposal for transuranic nuclear waste (in the southern area of the site), the northern area is dedicated for underground experiments. Geologically, the site is in a salt deposit, formed 250 million years ago by the evaporation of the Permian Sea. The experiment is located at the 2150 foot level (655 meter) which corresponds to 1585^{+11}_{-6} meters of water equivalent (mwe). The primary reason for EXO-200's presence in this location is for the cosmic ray shielding. Salt inherently contains less uranium and thorium than hard rock. The detector is located inside six class-1000 temperature and humidity controlled clean rooms. The cleanrooms are mounted on adjustable stilts to deal with the slowly but constantly shifting salt floor.

3.4.2 Lead

From Figure 3.9, the EXO-200 cryostat is surrounded on all sides with lead bricks of various shapes. The 25 cm thick lead (totaling about 500 lb) acts as a passive shield. On the east side of the cryostat, where the electronics and xenon transfer line feed through are located, a first wall of 25 cm thickness covers all the

area except for the feedthroughs. A second lead wall of 20 cm thick is present to shield the exposed openings due to the feedthroughs. The lead bricks used were designed with chevrons to ensure that gaps between the bricks due to small imperfections on the bricks should still result in no line of sight from outside the lead directly into the cryostat.

While ^{210}Pb found in the lead is a potential radioactive impurity contaminant, the α and the low energy γ 's (~ 800 keV but very low probability) are not expected to be able to contribute to the $\beta\beta 0\nu$ energy region of interest. γ 's of ~ 800 keV, however, are similar in energy to the two γ 's expected from the decay to the excited state. The HFE layer does provide some additional shielding of the potential γ 's originating from the lead.

3.4.3 Muon Veto

The vertical cosmic-ray muon flux at the WIPP site had been measured to be $(3.10 \pm 0.05 - 0.07) \times 10^{-7} \text{ s}^{-1}\text{cm}^{-2}\text{sr}^{-1}$ [76]. While muons traversing the TPC have large energy deposition and track-like signals that allow for easy rejection, muon bremsstrahlung and the prompt relaxation of nuclear excitations can mimic internal TPC events. To be able to discriminate these muon events from the events of interest, plastic scintillator muon panels are installed to tag coincidence with TPC events. Four of the six sides of the clean room holding the detector is covered by plastic scintillators panels. These muon veto panels have the dimensions of 5 cm thick by 65 cm tall by either 315 cm or 375 cm wide. On two ends of each

panel, four 2 inch photomultiplier tubes per end can measure the scintillations from passing muons.

From GEANT3 simulations, 31 ± 1 muon induced background events per year are expected in the $\beta\beta 0\nu$ channel if no external muon veto is employed. The experimental tolerance is only 3 events in that channel per year. This tolerance is achieved by the inclusion of the plastic scintillator muon veto panels in EXO-200 [77].

3.5 Electronics

The EXO-200 electronics are designed to minimize noise while still allowing for maximum flexibility of being modified. A schematic of the EXO-200 electronic setup is found in Figure 3.11. Wire charge and APD light signals are fed through kapton insulated flex cables to the front end electronics cards (FECs), which are at room temperature. Charge preamps amplify the signals, prior to the signals going into shapers and analog-to-digital converters (ADCs). The digitized signal is then fed into the data acquisition system (DAQ), which include the trigger event module (TEM) and a computer with a RAID (redundant array of independent disks) array for storage.

3.5.1 Signal Cable

The front end electronics for EXO-200 are maintained at room temperature, just outside the copper cryostat. Signal cables of about ~ 1 meter length are bundled together and run through the 6 TPC legs to connect between the signal wires (charge,

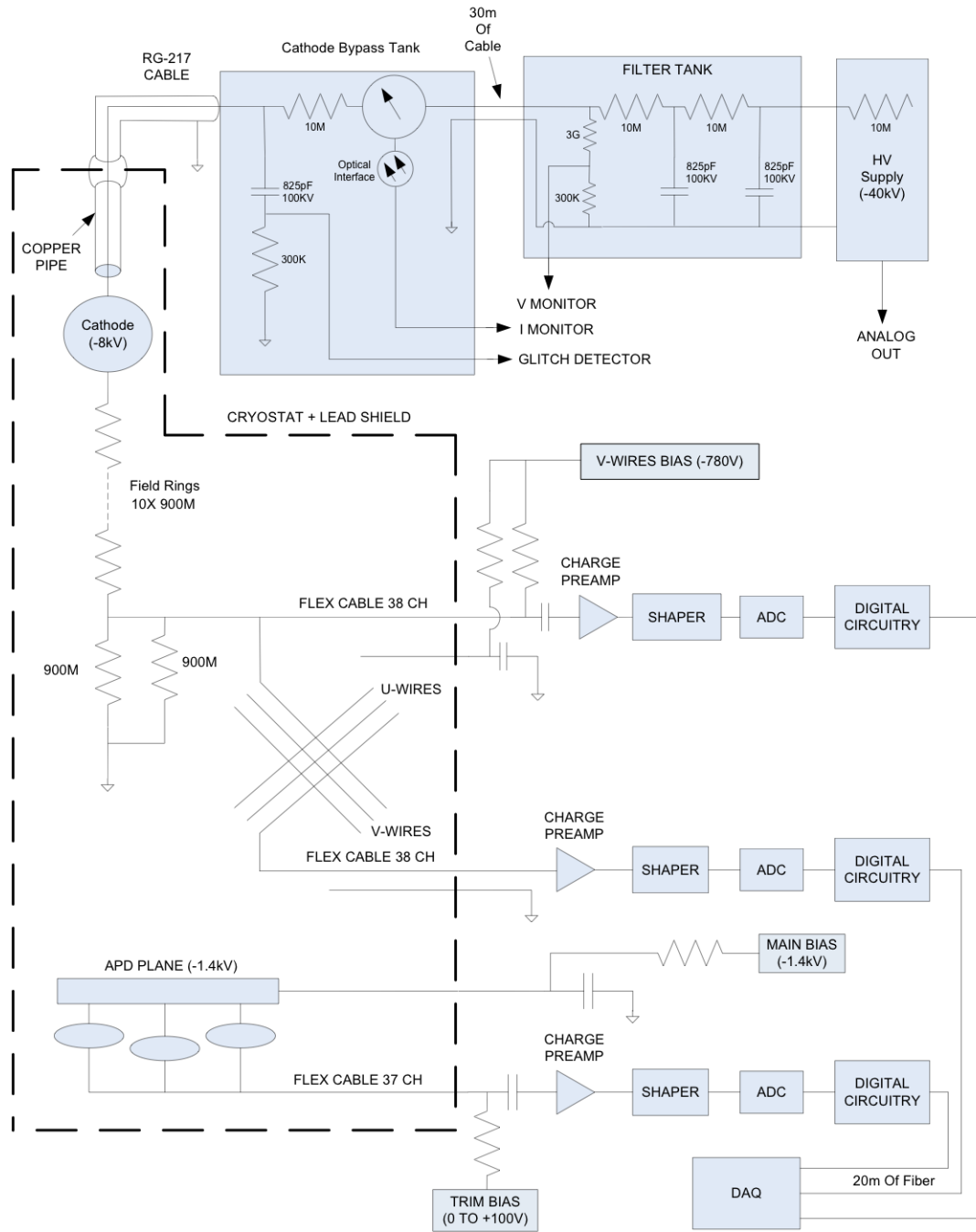


Figure 3.11: Schematic of the EXO-200 electronic system

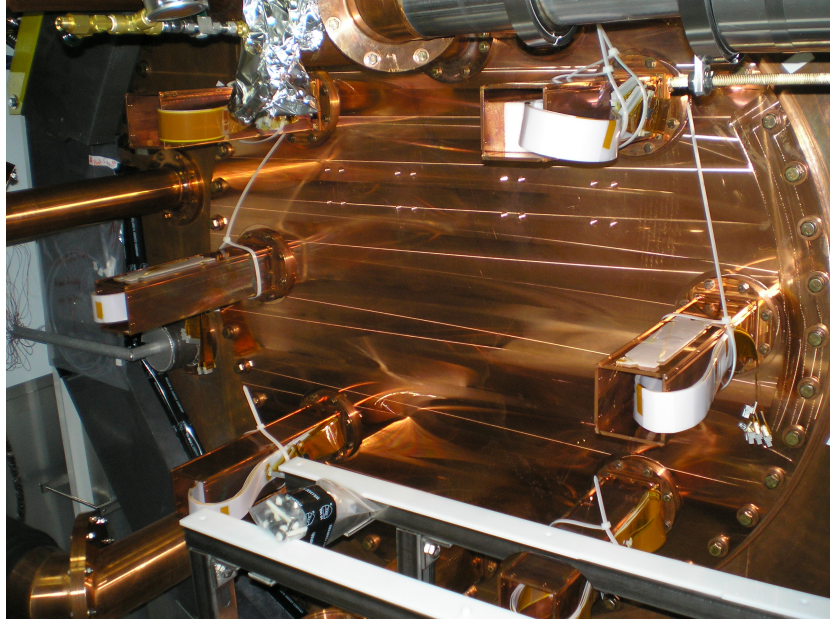


Figure 3.12: The signal cables coming out of the cryostat feedthroughs are visible here.

induction, and APD) and the front end electronics. They are visible in Figure 3.12. The shortness of the cable is designed to minimize electronic noise. These cables are manufactured via the photo-etching of polyamide coated copper strips. Each cable includes 19 channels for the wire planes. The 37 LAAPD channels per side is split into 6 cables. Additionally, the V-wire (up to -4 kV) and APD planes (up to -1.4 kV) bias voltages are applied through these cables.

3.5.2 Signal Shaping

At the FECs, the signals are next passed through a series of shapers. The effect of the shapers (2 integrators and 3 differentiators each) on a typical U-wire signal is illustrated in Figure 3.13. Different shaping times are applied depending on the signal type. Table 2.1 list the values of the various shaping constants applied

Table 3.1: Values of the shaping constants for the Front End Card integrators and differentiators used to read out signals from the TPC

Signal	Int1(μ s)	Int2(μ s)	Diff1(μ s)	Diff2(μ s)	Diff3(μ s)
U-Wire	1.5	1.5	40	40	measured (nominally 60)
V-Wire	3	3	10	10	60
APD	3	3	10	10	300

for the wires and APD signals. The purpose of these shapers is to create a band pass filter that eliminates noise outside the desired signal time of ~ 1 -100 μ s.

With the FECs being located outside the cryostats, the cards and consequently the various electronics shapers in the shaping circuit, are replaceable. The listed values here are the shaping times used for the data in this thesis. Each channel also includes a capacitor for the injection a fixed amount of charge. Charge injection calibration runs are done to measure the nominal 3rd differentiator shaping times.

This final shaping stage comes from the input to the field-effect transistor (FET). For the U-wires, this time constant is determined by a 1 pF feedback capacitor and a 60 M Ω resistor. A 1 pF capacitor is only accurate to within ± 0.5 pF, meaning this 60 μ s differentiation time can vary greatly from channel to channel. These last shaping times for the U-wires are measured separately for each channel. The more aggressive shaping times on the V-wires and the APDs lessen this issue for those channels.

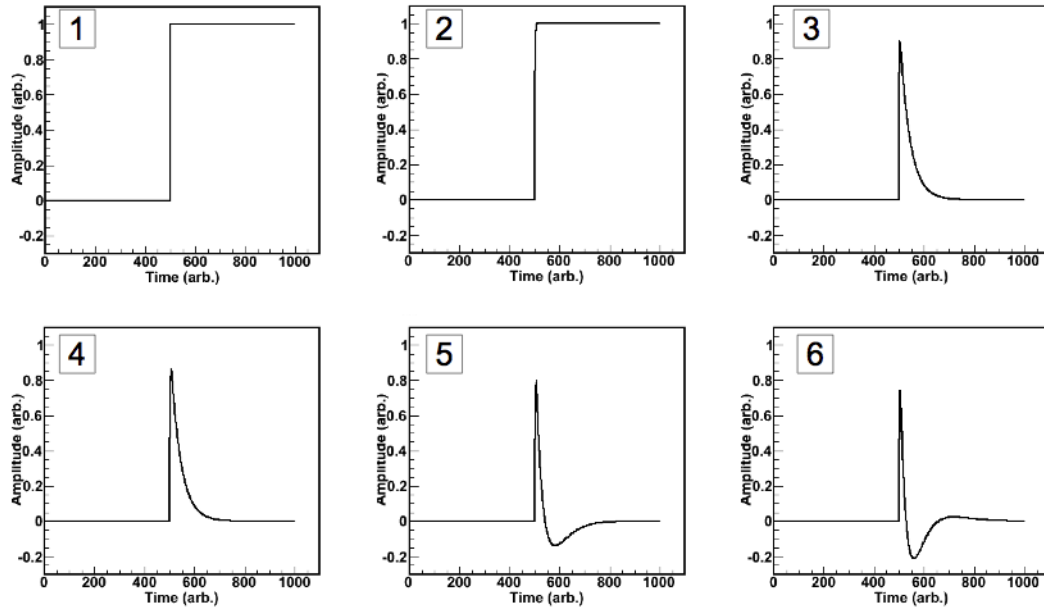


Figure 3.13: Pulse shaping of a U-wire signal. A raw pulse (1) is a step function. This pulse is shaped with a $1.5\mu\text{s}$ integrator (2), a $40\mu\text{s}$ differentiator (3), a second $1.5\mu\text{s}$ integrator (4), a second $40\mu\text{s}$ differentiator (5), and finally a $60\mu\text{s}$ differentiator to arrive at the final pulse shape (6). Figure taken from [7].

3.5.3 DAQ

An analog to digital converter (ADC) produces the digitized data and transfers it to a Trigger Electronics Module (TEM) through optical fibers. The TEM can trigger on individual channels or the sum of channels, when a signal exceed a certain set threshold. Typically, this means that either the TEM triggers on a single U-wire channel or on the sum of the signals from all the APDs on one side of the detector. The ADCs sample at 1 MHz and each waveform is $2048\mu\text{s}$ long. The trigger time is set to $1024\mu\text{s}$ so that each waveform contains 1 ms before and 1 ms after the trigger. A total of 152 wire channels (76 u-wires and 76 v-wires) and 71 APD channels are stored for each event.

The choice of the ~ 2 ms “frame” is sufficiently long to fully capture events since the expected maximum drift time for ionization in the TPC is ~ 100 μ s. Common correlated backgrounds such as the ^{214}Bi to ^{214}Po to ^{210}Bi decay sequence fits into one frame, as the ^{214}Po half-life is 165 μ s.

Chapter 4

Event Reconstruction

Since the EXO-200 detector is a TPC, events are expected to be reconstructed in 3 dimensions and in time. Event reconstruction is the process of translating the raw wire and APD signals for each event into usable information, mainly the position, time, and energies of the charge deposits for each event. This process is done in 4 stages.

- Signal Finding
- Parameter Extraction
- Clustering
- Position Determination

First, in signal finding, waveforms are scanned for signals to determine whether there exists a signal and when that signal took place. Then, signal amplitudes, which are proportional to the energies, are extracted. Clustering occurs next, which combines nearby signals to form single energy deposits. In the last stage, corrections are applied to the extracted parameters to determine the position of clusters in three dimensions.

4.1 Event Display

The EXO event display shows the event signals contained in a trigger window. Waveform amplitudes are illustrated as a function of time (X-axis) for each channel (Y-axis). The APD and wire channel data are separated in different 2D plots. The color code represents the amplitude in ADC counts, which is proportional to the deposited energy. An example of the event display for a low background event with just one cluster is shown in Figure 4.1. The first 38 channels are the U-wire charge collection channels of the TPC half at positive Z (TPC1) followed by the corresponding 38 V-wire induction channels. Channels 76-113 and 114-151 are the U- and V-wire channels, respectively, from the TPC half at negative Z (TPC2). The bottom panel shows the APD signals. The first 37 channels are the APDs in TPC1 followed by the 37 channels in TPC2. All the timing information can be ascertained from this figure.

Example wire signals for the U- and V- wires for the same event are shown in Figure 4.2. The U-wire is the collection signal while the V-wire is the induction signal. While the time difference between the two signals is small, the induction signal (V-wire) starts slightly earlier than the collection signal (U-wire), as expected. One of the goal of reconstruction is to figure out the actual energy deposition from the amplitude of these wire signals. The exact timing and energy determinations are done through a pattern recognition technique that requires good signal models for these two types of signals.

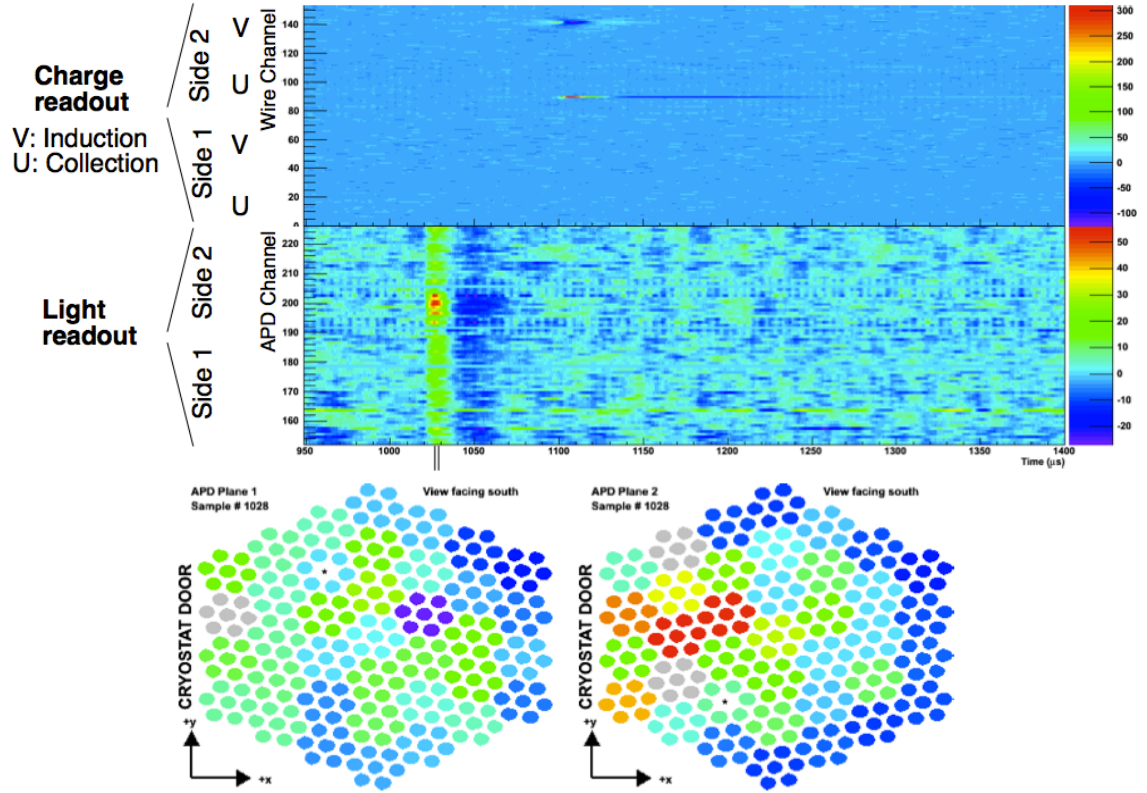
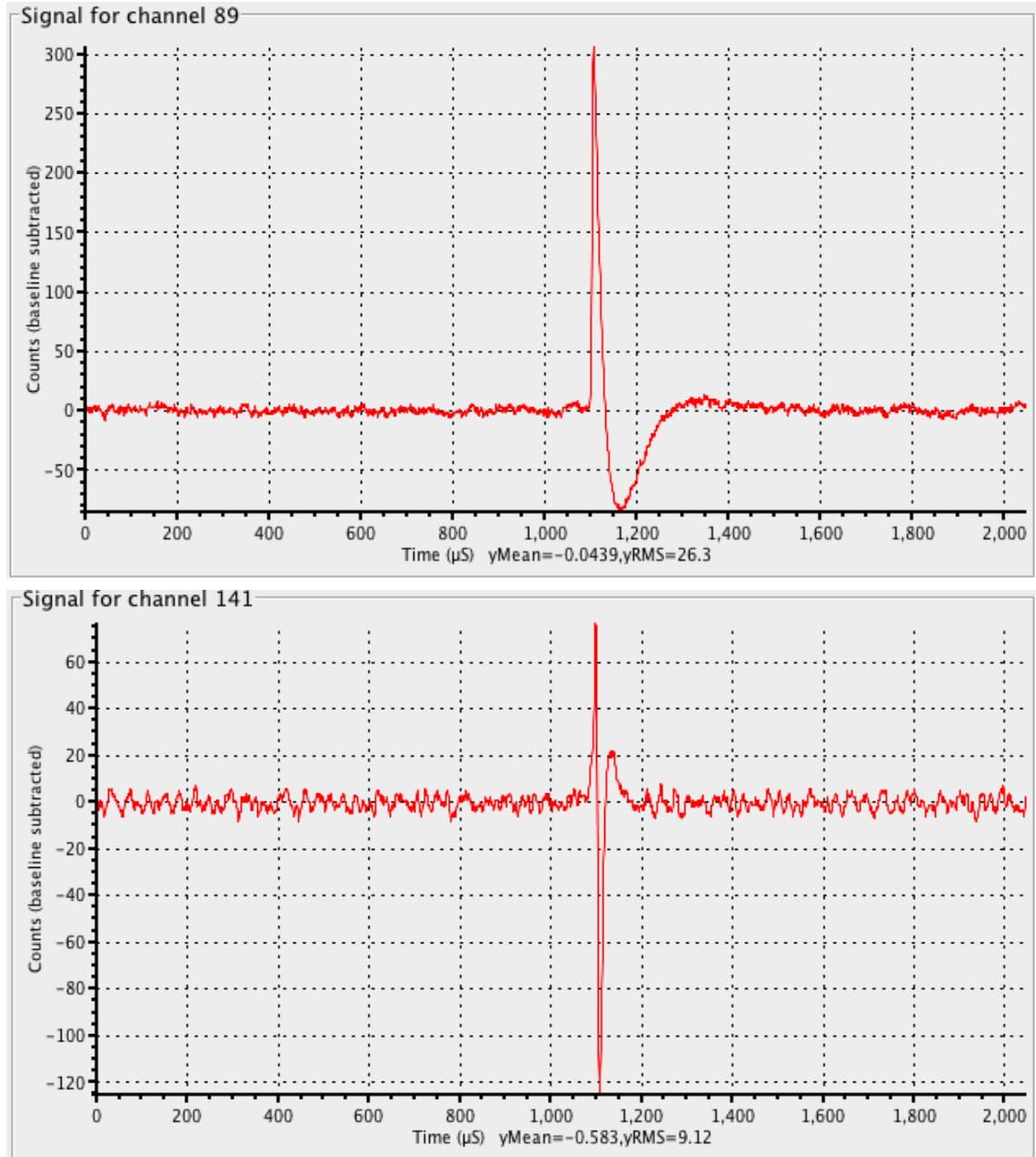


Figure 4.1: Event display output for an actual physics run signal. The wire and APD channels signal amplitude and time are shown on the top. The actual APD response from the two APD platters are shown on the bottom. The actual U- and V- wire signals for the two specific channels are shown in Figure 4.2.

Figure 4.2: Actual U- (top) and V- wire (bottom) signals for an actual low background physics signal. One specific U-wire channel (89) and one V-wire channel (141) are shown. The Y-axis is the background subtracted counts in analog-to-digital converters (ADC) units. The full wire and APD signal are shown in the event display of Figure 4.1.



4.2 Signal Models

In both the signal finding and the parameter extraction steps of reconstruction, a modeled signal shape called a template is used. The goal of the template is to be able to duplicate the true U- and V- wire signals as shown in Figure 4.2. For U- and V- wire signals, the template signals are based upon the electrostatic simulation result. Assuming that U- and V-wire are parallel to each other, both infinitely long, and perpendicular to the plane of calculation, the induced signal from a charge drifted from an arbitrary location in the detector is calculated using the electrostatic simulation package MAXWELL, following the Shockley-Ramo theorem [78, 79]. For the APD signals, the template signal used is simply a step function. These unshaped waveform are then filtered with the appropriate transfer functions corresponding to the relevant integration and differentiation shapers used by the front end electronics as listed in table 3.1. The templates used for U- and V- wire signals are shown in Figure 4.3 and Figure 4.6a, respectively.

4.3 Signal Finding

Even with the relatively high energy of 2458 keV for the main experimental target of $\beta\beta 0\nu$ events, the EXO-200 detector was designed to have as low of an energy threshold as possible. Since energy depositions do not necessarily all get collected together, due to effects such as the bremsstrahlung of a γ , a full energy measurement requires the ability to correctly identify all of the potentially low amplitude depositions for events that end up as multiple distinct charge depositions.

In particular, a low energy threshold is particularly important for the search for the decay to the excited states, where the signal consists of multiple depositions, including the two γ 's that are likely to Compton scatter within the detector and be detected as multiple charge clusters each with lower energies than the ~ 800 keV of the initial γ 's.

To identify better a low amplitude signal from noise of similar amplitude, a pattern recognition technique known as a matched filter is used to increase the signal to noise ratio based upon the waveform shape. After the matched filter is applied and a signal is found, a second pattern recognition technique called unshaping is applied to better identify multiple U-wire signals when they are in the same waveform.

4.3.1 Matched Filter

For a linear time invariant system with an output $r(t) = s(t) + n(t)$, where $s(t)$ is the signal and $n(t)$ is a white Gaussian noise, the matched filter is the optimal filter to maximize the signal to noise ratio (SNR),

$$SNR = \frac{|s_0(t_d)|^2}{|n_0(t_d)|^2} = \frac{|\int_{-\infty}^{\infty} H(f)S(f)e^{i2\pi ft_d} df|^2}{\frac{N_0}{2} \int_{-\infty}^{\infty} |H(f)|^2 df}, \quad (4.1)$$

where $s_0(t)$ and $n_0(t)$ are output signal and noise after filtering at some time t_d , $H(f)$ and $S(f)$ are the Fourier transforms of the filter and signal, respectively, and $\frac{N_0}{2}$ is the frequency independent Fourier transform of the noise.

SNR is maximized when

$$H(f) = k(S(f)e^{i2\pi ft_d})^* = kS^*(f)e^{-i2\pi ft_d}, \quad (4.2)$$

where k is an arbitrary constant. $H(f)$, the matched filter, is equivalent to a convolution in the time domain. So for the optimal SNR, the matched filter template is the signal shape itself. Scanning over time in the waveform, a signal shape template is convolved with the waveform. The optimal matched filter output is an amplified response at the same time sample as the pulse. This matched filter algorithm is applied to find signals on the U-wires, V-wires, and APDs.

In practice, the noise in EXO-200 is colored rather than white Gaussian, due to the noise being passed through the shapers and the non-white pickup noise. Consequently, the waveform has to first pass through a whitening filter, which is done by dividing the Fourier transform of the waveform, $R(f)$, by the magnitude of the noise frequency spectrum, $|N(f)|$. So the “whitened” response becomes

$$R'(f) = \frac{R(f)}{|N(f)|}. \quad (4.3)$$

The matched filter also needs to be “whitened” and becomes

$$H'(f) = \frac{H(f)}{|N(f)|}. \quad (4.4)$$

So finally, the optimal filter $H''(f)$ is

$$H''(f) = \frac{S^*(f)}{N^2(f)}. \quad (4.5)$$

4.3.1.1 U-wire signal

For U- and V-wires, the matched filter is applied individually for every channel of every event. For each channel, the matched filter is then applied at every time sample. Figure 4.3 shows a signal model for an U-wire signal. The signal model templates are generated by calculating the impulse function from a 2D drift simulation and passing it through the transfer function of the read out electronics.

The threshold is determined on the fly for each channel and each event to reduce sensitivity to channel- and time-based noise events. The peak search algorithm utilized is the following. If a signal, after matched filter is applied, is found to be 5 times the mean absolute deviation of the baseline, then that signal is accepted as a candidate event. The signal collection time is deemed as the time sample when the maximum matched filter response is obtained that exceeded the threshold. Figure 4.4a shows the waveform of an U-wire signal. The output of the matched filter is shown in Figure 4.4b as a comparison.

A separate U-wire template exists for each channel since the 3rd differentiation time, τ_3 , was allowed to float (rather than using the nominal $60 \mu s$ value, see section 3.5.2) while the shaping times, τ_1 and τ_2 , were fixed at their nominal values in the fits of U-wire calibration pulses to the analytic form. Figure 4.5 shows the distribution

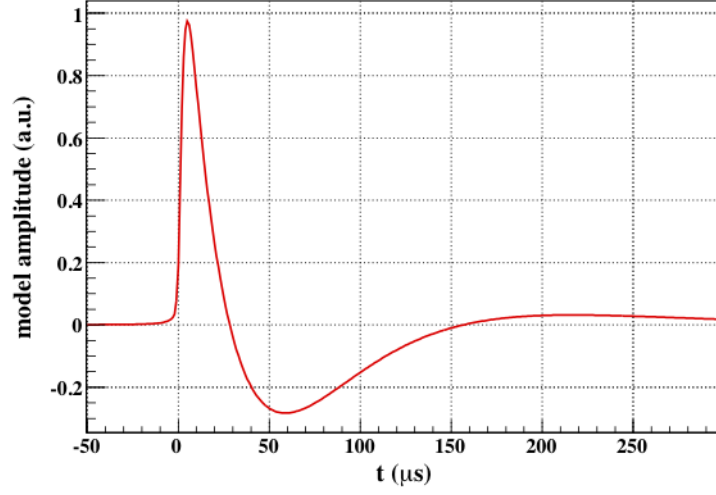


Figure 4.3: Signal model of the matched filter for an U-wire. The shaping time of the last differentiation stage of this particular channel is $57.9 \mu\text{s}$. Figure is taken from [6].

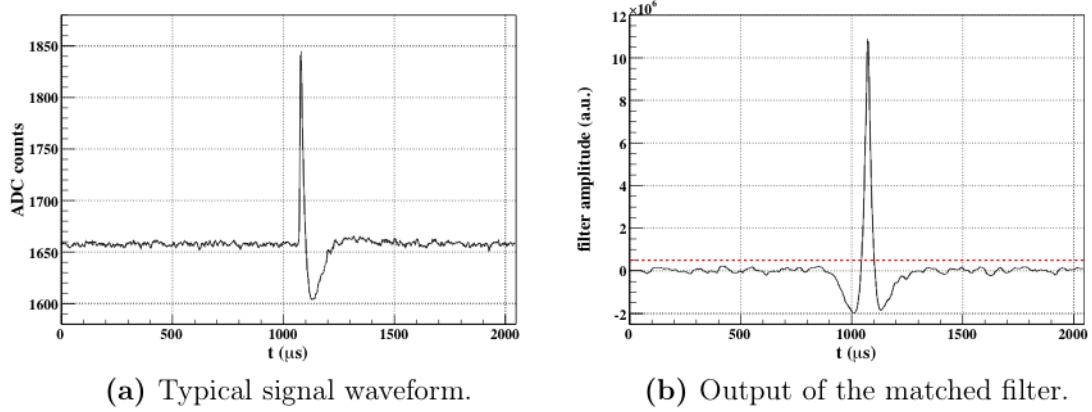


Figure 4.4: (a) A typical waveform of an ~ 1.5 MeV charge deposit on a single U-wire. (b) The spectrum after matched filter has been applied. The time of the signal is determined by searching for the local maxima above the threshold (red line). Figure is taken from [6].

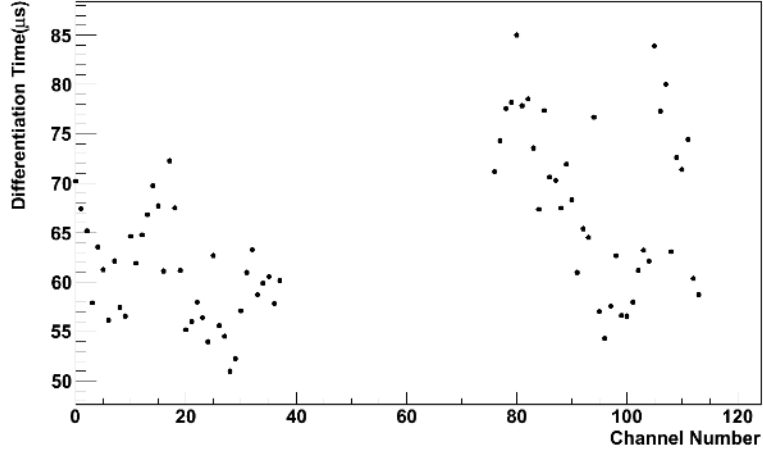


Figure 4.5: U-wire differentiation times for each u-wire channel. Figure is taken from [8].

of various differentiation time for this last shaper, τ_3 for all the U-wire channels.

For the data considered in this analysis, a separate unshaping algorithm was applied for channels where the matched filter method had found a signal to better deal with the cases where multiple signals are deposited in the same channel. Unshaping will be discussed in section 4.3.3.

4.3.1.2 V-wire signal

The matched filter algorithm is also applied on V-wire waveforms with the expected time of the V-wire signal given by the drift time (looking only at some specific time window before the charge collection). Figure 4.6a shows the template of a V-wire signal, which is used as the matched filter to search for actual V-wire signals, such as the one in Figure 4.6b. The normalized result of the convolution is used as the figure of merit. The output is maximal and above a set threshold of 20 for channels where the signal model matches with an actual induction signal. The

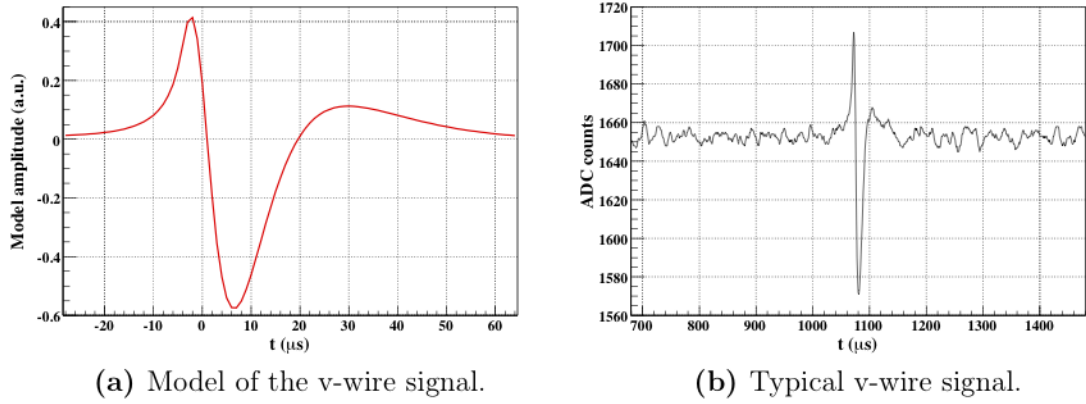


Figure 4.6: (a) Template for a V-wire signal. (b) An actual V-wire signal. Figure is taken from [6].

position in the V-coordinate is determined by the weighted average of channels above the threshold. For certain events with a found U-wire signal, however, it is possible for no corresponding V-wire channel to exceed the threshold. These events with missing the V-positions cannot have a full 3 dimensional position reconstruction. They are flagged and dealt with separately later in the analysis.

4.3.1.3 APD signal

For the APDs, a step function with the relevant shaping applied is used as the template model. All the APD signals from each half-TPC are summed to improve the signal-to-noise ratio for scintillation signals. The matched filter is then applied to both sums individually. If a signal, after matched filter is applied, is found to be 4 times the mean absolute deviation of the baseline, then that signal is accepted as a candidate event.

Charge clusters are associated to the scintillation cluster if their collection time is within a time window of the scintillation signal. Drift time is determined from the

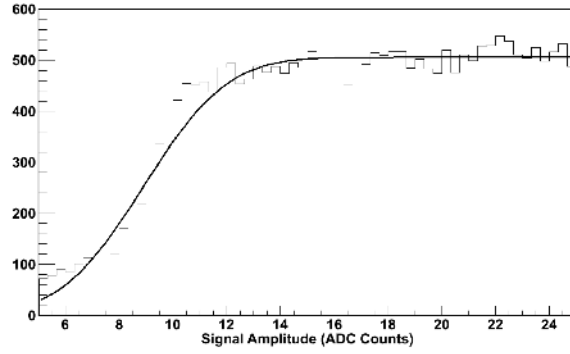


Figure 4.7: Fit of the low energy tail of reconstructed charge clusters to an error function to determine charge reconstruction threshold. Figure is taken from [8].

difference between the scintillation time and the collection time of the associated charge clusters.

4.3.2 Thresholds

The charge detection threshold on the U-wires using the matched filter can be determined from the source calibration data. For events with multiple clusters (multiple site) of at least 500 keV, the lowest amplitude clusters are binned and fit with an error function in Figure 4.7. Above 14 ADC counts (≥ 80 keV), 98% of charge clusters are reconstructed.

4.3.3 Unshaping

While the matched filter technique of using a template for a single U-wire signal does work quite well, the technique is flawed in identifying multiple signals on the same channel, separated in time. The matched filter technique broadens the signal and may cause the smearing out of signals that are close in time. Figure

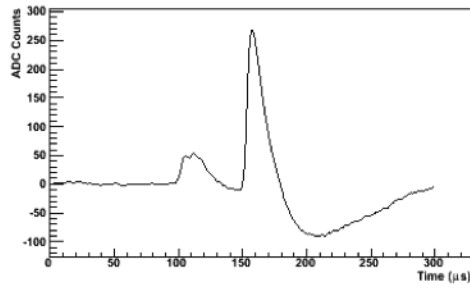
4.8a shows a raw U-wire signal with two pulses. With the standard matched filter output (Figure 4.8b), only one signal was found above threshold. To remedy this, a second algorithm known as *unshaping* is applied by reconstruction on channels that have already been determined to possess a signal by the standard matched filter technique described earlier.

Signals were lengthened in time by the electronic shaping, but better separation in time of multiple signals requires a narrower time response. Unshaping is the method to revert back the effects of the electronic shaping by sequentially applied the reverse of previous integrator and differentiators. Unshaping is performed on a $256\ \mu\text{s}$ section of an identified signal waveform. Figure 4.8c shows the unshaped waveform of that two pulse signal. After unshaping, a $2\ \mu\text{s}$ triangular filter is then applied. The result of the triangular filter is a waveform with two clear signals (Figure 4.8d).

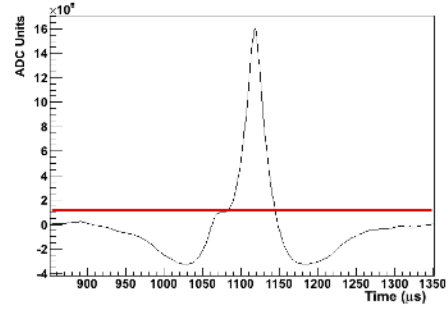
By applying unshaping, signals 3 to $5\ \mu\text{s}$ apart can be identified. The same threshold of 5 times above the baseline is then applied to the re-filtered result to determine how many charge signal candidates are present.

4.4 Parameter Extraction

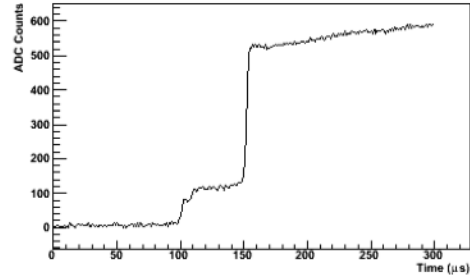
Once the signals have been identified, the energy and timing information are extracted from fitting the U-wire and APD matched filter template signals. As shown back in Figure 3.13, the template is made from a step function with the relevant shaping times (including the special 3rd differential time for U-wire signals



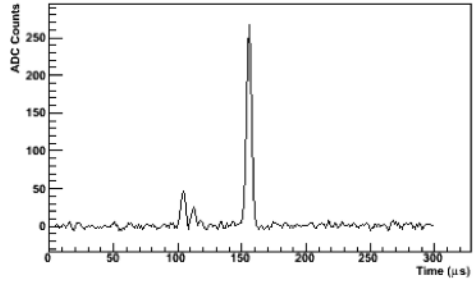
(a)



(b)



(c)



(d)

Figure 4.8: (a) a raw waveform from a U-wire channel with two pulses (b) the matched filter output for this waveform (c) an unshaped sub-trace of this waveform (d) the sub-trace after application of a $2\mu\text{s}$ triangular filter. Figure is taken from [8].

from fits) applied. The amplitude and the peak signal time are allowed to float in the fit of the template to an already identified signal channel, however. The resultant amplitude is the uncalibrated energy, and the peak signal time is the collection time of the signal. Due to how the induction signals are much smaller than the collection signals, V-wire signals are not fitted. The magnitude of the matched filter response amplitude is used as the signal amplitude.

4.5 Signal Clustering

The result of the U-wire pulse identification and signal fitting is a set of U-wire signals with amplitude, time, and channel information. The great discriminating power of the EXO-200 detector comes from its ability to differentiate between different type of energy depositions, particularly β and γ , from the size of the energy depositions. A single charge deposition can sometimes be split between two neighboring U-wire channels. *Clustering* is the algorithm used to combine certain U-wire signals together. U-wire charge collection signals on neighboring or the same wires are combined into a single cluster if they are separated by less than a clustering time, $t_{cl} = 3.5 \mu s$. The value of t_{cl} came from a comparison of data to Monte Carlo simulations. If a U-wires signal on a wire bundle and its neighboring channel occur within $10 \mu s$ of each other, they are also assigned to the same charge cluster. So a single charge cluster may span across two wire bundles, which are 18 mm apart, even though the algorithm is designed to find the cases where the energy deposition happened to occur between outside wires of a 3-wire bundle, mere 3 mm apart.

Events with only one single charge cluster are considered to be *single site* (SS). Events containing three or more U-wire signals or two non-adjacent U-wire signals are considered to be *multiple site* (MS).

For each U-wire signal, a V-wire is searched for in the $2\ \mu\text{s}$ window right before the U-wire signal time. For V-wires, however, a charge deposit can sometimes be induced across multiple wires. For certain low energy signals, there are cases where no V-wire signals are found.

4.6 Position Determination

Position information is determined from the location and the timing of the identified signals. Coordinates can be defined in the the plane of the wires, with the U- and V-axes defined as being perpendicular to the respective wires. The U and V coordinates of a signals are the coordinates of the nearest wire channels with signals above threshold. For the cases of signals on multiple wires, each signal is weighted according to the signal strength. The U-position is weighted by the amplitude of the signal; the V-position is weighted by the match filter response (the normalized result of convolution). Since the U and V wires are at an angle of 60° with respect to one another, coordinate transformation is necessary to switch from the U and V coordinates to the more common X and Y. The X, Y, and Z coordinates defined

here can be seen in Figure 7.1. The two sets of coordinates are related by,

$$x = \text{sgn}(z)(v - u), \quad (4.6)$$

$$y = (u + v)/\sqrt{3}. \quad (4.7)$$

where $\text{sgn}(z) = +1$ for TPC 1 and -1 for TPC 2. In these definition of X, Y, and Z, the X-axis is pointing horizontally into the TPC, while the Y-axis is pointing vertically up. Using the time difference between the charge collection and the associated scintillation signal, the Z position can be determined from knowing the drift time and the drift velocity. Drift velocity was measured during calibration runs to be $1.71 \text{ mm}/\mu\text{s}$. For events that are missing a V-wire signal, there are not enough positional information available to reconstruct the full three dimensional position of those events; only two dimensional spatial positions in U and Z are known for these events.

Chapter 5

$\beta\beta$ Decays Monte Carlo Simulations

The strategy to search for $\beta\beta 0\nu$ is by looking for a peak at the end point energy of the $\beta\beta 2\nu$ spectrum. Consequently, a very good understanding of the shape of the $\beta\beta 2\nu$ spectrum is of importance for the $\beta\beta 0\nu$ search. Two different theoretical spectra for $\beta\beta 2\nu$ are considered for EXO-200. Finally, the Monte Carlo simulation for the $\beta\beta 2\nu$ decay to the excited state of ^{136}Xe , which is based upon the same $\beta\beta 2\nu$ spectra with additional γ 's generated, is also discussed.

5.1 EXOsim double beta generator

The EXO simulation software (EXOsim) is a C++ based software package that generates simulated data via the Monte Carlo method with GEANT4. For all the nuclear decays within the EXO-200 detector, the GEANT4 Radioactive Decay Module is used. This module generates the appropriate α , β , and γ for a given parent nuclei, as well as further down the decay chain if the daughter nuclei are also radioactive.

Double beta decays (both $\beta\beta 2\nu$ and $\beta\beta 0\nu$) are not a part of the Radioactive Decay Module, however, so separate generators have been written to simulate them. The $\beta\beta$ decay generators in EXOsim follow the usual phase space calculations, taken from the book of Boehm and Vogel [32]. An approximation for the Fermi function is

applied for ease of calculations. EXOsim has the flexibility to simulate, by changing the Q-value and/or the atomic number of the final nuclei, the $\beta\beta$ spectra for other potential double beta decay nuclei, including ^{134}Xe . EXOsim can also simulate the double positron decays, such as the decays of ^{124}Xe . The $\beta\beta 2\nu$ spectrum from this method, referred to as the Vogel spectrum, is somewhat different from that of Kotila and Iachello [11]. A special generator using the Kotila/Iachello result is also included in EXOsim so the effect of the differences between the two theoretical $\beta\beta 2\nu$ can be explored in the final fit analysis.

5.1.1 Acceptance Rejection Method

The acceptance-rejection method is a basic pseudo-random number sampling algorithm that allows for the random generation of events that follow a distribution. The basic principle is that to sample a random variable one can just sample uniformly from the region under the graph of its density function. All the samplings which end up in the region above the graph of the density function are rejected. More specifically, the steps for this algorithm are the following:

- Sample a point (an x-position) from the proposal distribution.
- Draw a vertical line at this x-position, up to the curve of the proposal distribution.
- Sample uniformly along this line (i.e. uniformly from 0 to the maximum value of the proposal distribution), and reject points outside of the desired distribution (i.e. greater than the value of the desired distribution at this

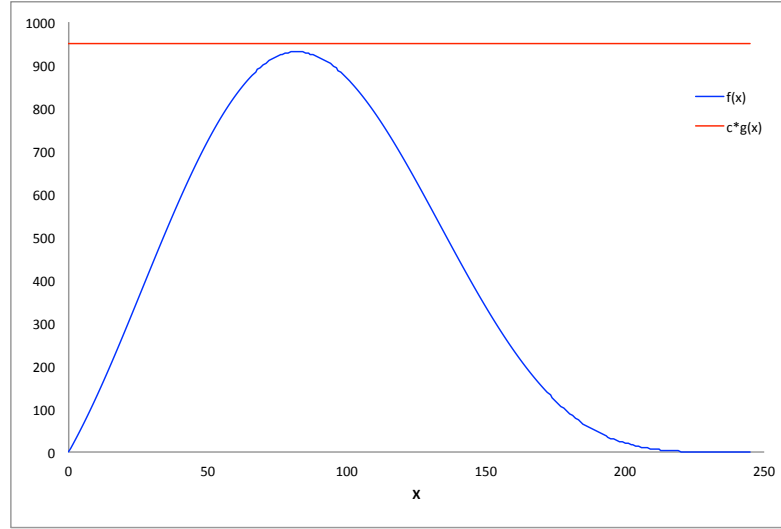


Figure 5.1: The graph showing a pdf of $f(x)$ (target distribution) and $c \cdot g(x)$ (proposal distribution) used for an acceptance-rejection example.

point).

In Figure 5.1, we start with two distributions: a target distribution, $f(x)$ in blue and a proposal distribution (which is uniform in this example), $g(x)$, multiplied by a coefficient, c , in red. First, a random point, x_0 is generated in the box bounded by the range of x and $c \cdot g(x)$, where c is chosen to ensure that the target distribution is not truncated. Then in this $c \cdot g(x_0)$ line, a sample is uniformly taken and compared to the probabilistic distribution function $f(x_0)$. If this second sample is less than the target distribution at that value, this sample is accepted; if the sample is outside (greater than) the target distribution, this sample is rejected. Consequently, only the fraction of $f(x_0)/(c \cdot g(x_0))$ is accepted at each point of x .

The drawback for this method is that if a sample has a special feature such as a very narrow peak (large value for $f(x_0)$), then there would be a lot of unwanted samplings at the rest of $f(x)$ where x is not x_0 . This problem could potentially

be remedied by a clever choice of the proposal distribution, $g(x)$. Fortunately for EXOsim, the $\beta\beta 2\nu$ spectrum does not have a feature such that this would be a problem.

5.1.2 Volume and Internal Detector Components

The double beta decay generators for EXO-200 are designed to simulate decay uniformly inside the “active liquid xenon” volume. This include most but not all of the liquid xenon in the EXO-200 detector. The active liquid xenon volume only radially extends out to the inner radius of the teflon reflectors; lengthwise, it extends out to the face of the APD platter. The rest of the liquid xenon is in the “inactive liquid xenon” volume, which consists of the LXe between the outside of the teflon reflector and the inside of the liquid xenon vessel radially, the LXe outside the APD platter in the Z-direction, and the LXe in the xenon vessel legs. The internal components inside the active liquid xenon that are considered by the simulation package used (GEANT4, see section 6.1.1) are shown in Figure 5.2.

For the regular $\beta\beta$ decays, the β ’s are not expected to travel very far or through the teflon layer. For the decay to the excited state, however, the two $\sim 800\text{keV}$ γ ’s can be generated from the non-fiducial xenon region but still deposit energy inside the fiducial volume due to the gamma interaction length being a few centimeters (see Figure 6.1). The possibility of decays to the excited state from the inactive liquid xenon volume changing the expected signal within the active liquid xenon volume is considered in section 8.4.

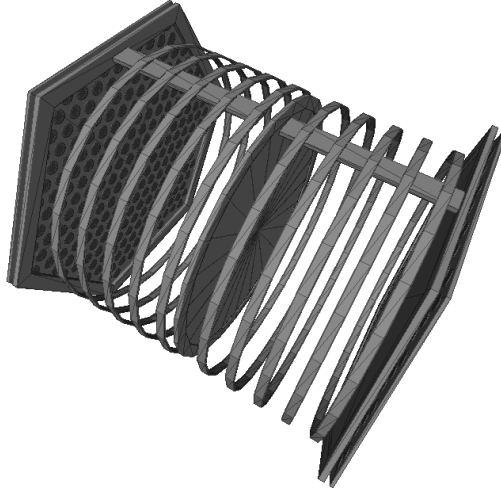


Figure 5.2: The TPC interior components as rendered by GEANT4 simulation package. The teflon reflectors are suppressed to show the internal components. Also, only half (every other one) of the field shaping rings are shown. Figure taken from [1].

5.2 Generating $\beta\beta$ Decay Spectra

The differential beta decay spectra Equation 2.17 and Equation 2.18 were defined in section 2.3.4. The differential decay rate for both the $\beta\beta 0\nu$ and the $\beta\beta 2\nu$ cases are dependent upon the momenta and total energies of the two β 's and the energy-dependent Fermi functions. Of course, the momentum and the total energy are related to each other by

$$E = \sqrt{p^2 + m_e^2}, \quad (5.1)$$

where p is the momentum of the β and m_e is the mass of the electron, in the units where the speed of light, $c = 1$. The kinetic energy of the β , T , is then defined simply as $T = E - m_e$.

The EXOsim double beta generator code determines the energies of the two

β 's by considering their individual kinetic energies (T_1 and T_2). The two β kinetic energies are actually sampled based upon their sum (K) and the difference (D). More specifically, the relationships between these energies are:

$$K = T_1 + T_2, \quad (5.2)$$

$$D = T_1 - T_2, \quad (5.3)$$

so that

$$T_1 = \frac{K + D}{2}, \quad (5.4)$$

$$T_2 = \frac{K - D}{2}. \quad (5.5)$$

For $\beta\beta 0\nu$, the sum electron spectrum is simply the end point energy (at the Q-value). The code randomly generates the difference of the two beta kinetic energies based on the phase space constraint, equation 2.17. The acceptance-rejection method is applied here to constrain the desired probabilistic distribution function (from phase space calculations) upon the generated energy differences. Once there is an acceptable energy difference, it is trivial to determine the two beta energies using equations 5.4 and 5.5. As for the angular distribution of the betas, [32] states

that for the $0^+ \rightarrow 0^+$ transition,

$$f(\cos) = 1 - \beta_1 \beta_2 \cos(\theta_{12}) \quad (5.6)$$

where $\beta = p/E$. This relation is used to constrain the angle (θ_{12}) between the two electrons, again evoking the acceptance-rejection algorithm. This $\beta\beta$ angular correlation is not observable in EXO-200.

The method for generating $\beta\beta 2\nu$ is similar. First, the algorithm generates randomly a sum kinetic energy, K , that satisfies the dN/dK spectrum. The dN/dK spectrum is based on phase space consideration from equation 2.18 for the default version of EXOsim or read in from a table for the Kotila/Iachello spectrum. Then, the code randomly generates the difference of the two beta kinetic energies that is consistent with the previously determined sum energy. After these steps, the two kinetic energies of the β 's are calculated using equations 5.4 and 5.5. Their momenta are calculated after requiring angular correlation that fits equation 5.6.

5.2.1 Fermi Function Parameterization

As introduced in section 2.3.5, the Fermi function, describing the Coulomb effect between the final-state beta particle and the final-state nucleus, is a part of the $\beta\beta$ decay rate calculations. The Fermi function is a part of the exactly calculable phase space factor. Typically, the non-relativistic Coulomb expression of the Fermi function is used; the Primakoff & Rosen form is

$$F(E, Z) = \frac{E}{p} \frac{2\pi Z\alpha}{1 - e^{-2\pi Z\alpha}}, \quad (5.7)$$

where α is the the fine structure constant and Z is the atomic number of the final-state nucleus. This expression is easily integrable and often cited in the literature. However, the non-relativistic regime corresponds to light nuclei (small Z). For heavy nuclei such as the Barium ($Z = 56$) daughter ion from the Xenon double beta decays, the relativistic form is needed. The exact relativistic expression of the Fermi function is

$$F(E, Z) = 2(1 + \gamma)(2pR/\hbar)^{-2(1-\gamma)} e^{\pi\nu} \frac{|\Gamma(\gamma + i\nu)|^2}{\Gamma(2\gamma + 1)^2}, \quad (5.8)$$

with

$$\nu = Ze^2/\hbar v, \quad (5.9)$$

$$\gamma = [1 - (Z\alpha)^2]^{1/2} \quad (5.10)$$

where α is again the the fine structure constant, Z is again the atomic number of the final-state nucleus, Γ is the complex gamma function, R is the nuclear radius (which often has to be approximated in some way), and p is the electron momentum. There

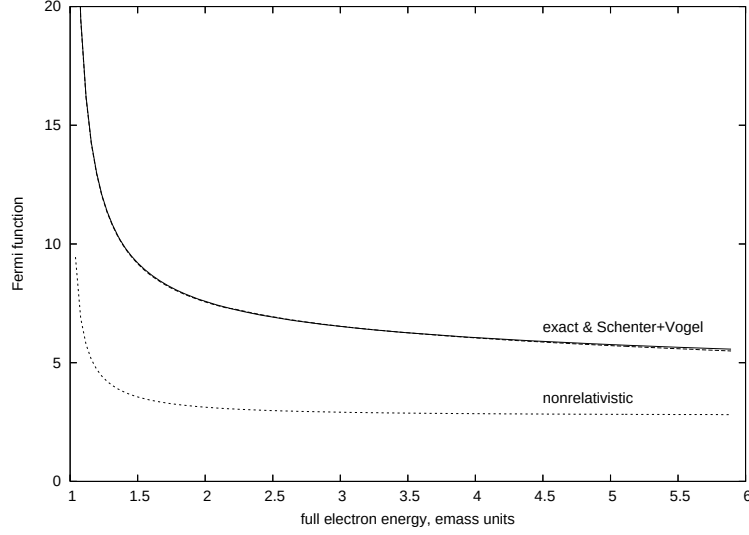


Figure 5.3: Comparison of the exact fermi function, the Schenter-Vogel approximation, and the non-relativistic fermi function for $Z = 56$ (the daughter nucleus of Xe-136 double beta decay).

is a significant difference between the non-relativistic and the relativistic form of the Fermi function as illustrated in Figure 5.3.

The complex gamma function in equation 5.8 makes it somewhat cumbersome to calculate. Consequently, a parameterization is used to speed up the calculations. Currently, EXOsim uses the parametrization of Schenter and Vogel [9], which is

$$F(E, Z) = \frac{E}{p} \exp[\alpha(Z) + \beta(Z)(E/m - 1)^{1/2}], \quad (5.11)$$

where for $E/m < 2.2$,

$$\alpha(Z) = -0.811 + 4.46 \times 10^{-2}Z + 1.08 \times 10^{-4}Z^2, \quad (5.12)$$

$$\beta(Z) = 0.673 - 1.82 \times 10^{-2}Z + 6.38 \times 10^{-5}Z^2, \quad (5.13)$$

but for $E/m \geq 2.2$,

$$\alpha(Z) = -8.46 \times 10^{-2} + 2.48 \times 10^{-2}Z + 2.37 \times 10^{-4}Z^2, \quad (5.14)$$

$$\beta(Z) = 1.15 \times 10^{-2} + 3.58 \times 10^{-4}Z - 6.17 \times 10^{-5}Z^2, \quad (5.15)$$

where E is the total electron energy and m is the mass of the electron.

The Schenter-Vogel parameterization is accurate to within 2% of the analytic form. A comparison of the Schenter-Vogel Fermi function and the analytic form with a correction by Wilkinson [10] are shown in Figures 5.3 and 5.4. The Wilkinson correction adjusts for the size of the nucleus, which is particularly important for large Z nuclei such as ^{136}Xe . At low energy (< 600 keV, equivalent to the change in parameterization at $E/m = 2.2$), Schenter and Vogel results differs from the analytic form by about 2%. The difference drops to 0.5% above the change in parameterization. Figure 5.5 compares the two $\beta\beta 2\nu$ sum energy spectra calculations by their fractional difference. Both calculations are identical with the exception of the Fermi function: one uses the Schenter-Vogel parameterization [9] and the other uses the analytic form with the Wilkinson correction for nuclear size [10]. By using the Schenter-Vogel approximation, a difference of at most 2.5% in the $\beta\beta 2\nu$ spectra is obtained with most of the difference within 0.5%.

5.2.2 Comparison of Two Theoretical Models

The Kotila and Iachello calculation was also considered for EXO-200. In this calculation, the phase space factors were calculated using newly improved numerical evaluation of the Dirac wave functions. Rather than considering the phase space factors in terms of the Fermi functions, the Kotila/Iachello calculation starts with the radial form of the Dirac equations and retains this radial form to be evaluated by the package RADIAL [11].

A separate generator for $\beta\beta 2\nu$ using the Kotila/Iachello model was added to EXOsim to allow for a different $\beta\beta 2\nu$ fit. Since the search for $\beta\beta 0\nu$ is sensitive to the spectral shape of $\beta\beta 2\nu$, particularly at the tail, the potential fit difference due to the two different theories must be checked. We obtained a 2D table of electron probability (Figure 5.6) directly from Kotila and Iachello. From this table, the dN/dK distribution, based upon the energies of the two electrons, is used through the acceptance-rejection method again to generate a $\beta\beta 2\nu$ spectrum.

Figure 5.7 plots the normalized $\beta\beta 2\nu$ spectra for the two different calculations: the Vogel calculation is in gold and the Kotila/Iachello calculation is in blue. In this plot, one cannot discern any difference between the two spectra, including the location of the peak. Using the fractional difference as the figure of merit, Figure 5.8 shows the small variations between the two calculations. To ensure that the difference between the two spectra is not due to the Q-value, both calculation used the same exact value of 2.45783 MeV for the Q-value of ^{136}Xe as measured by [54]. At the very tail, the difference is as much as 5% while the bulk of the spectra are in

agreement to within 2%. The minimum fractional difference is found at 0.89 MeV, very close to the peak for both spectra at 0.82 MeV.

$\beta\beta 2\nu$ distribution from both theories were used separately to fit the final results. The comparison of the fit results will be discussed in section 8.5.3.

5.3 $\beta\beta 2\nu$ Decay to Excited State

As described in earlier section 2.4, the ^{136}Xe decay to the excited state is effectively a $\beta\beta$ decay with a smaller Q-value (879 keV) plus the emission of two γ 's (760.5 keV and 818.5 keV) from the de-excitation from the excited state. Since the de-excitation stages have half-lives in the picoseconds, much shorter than the sampling time of the EXO-200 detector, the emission of the two γ 's can be considered as happening simultaneously as the $\beta\beta$ decay to the excited state.

The simulation of the decay to the excited state for ^{136}Xe in EXOsim first generates a $\beta\beta 2\nu$ with a 879 keV Q-value used for the phase space calculation and the Schenter-Vogel approximation applied for the Fermi function. For this first analysis, the two γ 's were generated with no angular correlation between the γ 's or between the γ 's and the β 's. The two uncorrelated γ 's have equal probabilities to be emitted in any direction. This decay to the excited state with simultaneous emission of the $\gamma\gamma$ at the same location can also be applied to the $\beta\beta 0\nu$ and the $\beta\beta 2\nu X$ decays to simulate the neutrinoless double beta decay to the excited state and the neutrinoless double beta Majoron decay to the excited state.

5.3.1 Angular Correlation

The two γ 's from the de-excitation of the $\beta\beta 2\nu$ daughter excited state in the $0^+ \rightarrow 2^+ \rightarrow 0^+$ have an angular correlation due to angular momentum considerations. The $\gamma\gamma$ angular correlation is

$$W(\theta) = \frac{5}{8} \times (1 - 3\cos^2\theta + 4\cos^4\theta) \quad (5.16)$$

where θ is the angle between the two γ 's. The two γ 's have a preference to be either emitted in the same direction (angle 0) or in complete opposite direction (angle π) [3].

The excited state decay search described in Chapter 8 does not make use of this angular correlation, and it is not included in the simulations used in that analysis. Using the same acceptance-rejection algorithm that sets the $\beta\beta$ angular correlation, the $\gamma\gamma$ angular correlation has since been added to the excited state simulations. The angular correlation included excited state simulation is used for the position dependent fit shown in section 9.1.3.

The first γ has the freedom to be uniformly pointing in any direction while the momentum vector of the second γ is constrained by this angular correlation equation relative to the first vector. Figure 5.9 shows the comparison between the simulated angles of the $\gamma\gamma$ with the angular distribution from equation 5.16 for 50000 events. The simulated total energies in the detector (the variable that is fitted in this analysis) was found to be the same with and without the angular correlation, although the angular correlation may play a pivotal role in future analyses.

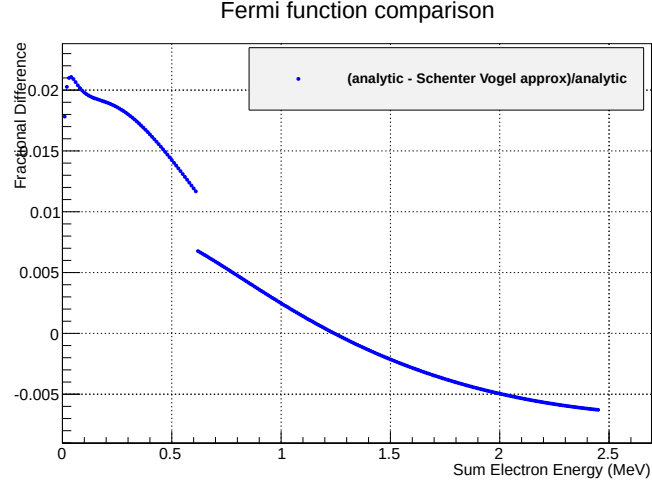


Figure 5.4: Comparison of Fermi functions, for $Z = 56$, of the Schenter Vogel parameterization [9] and the exact analytic form with the Wilkinson correction [10] in terms of fractional difference: $(\text{analytic} - \text{Schenter Vogel approx})/\text{analytic}$. Note that the discontinuity at around 0.6 MeV corresponds to the change in parameterization for the Schenter Vogel approximation. The EXO-200 analysis threshold is 700 keV.

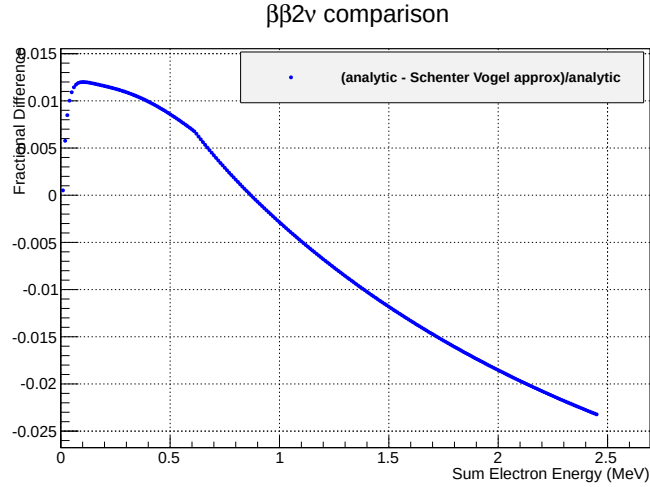


Figure 5.5: A comparison of two $\beta\beta 2\nu$ sum energy spectra calculations by their fractional difference. Both calculations are essentially identical with the exception of the Fermi function, Schenter-Vogel parameterization [9] and the analytic form with the Wilkinson correction [10]. By using the Schenter Vogel approximation, a difference of at most 2.5% difference in the $\beta\beta 2\nu$ spectra is obtained.

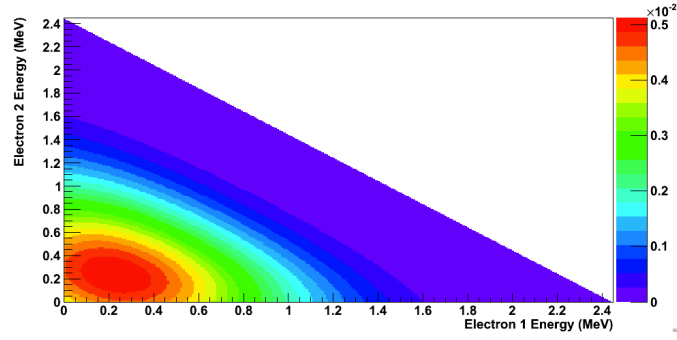


Figure 5.6: 2D plot of the electron probability table based on electron energies used for the Kotila/Iachello $\beta\beta 2\nu$ spectrum generation [11].

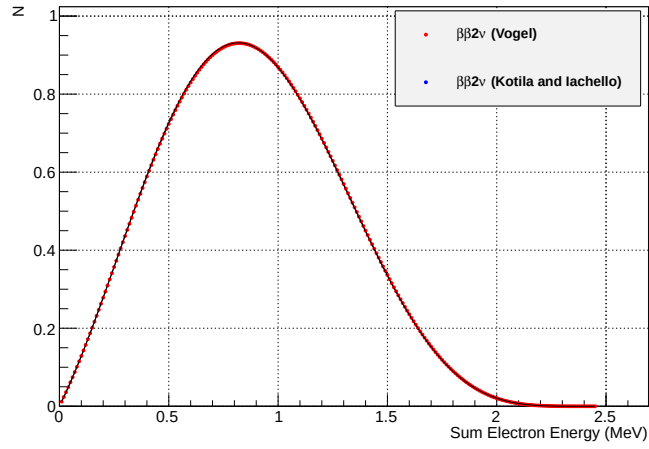


Figure 5.7: $\beta\beta 2\nu$ spectra (normalized to 1) for both the Vogel 2012 calculations (in gold) and the Kotila/Iachello calculations (in blue) [11].

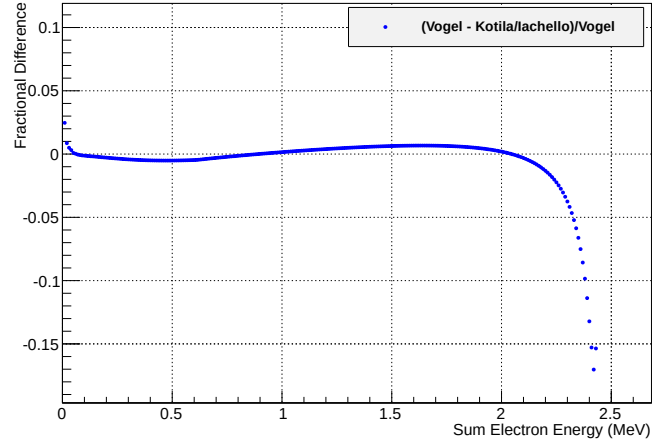


Figure 5.8: Fractional difference comparison of the Vogel (default EXOsim) and the Kotila/Iachello calculations [11]. Fractional difference is defined as $(\text{Vogel} - \text{Kotila/Iachello})/\text{Vogel}$. There is as big as a 15% difference at the very tail (due to roundoff errors for two very small numbers) while the bulk of the spectra agree to within 2%.

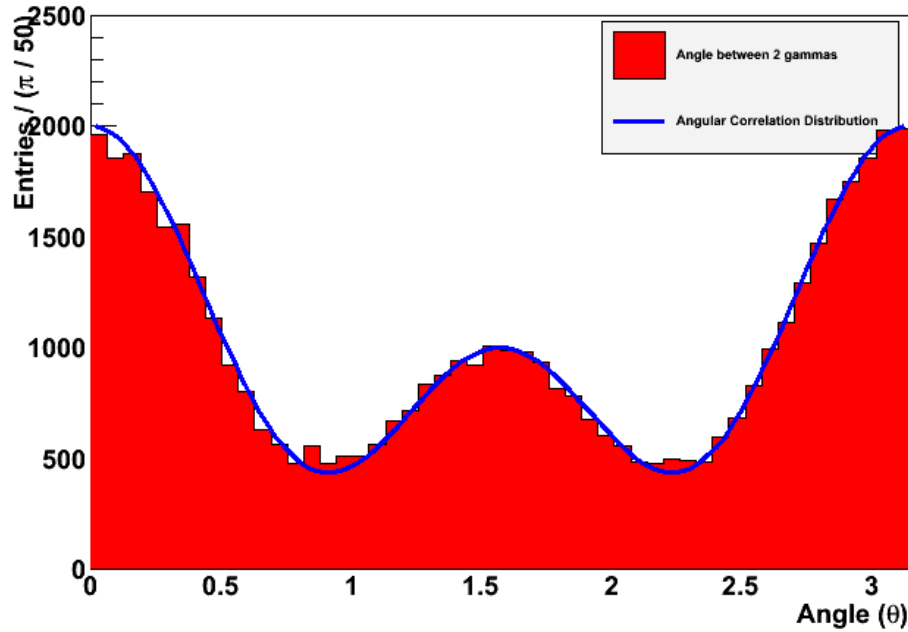


Figure 5.9: Comparison of the histogram of the angle between $\gamma\gamma$ for 50000 events and the theoretical $W(\theta)$ from equation 5.16 (blue line) scaled for the same number of events.

Chapter 6

Background Monte Carlo and PDF Generations

Chapter 5 described the double beta decay event generators. This chapter will cover the generation of background Monte Carlo used in the analysis and the generation of the Probability Density Functions (PDFs) for both the signal and the various backgrounds considered. GEANT4 was used to generate the MC events and simulate how the resultant particles travel through the different types of materials found in the detector and the support structures. Then, digitization and reconstruction are applied to the simulation to produce simulated energy spectra. These simulated energy spectra, one for single-site (SS) and one for multi-site (MS) for each signal and background events, are converted into PDFs. The PDFs are used in the fitting of the low background physics data to determine process rates.

6.1 Monte Carlo

An accurate simulation of the detector behavior is pivotal for the EXO-200 analysis. The experimental geometry, replicated in the simulation with some omissions, includes the detector (shown in Figure 5.2), the HFE, the cryostat, the lead, and the walls of the salt mine. The output of the simulations are pixelated charge deposit informations inside the detector from the various backgrounds. Next, the transport of ionization within the drift volume is simulated to create the induction

signals on the V-wires and the charge collection signals on the U-wires. The charges collected on each wire and their associated induction signals are then translated into digital signals (waveform) according to the response of the readout electronics. Since the bulk of the EXO-200 analysis power comes from the discrimination of events based upon multiplicity (see Chapter 7.5.3), the multiplicity of the Monte Carlo events also needs to be accurately determined. Therefore, a good simulation of events on the waveform level is required so that the same reconstruction algorithm (and its associated systematics) can be applied and compared for both data and MC. For each background and signal processes, two PDFs are generated, one for single site events and one for multiple site events.

6.1.1 GEANT4

GEANT4, which stands for or GEometry ANd Tracking, [80] is a C++ based platform for “the simulation of the passage of particles through matter,” using the Monte Carlo method. The version used for this analysis is GEANT4.9.4. Designed for high energy physics, GEANT4 includes the Radioactive Decay Module to simulate most of the known nuclear decays. Taking the half-lives, branching ratio, and energies from the Evaluated Nuclear Structure Data File (ENSDF) [13], α , β^- , β^+ , and Electron Capture (EC) are simulated. In addition to creating the particles to follow certain energy (and sometimes angular) distributions, GEANT4 can track the particles inside the detector, accounting for the interaction with the various internal parts of the detector. Particle attenuation lengths for various particle types and

energies through different materials are considered in the simulations. GEANT4 is also capable of simulating optical processes, however, this is not currently employed by EXO-200. Instead, a parameterized optical response is employed.

6.1.2 Particle Tracking

After the radiation events from either the customized $\beta\beta$ generator (see Chapter 5) or for radioactive nuclei through the GEANT4 Radioactive Decay Module are generated, GEANT4 simulates the interaction inside the detector until termination. The attenuation of particle energies through the interactions with detector components is simulated based upon the various cross sections of particles in different materials. Then, the final charge deposits are recorded for each $0.167 \text{ mm} \times 0.167 \text{ mm} \times 0.167 \text{ mm}$ voxels. For comparison, the separations between U and V wire gangs are 9 mm from the actual physical readouts. For a given event, each voxel with energy deposition has its position, total deposited energy, and the U-wire on which its charge is collected (if any) recorded.

Different types of radiations, for this particularly analysis (β and γ) have different interaction cross sections with the liquid xenon in the detector. As indicated in Figure 6.1, at the end point energy of $\beta\beta 0\nu$, the γ interaction is dominated by Compton scattering. The Compton scattering will often result in multiple charge deposits that are spread out over a wider area. Consequently, multiplicity allows for the separation of the $\beta\beta$ events from the background γ 's for the main EXO-200 $\beta\beta 0\nu$ analysis.

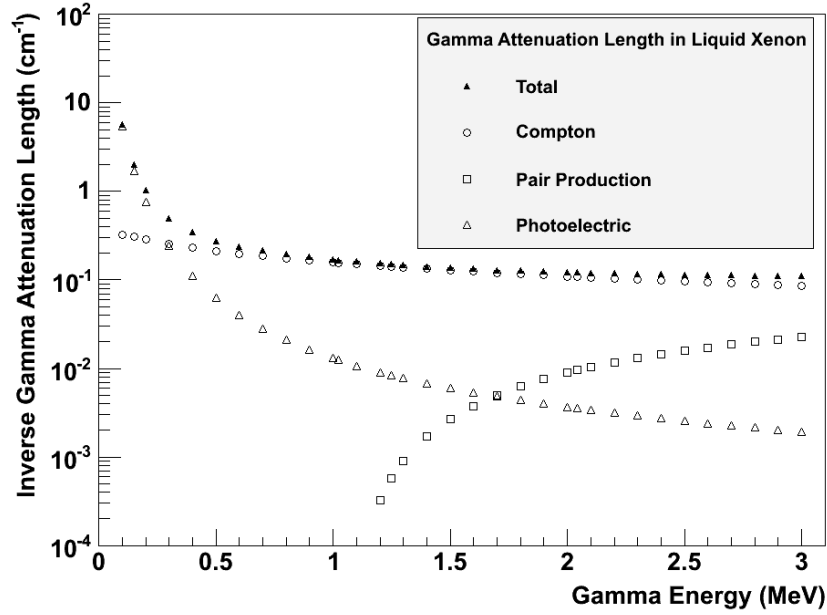


Figure 6.1: Gamma attenuation lengths in xenon for energy-depositing processes. Figure taken from [1], data value taken from [12].

The α 's are much more easily identifiable from the β 's. α particles ionize smaller regions as compared to their β and γ counterparts to produce higher light yields. They can be easily discriminated from considering the ionization/scintillation ratio.

6.1.3 Digitization and Reconstruction

After GEANT4 has simulated the pixelated charges for an event, digitized waveforms for the wire and the APD signals are next created. An electrostatic software package, MAXWELL, was used to calculate the wire planes' weighting field, an electric field that represents the response of the electrode to the presence of charges in the detector. This 2-dimensional electrostatic simulation result is used to determine the drift trajectories of the individual pixelated charge deposits to the

wires. For each event, the induction and charge collection signals on the U-wires and induction signals on the V-wires are simulated. Raw waveforms are first generated with a fine sampling time of $0.05\ \mu\text{s}$. Wire signals are calculated using the pixelated charge deposits using Ramo's Theorem [79], and APD signals are taken as step functions. The signals are then resampled with a $1\ \mu\text{s}$ sampling time to match the output of the physical DAQ. Noise, taken from calibration runs, is added in so that reconstruction (mainly the matched filter algorithm) would yield similar efficiency. Finally, the digitized signals are run through the same reconstruction algorithm as data.

6.1.4 Scintillation Monte Carlo

For EXO-200, the scintillation information from Monte Carlo is not used for two reasons. First, photon tracking is computationally expensive. Second, the reflectance of the Teflon tiles in the simulation also has a large uncertainty. These two factors combine to make scintillation simulation in the TPC difficult and its accuracy quite questionable. Additionally, no model of charge recombination is available to accurately simulate the anticorrelation between charge and scintillation.

6.2 Background Model

Figures 6.2 and 6.3 show the two main decay chains of interest for EXO-200 in ^{238}U and ^{232}Th . These two chains, along with ^{40}K are common long lived radioactive isotopes and typical backgrounds for low radioactivity experiments. For EXO-200,

^{40}K , a beta emitter that effectively emit a gamma with an endpoint of 1460 keV, is typically a background for the $\beta\beta 2\nu$ decay. However, the ^{232}Th decay chain has a 2615 keV gamma from ^{208}Tl and the ^{238}U chain has a 2448 keV gamma from the ^{214}Bi decay. These backgrounds are troublesome for the $\beta\beta 0\nu$ search at the energy of 2458 keV. All three of these isotopes can be present in the copper vessel, the APD planes, and the signal cables. Given the shielding ability of the HFE, the presence of these isotopes in the Inner Cryostats was not used in the background model, although they have been simulated and studied. Any possible contributions from outside the LXe vessel would be added by the fit to the corresponding vessel PDFs.

The following list contains all backgrounds considered in the fitting of the low background data:

- ^{238}U in the vessel
- ^{232}Th in the vessel
- ^{40}K in the vessel
- ^{60}Co in the vessel
- ^{54}Mn in the vessel
- ^{65}Zn in the vessel
- ^{222}Rn in the active LXe
- ^{135}Xe in the active LXe

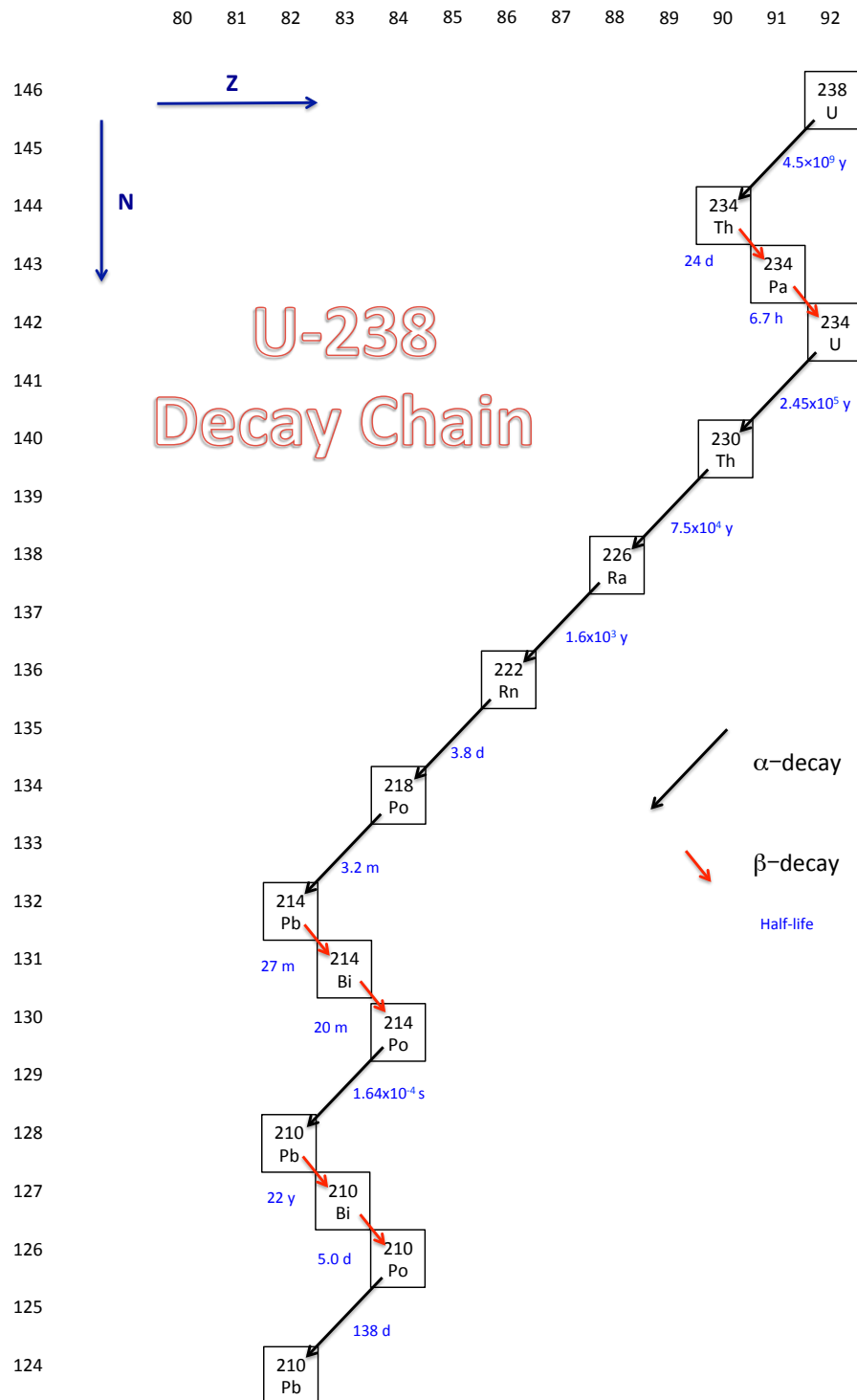


Figure 6.2: Decay chain diagrams for ^{238}U . Decays in the Uranium chain with branching ratios $< 0.1\%$ are omitted for simplicity. The decay half-lives are taken from Table of Isotopes, which have data from ENSDF [13].

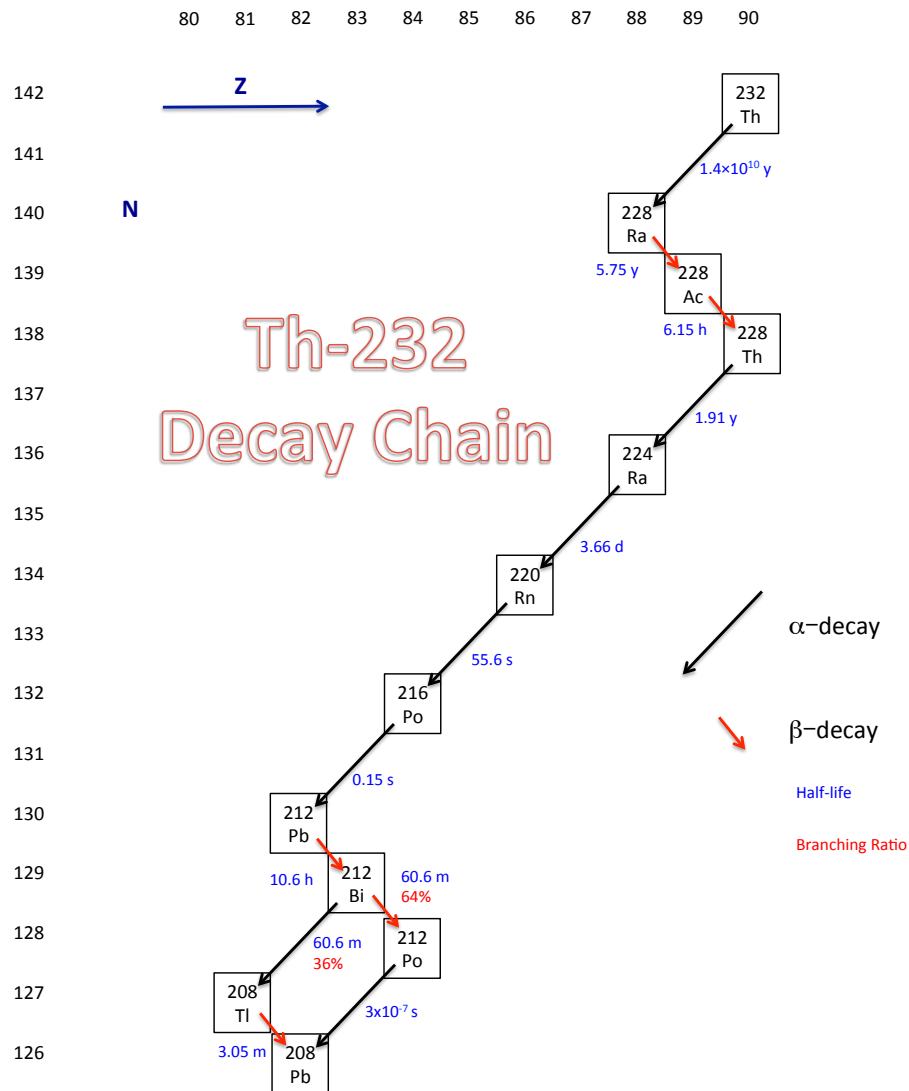


Figure 6.3: Decay chain diagrams for ^{232}Th . The decay half-lives are taken from Table of Isotopes, which have data from ENSDF [13].

- ^{222}Rn in the inactive LXe
- ^{214}Bi on the cathode
- ^{214}Bi in the airgap

Few of the cosmogenically activated isotopes with long half-lives are plausible to still exist in the copper of the liquid xenon vessel during the data taking. Although ^{54}Mn (half-life of 312 days) and ^{65}Zn (half-life of 244 days) are γ emitters with end points well below the Q-value of ^{136}Xe , ^{60}Co (half-life of 5 years) has a sum peak at 2506 keV. Since these energies are emitted as γ 's, they are most likely going to Compton scatter and become multiple site events. While these same cosmogenics background can exist in the cryostat and beyond, the self shielding ability of the liquid xenon and the shielding power of the HFE make those contributions negligible.

With the liquid xenon being constantly repurified, non-noble cosmogenics are expected to be taken out from the liquid xenon. However, noble gas related backgrounds that originated from the liquid xenon still need to be considered. Radon, to be discussed below, can dissolve in liquid xenon. The other possibilities to be considered are the xenon isotopes created by neutron capture. Neutron capture of ^{134}Xe and ^{136}Xe can lead to ^{135}Xe and ^{137}Xe . There is some evidence for the presence of ^{135}Xe in the data, but little evidence for ^{137}Xe . Only ^{135}Xe is considered in the background model.

It should be noted here that the measured rates from the material screening are often only upper limits; this makes it difficult to properly constrain them in the fit as multiple components are merged into the same PDF.

6.2.1 Radon

A background simulation that requires special attention is that of ^{222}Rn in the LXe. Radon decays inside the detector are mostly measurable from the α -spectroscopy analysis. Three separate PDFs (^{222}Rn in active LXe, ^{222}Rn in inactive LXe, and ^{214}Bi on the cathode) are used to represent the radon in the liquid xenon. Given the Rn-222's half-life of 3.8 days, radon may find its way into the active xenon volume. The daughter nuclei of Rn-222 have half-life on the order of several minutes. Because these positively charged daughter ions in the active volume may slowly (relative to the electrons) drift towards the cathode, the PDFs to represent the radon in LXe are more complicated to build than for other backgrounds. ^{214}Bi on the cathode is considered a part of the ^{222}Rn in the LXe given how some of the daughter ions may drift to the cathode and stay on the surface. Radon is discussed further in section 8.5.1.1.

6.3 PDF Generation

The simulations generate spectra of the total energy deposited in the liquid xenon assuming perfect energy resolution. To make the PDFs more realistic, therefore, these simulated spectra must be convolved with a detector energy resolution function. This energy dependent function is determined from calibration runs. Furthermore, given the existence of “dead regions” within the detectors, not all of the simulated pixilated charges in the liquid xenon will be observed by the wire grids in real data. Some of the pixilated charges in the Monte Carlo must be manually

culled prior to being used in the PDFs for the data and simulation to match. The detail of this “fiducial volume” determination and the corresponding “cluster cull” algorithm will be discussed in section 8.1.5.

For each charge deposit in an event, the deposit is counted as a part of the total detected energy if and only if its corresponding U-wire signal survives the “cluster cull” cut. Assuming that the desired energy resolution function is known, the summed total of all the surviving charge deposits is convolved with a gaussian PDF whose width is the energy resolution, determined from the energy resolution function for that total energy. To perform this convolution, a modified version of the gaussian convolution is used. For our purpose, we want the convolution to result in the width of the specific energy resolution, following an energy dependent formula. This is achieved by defining the convolution between a function h and a gaussian $g(E)$ with energy dependent width $\sigma(E)$ as

$$(g * h)(E) = \int e^{-Q^2/2\sigma^2(E)} h(E - Q) dQ. \quad (6.1)$$

In the normal definition, the energy-dependent width σ term is a function of Q and integrated out. With our definition, if one convolves a δ -function $h(E) = \delta(E - E_0)$, one ends up with a gaussian around E_0 with the energy dependent width of $\sigma(E)$. ROOT’s interface to the FFTW3 package [81] is used to perform this modified convolution.

Figure 6.3 shows the PDFs for all of the backgrounds considered with the energy resolution smearing from the expected anticorrelated energy resolutions -

both the single site (SS) in red and multiple site (MS) in blue are plotted. Figure 6.3 shows the PDFs for the various $\beta\beta 2\nu$ signals. Each of the PDFs is individually normalized to one in these plots to better show the energy spectral shapes.

One of the variables considered during the fit is the “beta scale” - an energy scaling to compensate for applying calibrations from solely the γ 's to the β 's. In order to do a profile likelihood based on the beta scale, a different set of PDFs has to be used, where every relevant beta-like PDF (mainly $\beta\beta 2\nu$) is scaled in energy by this scaling factor. Beta scale will be discussed more in detail in section 8.5.2.

Figure 6.4: Background PDFs generated from Monte Carlo simulations. The spectra are between the energy range of 700 keV and 3500 keV. Red is the single site spectrum and blue the multi site spectrum. An energy resolution, determined from calibration runs, has been included in these PDFs

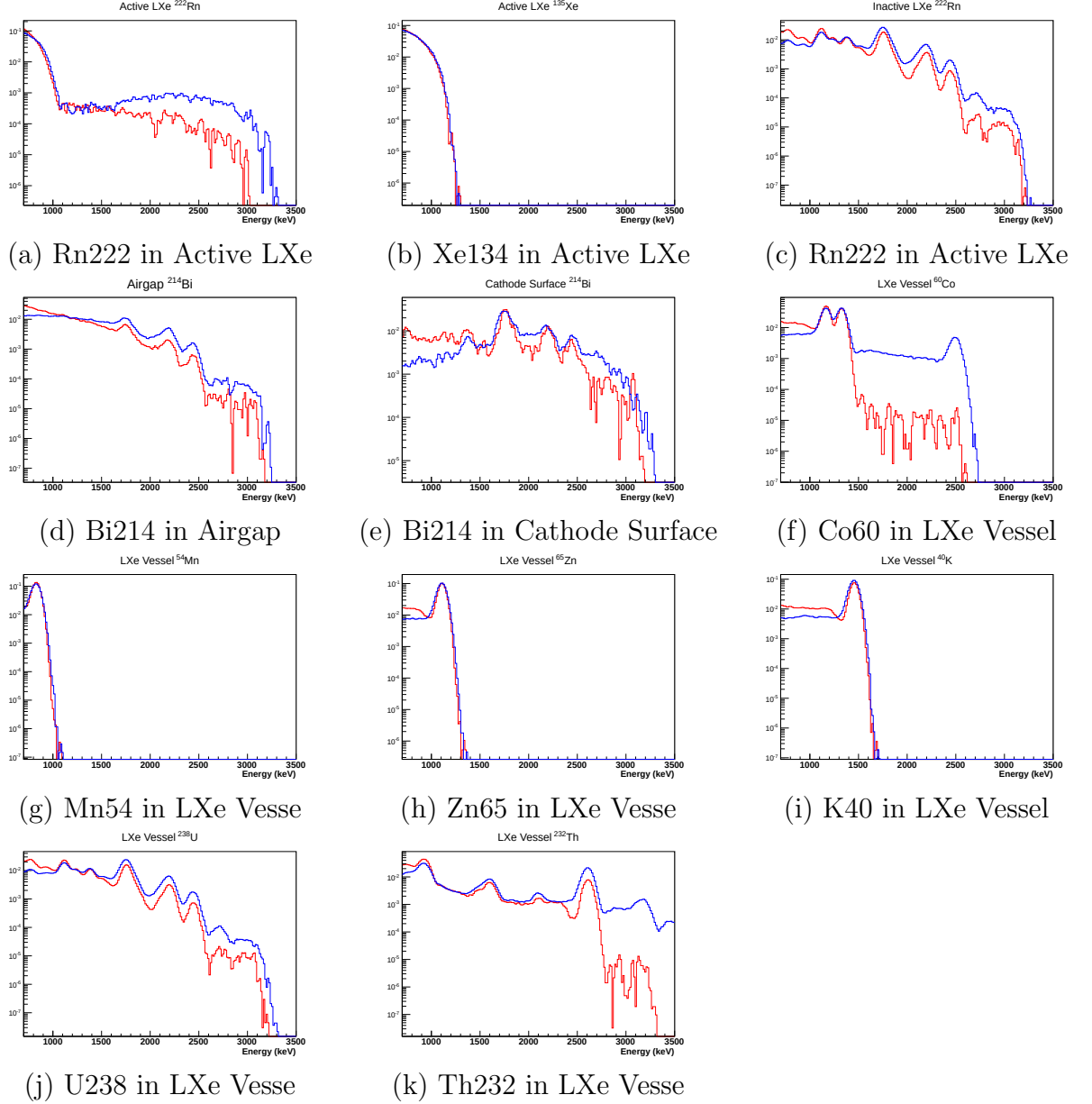
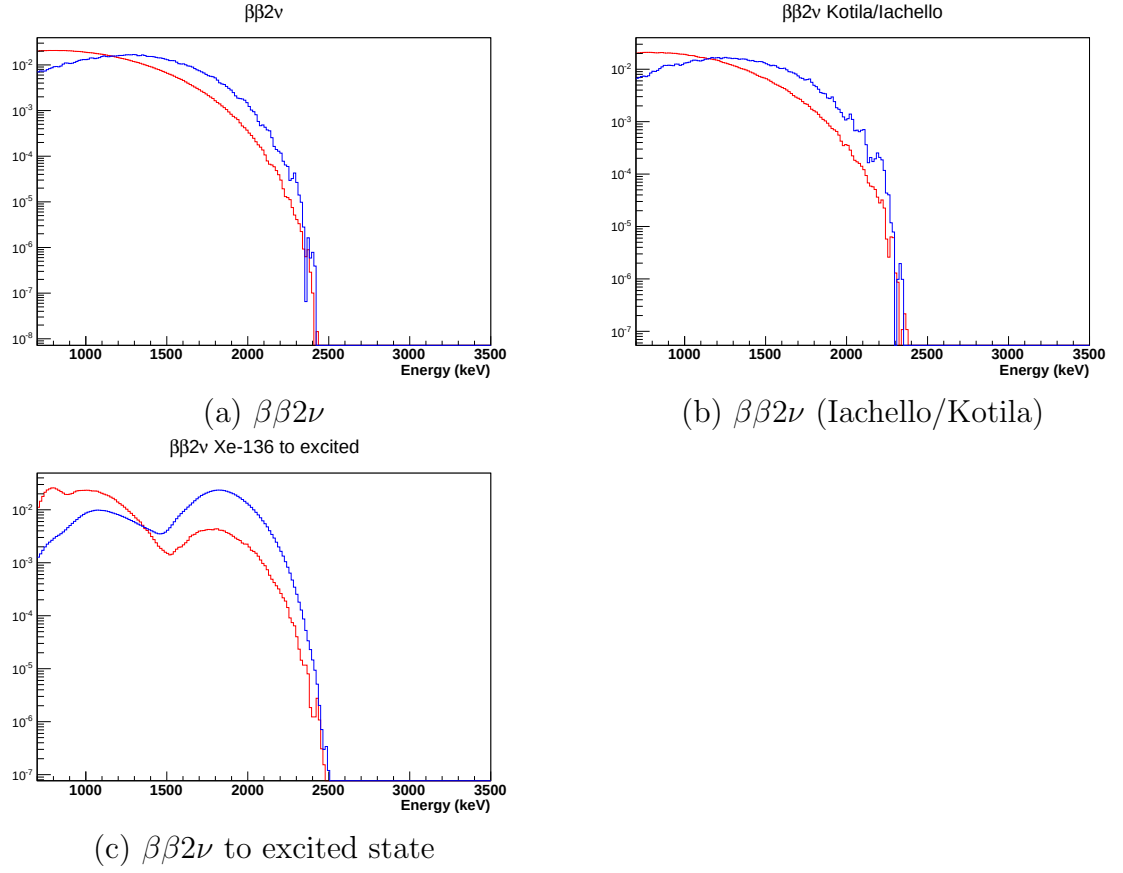


Figure 6.5: Signal PDFs generated from Monte Carlo simulations. The spectrum are between the energy range of 700 keV and 3500 keV. Red is the single site spectrum and blue the multi site spectrum. An energy resolution, determined from calibration runs, has been included in these PDFs



Chapter 7

Calibration

The response of the detector to ionizing radiation is calibrated with external γ sources placed near the TPC. For EXO-200, the three types of external calibration sources used are ^{60}Co , ^{137}Cs , and ^{228}Th . From these three calibration sources, 4 γ -lines are obtained for calibration: 661.7 keV from ^{137}Cs , 1173.2 keV from ^{60}Co , 1332.5 keV from ^{60}Co , and 2615.5 keV from ^{208}Tl , which is a part of the ^{228}Th decay chain. These three sources cover the full energy scale of interest (500 keV - 2500 keV). The half-lives of these sources are 30.2 years for ^{137}Cs , 5.3 years for ^{60}Co , and 1.9 years for ^{228}Th .

7.1 Calibration Hardware

To calibrate the detectors with these γ -sources, a 1/4 inch (outer diameter) copper guide tube is installed inside the inner cryostat, just outside the liquid xenon vessel. The calibration tube system is shown in Figure 7.1. From outside the cryostat, at room temperature, different sources can be inserted into the calibration tube and moved around the TPC. The calibration sources are 0.7mm in diameter and attached to the end of a flexible steel cable. Based upon how far the calibration sources have been inserted into the tube, their relative positions around the TPC are determined and can be repeated. For the most part, calibrations are taken either

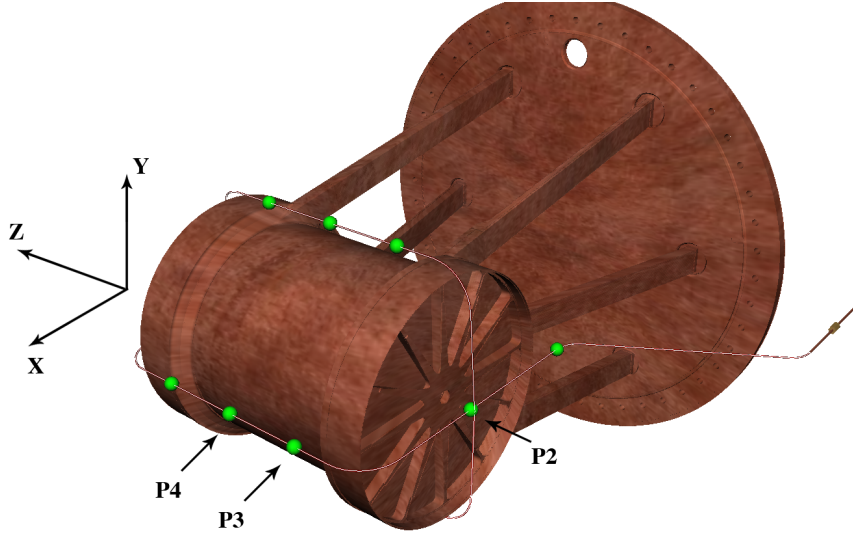


Figure 7.1: The calibration system consists of a guide tube around the LXe vessel. Green dots show the designated locations for calibration sources. The label points: P2, P3, and P4 are the main calibration position used.

at the anode (end cap of the cylinder that is the liquid xenon vessel, labelled as P2 in Figure 7.1) or at the cathode (in the center of the cylinder, labelled as P4 in Figure 7.1). The standard positions are listed in Table 7.1. The calibration source can be swapped even while the cryostat is still cold, as all the relevant components are out at room temperature. Care must be taken, however, to ensure that dry air is flushing the calibration tube so that no water can enter the calibration tube to form ice inside the cold sections.

At these energies, the interaction length of the γ 's from these sources is long enough for a large fraction to penetrate the HFE between the tube and the TPC vessel as well as the copper vessel itself before being fully absorbed inside the active liquid xenon volume. Nevertheless, the density of interactions does fall off the further the γ 's have to travel, few interactions are observed on the opposite side

Source Position	Source Position Name	Nominal Coordinates (cm)
S2	P2 nz	(0, 0, -30.4)
S5	P4 px	(25.4, 0, 0)
S8	P2 pz	(0, 0, 30.4)
S11	P4 py	(0, 25.4, 0)
S17	P4 ny	(0, -25.4, 0)

Table 7.1: The 5 standard calibration source positions. Given the cylindrical symmetry of the xenon vessel, two distances P2 (anode) and P4 (cathode) are used. The P2 and P4 in Figure 7.1 correspond to positions S2 and S5.

of the active liquid xenon volume. To achieve calibration measurements that are position-dependent (mainly for the light map, see section 7.3.2), the sources have to be movable to reach the different areas of the TPC. Among the available standard positions used and listed in Table 7.1, the same relative position (given the cylindrical symmetry of the TPC) but opposite sides are achievable by the sources.

For each of the three types, two sources of different strengths were made (weak and strong) although only the weak sources were used for the bulk of the calibration runs. Too many “pile-up” events, where multiple decays occur in one trigger window, were found in the strong source runs. The weak source runs can be triggered similarly to the low background physics runs, however; the possible physics triggers used were the APD sum signal (threshold 800 ADC counts), individual signal (threshold 1750 after baseline correction), single U-wire signal (1617 ADC counts), and 0.1 Hz random trigger.

7.2 Calibration Data Selection

The goals of the calibration runs are to determine the necessary data correction and data selection criteria. For each run, a large number of events in the least amount of time (to minimize the loss of physics data livetime) is preferred to reduce statistical fluctuations. Most source runs are taken with a forced trigger at 50 Hz, the maximum frequency the DAQ can handle. A few runs used for source agreement studies are taken with the same physics trigger as the low background data in order to have the same conditions for comparison. The strength of the sources are large enough to sometimes produce “pile-up”: for example, multiple γ ’s interactions within a trigger window. To deal with this, any scintillation signal must be separated by more than $120\ \mu\text{s}$ (more than the maximum drift time) from others to be accepted. A similar set of analysis selection cuts (see section 8.1) is applied to the calibration data. The surviving data have to be from the fiducial volume and be reconstructed in three dimensions.

7.3 Data Correction

From the source calibrations runs, position dependent corrections are inferred and made onto all runs, both source calibration and low background physics. Three ionization corrections are made to adjust for the electron lifetime (Z dependent since drift time is related to distance to the anode), V-wire shielding inefficiency (also Z dependent), and U-wire channel dependent gain (U dependent). A light map correction is applied to the scintillation signal. No additional signal corrections

are done after this stage. The corrected ionization and scintillation signals are next used to find the energy resolution minimizing the anticorrelation parameter of rotated angle. A summary of all of the energy corrections applied is shown in Table 7.2.

7.3.1 Ionization Corrections

7.3.1.1 Electron Lifetime

Electronegative impurities in the liquid xenon can absorb ionization charges based on the amount of time that the ionization exists. A correction is made on the total charge detected based upon the drifting distance/time of the electrons.

$$Q_{collected} = Q_{deposit}e^{t_d/\tau}, \quad (7.1)$$

shows the relationship between the deposited charge and collected charge given an electron lifetime of τ and drift time of t_d .

The electron lifetime is determined from looking at the full-absorption peak from radioactive source calibration spectra, mainly the 2615.5 keV peak from ^{208}Tl of the ^{232}Th runs. By looking at how the amount of charge collected decreases as the distance of the interaction site from the anode increases (distance in Z), a relationship of the change in full-absorption peak position with drift time is used to get the electron lifetime. In this “peak method”, events are divided by drift time into 24 even bins of $6.875 \mu\text{s}$, with 12 bins in each TPC half. Events in each bin are

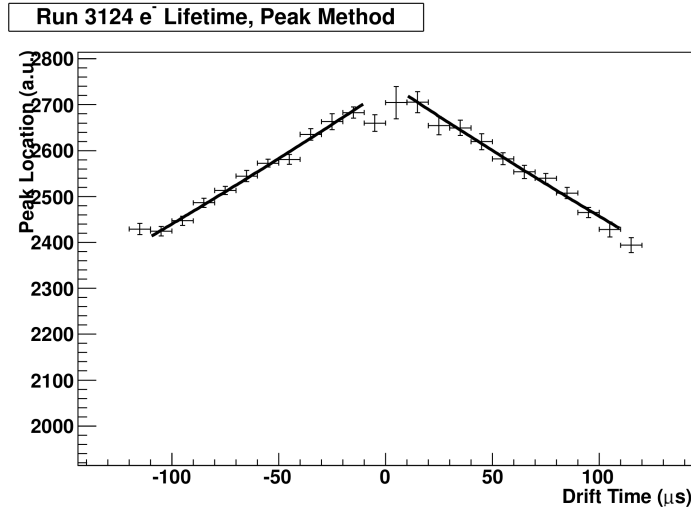


Figure 7.2: Fitted peak position versus drift time (but essentially Z) for a ^{232}Th source calibration, which is fit to an exponential to extract the electron lifetime.

within a radial distance of $r < 160$ mm and above a scintillation threshold of 2000 ADC count for Th source. By fitting (discussed in more details in section 7.4.2) for the full absorption peak separately in each bin, the variance of the peak position is then compared to the drift time and shown in Figure 7.2. A fit of the slope allows the electron lifetime to be extracted.

For EXO-200, the electron lifetime of the xenon is found to be strongly correlated to the xenon recirculation rate. Since the xenon is constantly being pushed through a purifier, this correlation is to be expected. Figure 7.3 shows both the measured electron lifetime and the flow rate with respect to time.

7.3.1.2 V-wire shielding inefficiency

Because the V-wires do not perfectly shield the U-wires from the charge deposited, the slowly drifting positive charges (the positive ions that are virtually not

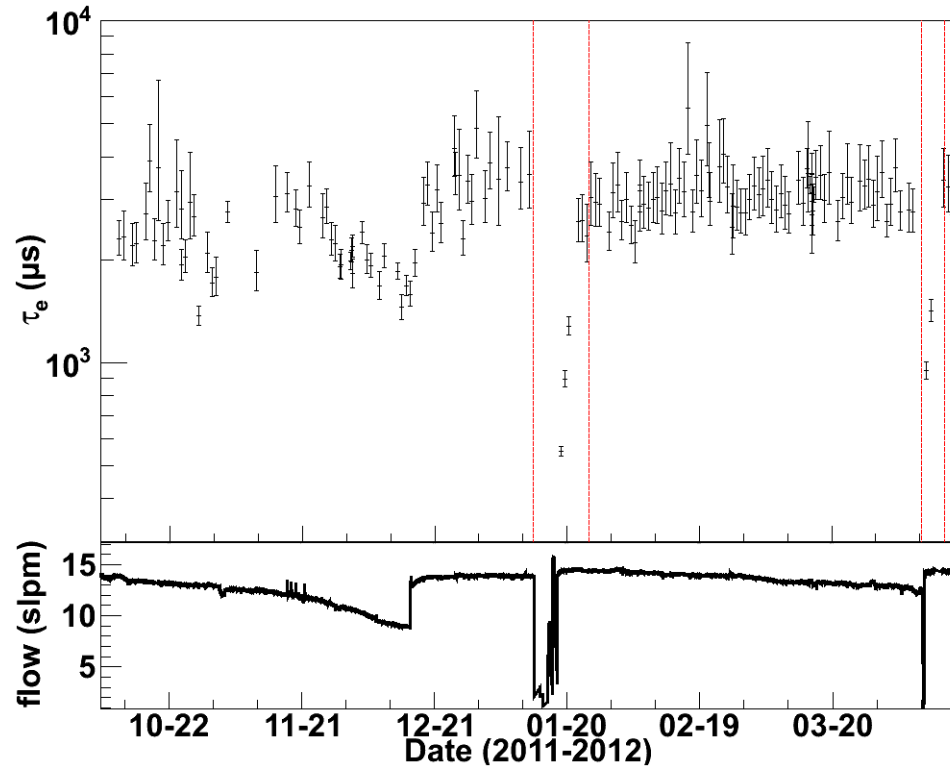


Figure 7.3: Top: Electron lifetime measured using peak method, with both TPCs combined. Bottom: xenon recirculation rate during the physics run. There is a strong correlation between the two.

moving due to their mass, compared to the drift times of the electrons) can affect the measured charge collected due to induction effects. The expected induced charge is modeled as linear relative to the location of the positive charge (taken to be the location when the charge deposition took place). Thorium calibration data are fit to this model to determine the correction.

To find the correction, total ionization energies of the events were corrected for purity and divided into 75 spectra, each containing events in a 2.5 mm range of Z . To increase statistics while retaining the small bin size, events from both TPCs were mixed. The full absorption line from the Th runs is again being fitted for (discussed in more details in section 7.4.2), with the fit peak location plotted versus absolute value of Z in Figure 7.4. The plot of the best-fit peak energy versus absolute value of Z is then fit to a function of the form:

$$E = E_{measured} \left(1 - \frac{B}{Z_0 - Z} \right), \quad (7.2)$$

where B and Z_0 are parameters allowed to float, and $E_{measured}$ is the purity corrected measured energy. The fit value of Z_0 correspond to the distance between anode and cathode. The value of B represents the inefficiency. A similar effect is observed in the Monte Carlo. Figure 7.4 shows the data and the fits for all events from a run. However, when the data is limited to just the single U-wire events and the two U-wire events, the fit value for B is almost doubled in the two U-wire events. This finding supports the idea that the V-wire inefficiency is related to the number of collection wires.

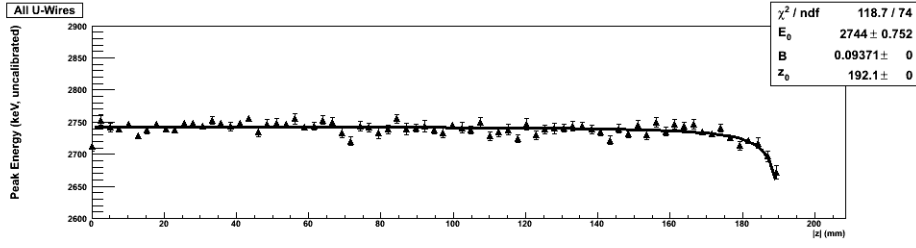


Figure 7.4: ^{228}Th mean peak position in various Z-bins, taken from dedicated calibration runs. Induction effects lead to a decrease in peak position, most noticeably at large values of Z (far from the cathode). Signals striking any number of U-wires are included. A fit of the form $1/Z$ is also included. Figure taken from [1].

7.3.1.3 U-wire gain correction

From source calibration data, the gains of the U-wires are measured. Using the ^{228}Th calibration runs specifically, the pair production double escape peak of ^{208}Tl was studied. The origin of the pair production peak is discussed in section 7.4.5. While the full absorption photo peak has higher energy and is more likely to be spread out across multiple U-wire triplets, the lower energy and β -like pair production double escape peak is more likely to be found at just one single U-wire triplet. Looking at events where charge is only detected on an single U-wire channel, the pair production double escape peaks were found to be at different positions depending on the U-wire channel, see an example in Figure 7.5. A relative correction factor is determined from these fits.

7.3.2 Scintillation Correction

For the scintillation signal, a light collection efficiency correction is applied based on the location of the signal (determined from the charge information). The

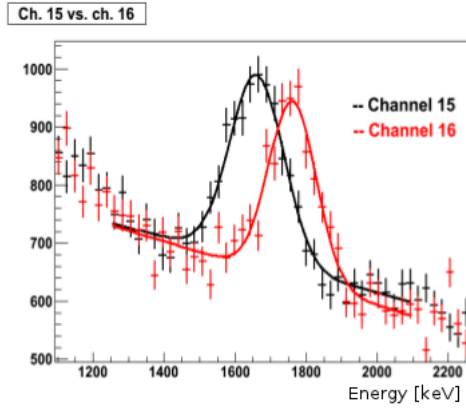


Figure 7.5: An example of the fits to the ^{208}Tl double escape peak two different U-wire channels in the same ^{228}Th calibration run. Correction is made to adjust for the relative difference between the U-wire channels. Figure taken from [8].

need for a scintillation correction comes from variations in APD gains, as well as differences in the solid angle subtended by the APD planes. Shadowing effects from detector edges or internal components are causes for additional minor location-dependent corrections.

The light collection efficiency is determined from isolating the 2615 keV full-absorption peak events from the ^{228}Th calibration runs for different regions of the detector based on the ionization signal only. The corresponding scintillation response of these events are then used to produce a light collection efficiency map in 3 dimensions, called *light map*, for the detector. Figure 7.6 shows the light map in 2 dimensions (R and Z of a cylinder), where the azimuthal bins are averaged over. The scintillation light response is the highest near the anode (and the APD platters) center while there is a “dead” spot at the outer edge of the cathode. From the light map, scintillation signals are corrected based on the location of the reconstructed ionization cluster. For multiple cluster events, an energy weighted sum of

the correction for each cluster is used.

The light map used for the EXO-200 analysis came from Th calibration runs from all 5 source positions, to ensure as uniform a position distribution as possible for TPC events. Only single-site events (as determined from the charge signal) are used. The detector was divided non-uniformly into 1352 voxels, formed by 13 radial divisions, 13 division along the Z axis, and 8 azimuthal divisions. The voxels are chosen to include sufficient statistics in every bin. For each voxel, the mean peak energy that is normalized to 2615 keV, was taken as the light map value for that voxel.

Table 7.2: Summary of corrections made to the reconstructed charge and scintillation energies. Corrections are applied initially to the wire signal energies, Q_{rec}^{wire} , and the scintillation clusters, E_S^{recon} . Table taken from [1].

Correction	Correction Factor	Notation
U-wire response	ξ	$E_{uc} = \sum \xi \cdot Q_{rec}^{wire}$
Electron lifetime	κ	$E_{pc} = \kappa \cdot E_{uc}$
Shielding grid inefficiency	λ	$E_{gc} = \lambda \cdot E_{pc} = \lambda \cdot \kappa \cdot E_{uc}$
Total charge cluster energy	N/A	$E_Q = \sum E_{gc}$
Light map	$f_{light}(r, \phi, z)$	$E_S = E_S^{recon} / f_{light}(r, \phi, z)$

7.4 Calibration Parameter Extractions

While a 2 hour calibration run (typically the weak Th source) is done everyday, the calibration parameters are extracted from a specific subset of calibration runs. For each of these sources, the data are subjected to the event selection cuts (see section 7.2), processed with purity and light map corrections (see section 7.3 or

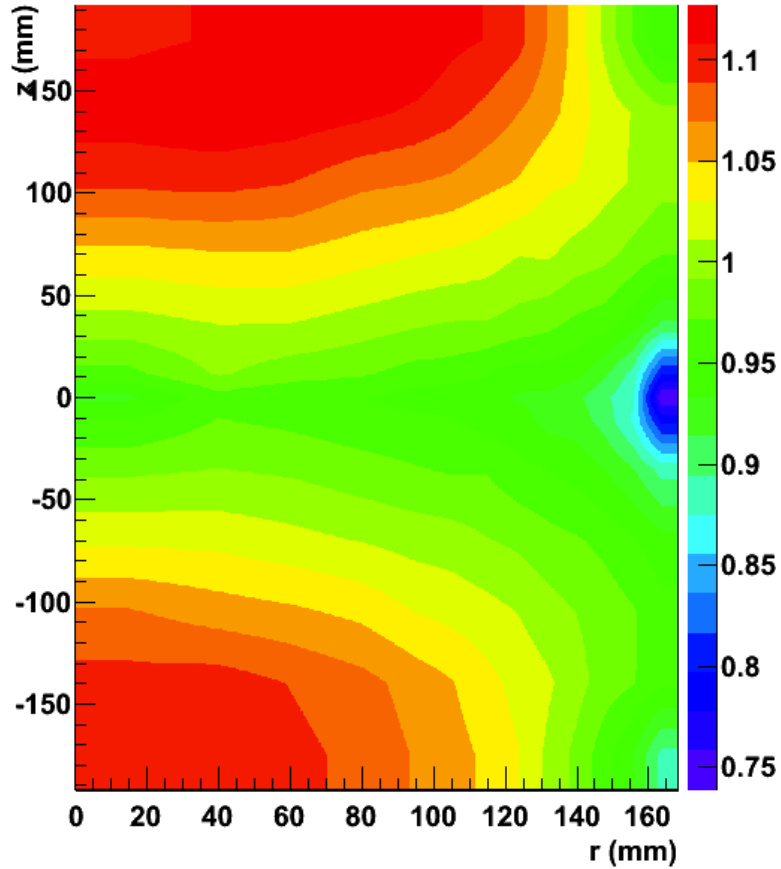


Figure 7.6: Light map correction function, averaged over all azimuthal bins. Heat intensity shows the relative scintillation response to events in that voxel. The light map is measured from the full-absorption peak in ^{228}Th calibration. Noticeable features are the higher response right by the center of the anodes (high absolute value of Z and low R) and the lowest response right by the cathode support ring ($Z = 0$ and high R). Figure taken from [1].

Table 7.2), and separated into single and multisite spectra. To take advantage of the enhanced energy resolution from utilizing the anticorrelation between the ionization and scintillation energies, a linear combination of the uncalibrated energies is used to generate a rotated energy.

7.4.1 Rotated Energy

Rotated energy is defined as,

$$E_{rotated} = E_{Ionization} \cos \theta + E_{Scintillation} \sin \theta. \quad (7.3)$$

The various linear combination of charge ($E_{Ionization}$) and light ($E_{Scintillation}$) are parameterized by a single variable: rotated angle θ . From the 2615 keV full-absorption peak of the ^{228}Th calibration data, the optimal θ is identified by minimizing the resolution of the full-energy peaks. SS and MS are treated separately, so there is a different optimal angle θ for the two cases. Figure 7.7 shows the fits that was done to get determine these θ_{min} 's. With the two different rotation angles for the SS and MS cases, rotation energy can be better defined as

$$E_{rotated} = \begin{cases} E_{Ionization} \cos \theta_{SS} + E_{Scintillation} \sin \theta_{SS}, & \text{(single-site)} \\ E_{Ionization} \cos \theta_{MS} + E_{Scintillation} \sin \theta_{MS}. & \text{(multi-site)} \end{cases} \quad (7.4)$$

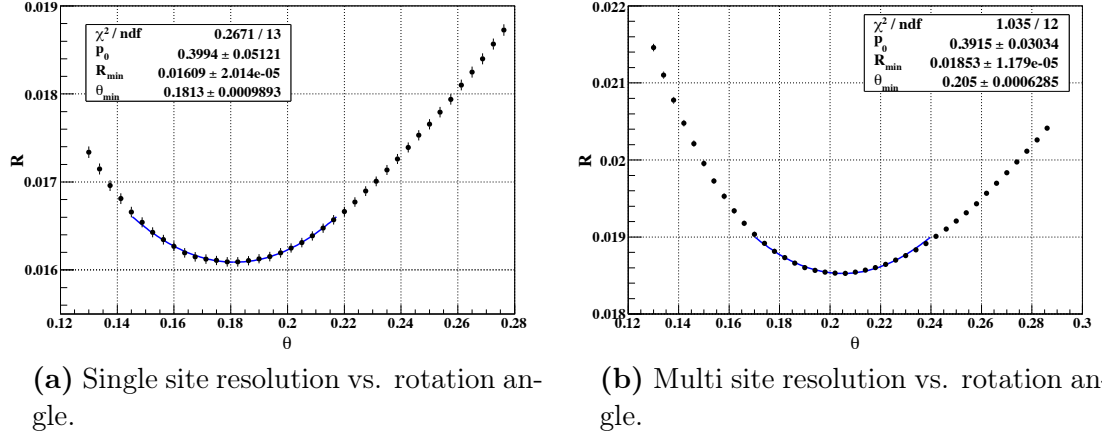


Figure 7.7: Resolution of the ^{228}Th full absorption peak versus rotation angle. A different rotation angle, taken to the minimum resolution, is obtained for SS and MS. Figure taken from [6].

7.4.2 ^{208}Tl Full-Absorption Peak Fitting

After all the selection and corrections, the full-absorption peaks in the rotated energy space of each calibration runs are fitted to the sum of a complementary error function and a Gaussian:

$$f(E) = A[0.5\epsilon(1 + \text{erf}(\frac{E - E_0}{\sqrt{(2)\sigma}})) + e^{\frac{E-E_0}{2\sigma}}], \quad (7.5)$$

where the error function (erf) is meant to represent the Compton background not resolved from the peak (represented by the Gaussian), and the same parameters E_0 and σ are used for both functions. The parameter ϵ fixes the ratio of the error function to the amplitude of the Gaussian. Figure 7.8 shows the rotated spectra for the calibration sources as well as the results of the fits to the full absorption gamma peaks. For the charge only case, ^{60}Co has two peaks that are not fully resolved. The same fitting method (an error function and a Gaussian) is still applied, however. In

the rotated energy space with the better energy resolution, the two ^{60}Co peaks are fully resolved.

From these fits, done separately for the single site and the multiple site data, we get the position and the width of the peaks at the 4 energies. A fit of the positions set the energy scale. A fit of the widths give the energy resolution function.

7.4.3 Energy Scale

Initially, the energy scale was expected to be linear. However, the linear fit of the rotated energy yielded a poor reduced χ^2 , unlike the case for charge only energy (see section 9.2.1). A quadratic function is used instead to set the energy scale. Both of the fit results, including the best fit parameters, are shown in Figure 7.9.

The nonlinear nature of the energy scale may be due to the nonlinearity in which the ionization and scintillation information are used in anticorrelation. Only with the much better energy resolution in the rotated space, does the need to do a quadratic fit occur. A typical quadratic fit has the form of

$$E_{rotated}^{cal} = a_0 + a_1 E_{rotated} + a_2 E_{rotated}^2, \quad (7.6)$$

where a_i are the parameters of the fit. It is also plausible that the better energy resolution is showing some small nonlinearity in detector behavior.

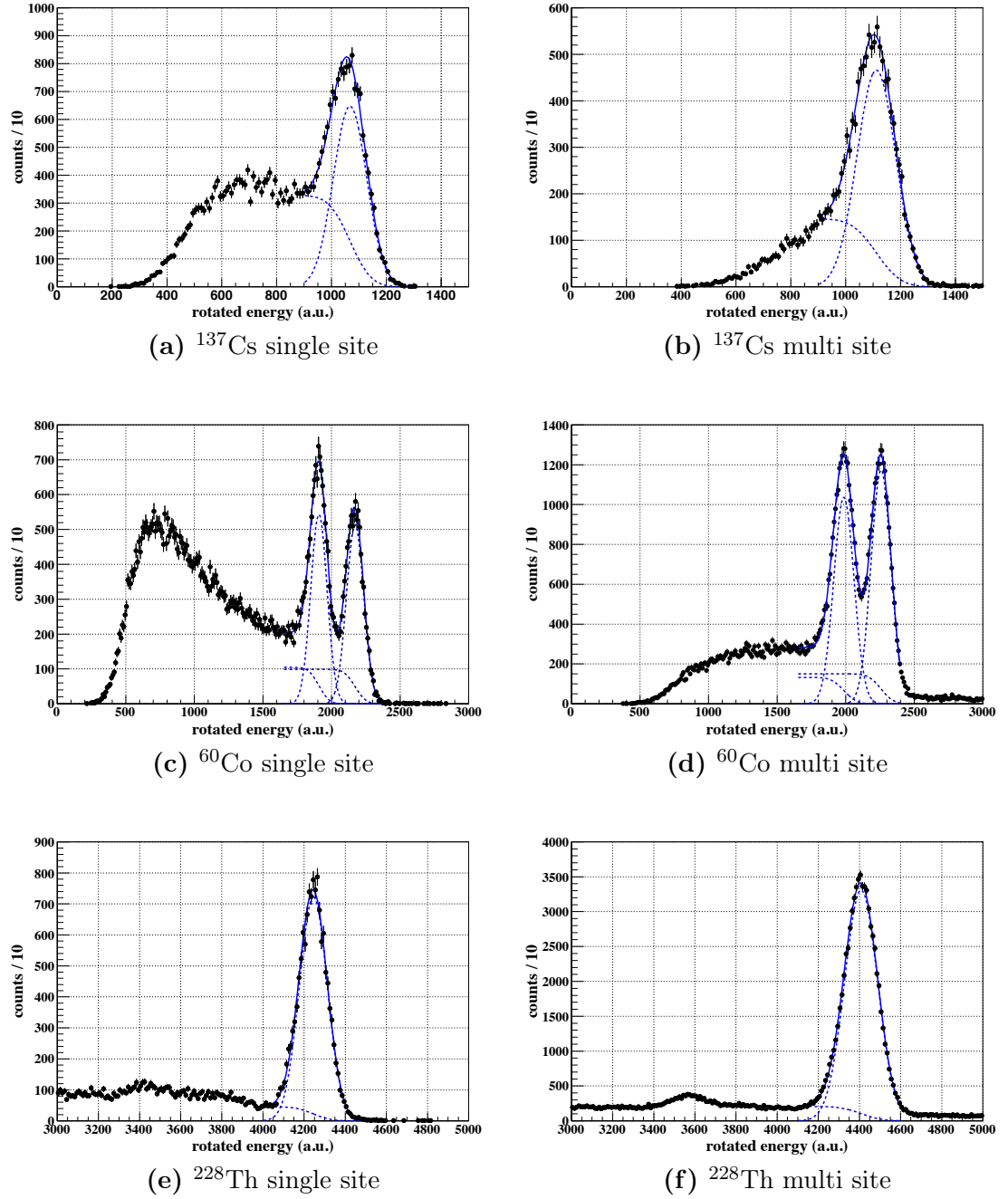
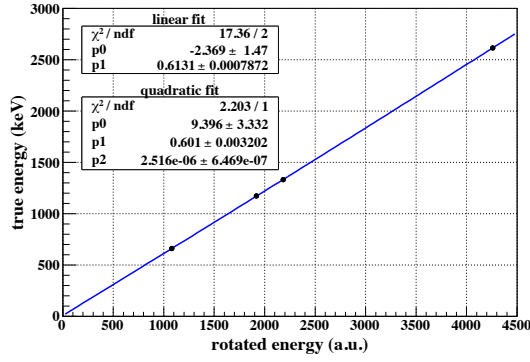
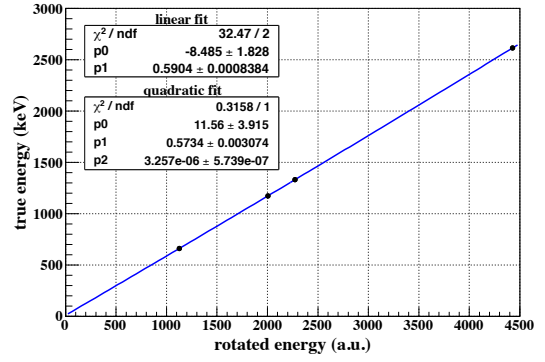


Figure 7.8: Rotated spectra and fit results of the γ peaks for the three calibrations sources. Again, separate fits were done for the SS and the MS cases. Fit results are used to extract energy scale and energy resolution parameters. Figure taken from [6].



(a) Single site calibration.



(b) Multi site calibration.

Figure 7.9: Calibration of rotated energy scale for SS (a) and MS (b). Figure taken from [6].

7.4.4 Energy Resolution

Using the four energy resolutions at four different energies (see Table 7.3) for the single site or the multiple site case, separately, resolution functions $\sigma(E)$ with three parameters can be obtained from the fits. The energy resolution function can be written as

$$\begin{aligned}
 \sigma^2(E) &= \sigma_{stat}^2 + \sigma_{noise}^2 + \sigma_{drift}^2 \\
 &= p_0^2 E + p_1^2 + p_2^2 E^2 \\
 &= (\sqrt{wFE})^2 + (w\sigma_e)^2 + (kE)^2.
 \end{aligned} \tag{7.7}$$

The first term, σ_{stat} , is due to statistical fluctuations in the number of electrons and photons collected; scaled as $\sqrt{E}$, this term is dependent on the energy deposited. The next term, σ_{noise} , is due to electronic noise and independent of deposit energy. The last term, σ_{drift} , comes from the resolution broadening time variations in the electronic gain and scales as E . These three components are independent of one

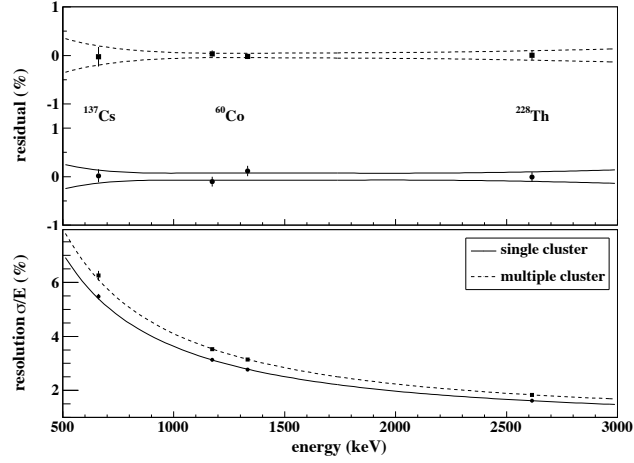


Figure 7.10: Top: systematic uncertainty bands on the energy calibration residuals for the three γ sources. For both SS (solid) and MS (dashed) the position of the four γ lines is consistent with the calibration model within $\leq 0.1\%$. Bottom: energy resolution curve with the energy resolutions from the sources along with a fit to the empirical model. Figure taken from [14].

another and add in quadrature. They can also be expressed in terms of related physical parameters: $w = 0.0187$ keV is the W-value, or average energy required to liberate a single electron from liquid xenon; F is the Fano factor, which enters into the statistical fluctuations term; $\sigma_E = 800$ is the number of electrons produced by noise; and k is a constant parameterizing the amount of electronic drift.

Table 7.4 lists the best fit values. The resolution is dominated by the constant (noise) term whereas the square root term (statistical term, p_0 , that scales as $\sqrt{E}$) is negligibly small.

7.4.5 Pair Production

An additional peak can be used for calibration. The 2615 keV line from Tl208 decay of Th228 can pair produce and form a pair production peak at 1593 keV. In

Table 7.3: Measured values of the rotated energy resolution for each calibration peak.

Source	σ/E (SS) (%)	σ/E (MS) (%)
^{137}Cs	5.50	6.23
^{60}Co (1)	3.12	3.53
^{60}Co (2)	2.77	3.15
^{228}Th	1.62	1.84

Table 7.4: Best fit values for the rotated energy resolution parameters.

Number of Sites	p_0	p_1	p_2
Single	0	35.16 ± 0.34	$8.95\text{e-}3 \pm 3.78\text{e-}4$
Multi	0	39.7 ± 0.39	$1.03\text{e-}2 \pm 3.38\text{e-}4$

a pair production event, a γ , in the presence of a nucleus, generates an electron-positron pair. The total energy of this pair is the full energy of the γ minus twice the mass of the electron (1593 keV in this particular case). The positron will quickly annihilate within the liquid xenon to form two 511 keV γ 's. The 511 keV γ 's, emitted back to back, can both escape the detector region to leave behind the 1593 keV energy deposition in the detector, that is β in nature, just like the physics process of interest for EXO. Additionally, if the energy threshold is lowered, the 511 keV γ can also be observed as a peak for cases where the second 511 γ and the 1593 keV β have escaped the detector. Even when the event is fully captured in the fiducial volume, the pair production events can be selected by requiring three collinear charge clusters. Figure 7.11 show how the 1593 keV and 511 keV peaks can also be fitted to get two more data points for the energy scale and energy resolution fits. A energy calibration residual plot including these two additional energies is

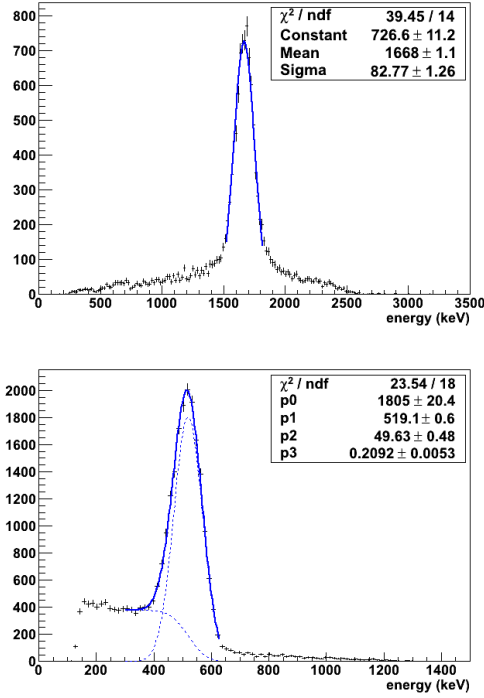


Figure 7.11: Top: 1593 keV peak from pair production events of 2615 keV gamma of a ^{228}Th source with a fit (gaussian peak only). Bottom: 511 keV peak can also be observed and fitted (gaussian peak and a complementary error function for background). Both of these plots shown are charge only peaks from specially selected pair production events that required the golden geometry of having three collinear clusters with the largest cluster in the center. Figure taken from [7].

found in Figure 7.12. The β nature of the 1593 keV peak does not follow the energy calibration of γ 's in the detector. This may indicate that the charge calibration for the more point-like β events, including $\beta\beta 0\nu$ and $\beta\beta 2\nu$, may differ from that of the larger γ events. A β -scale is included as a parameter in the analysis to accomodate this discrepancy (see section 8.5.2).

7.5 Source Agreement

How well the Monte Carlo simulation can reproduce the data energy spectra is evaluated for the calibration sources. Before the PDFs of the various backgrounds

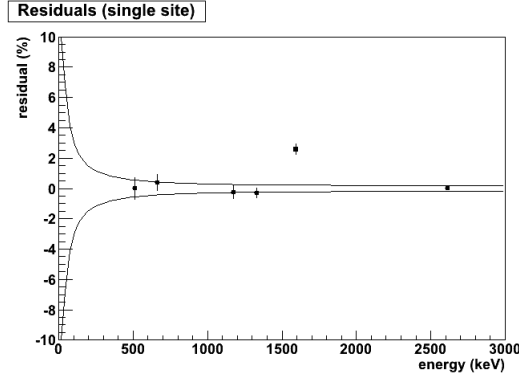


Figure 7.12: Systematic uncertainty bands on the energy calibration residuals for the three γ sources just like Figure 7.10, but also including the 511 keV and 1593 keV peaks from pair production events. Note how the β nature of the 1593 keV peak cause it to be outside the uncertainty band of the γ events. Figure taken from [7].

and for the physics signal are fitted to the low background data, it is imperative that the same Monte Carlo is able to reproduce the source calibration data. Source agreement needs to match for three aspect of the calibration data. First, the spectral shape of the simulation and data has to match for the entire energy range of interest of the fit. Two goodness-of-fit criteria (reduced χ^2 and Kolmogorov-Smirnov (KS) test) were used to determine this. Second, the total rate of the sources as measured by external methods must match the source rate determined from the calibration run, based upon the efficiency given by the Monte Carlo. Finally, since the low background fit will be done as a simultaneous fit on both the SS and MS, the ratio of the single site, defined as the number of single site events divided by total events, must also match between MC and data.

Only the ^{60}Co and ^{228}Th sources are used for the source agreement checks, since the ^{137}Cs source full energy deposition peak of 612 keV is below the analysis

threshold of 700 keV. Additionally, only source calibration runs at the cathode are used in these source agreement studies.

7.5.1 Source Shape Agreement

Figure 7.13 and figure 7.14 show the source agreement plots of MC (blue lines) and data (black dots with error bars) for ^{60}Co and ^{228}Th source calibration runs. Source PDFs are fit to the data allowing overall normalization to float freely. Energy scale offset and resolution parameters are constrained by dedicated calibration measurements. The first goodness of fit result, χ^2 per degree of freedom (d.o.f) or reduced chi-square, is also listed on these figures. The reduced χ^2 is computed separately for the single site and the multiple site fits. All four reduced χ^2 values are around 1. It should be noted, however, that only the statistical errors for each bin are considered in this calculations.

A second goodness of fit method used to check source shape agreement is the Kolmogorov-Smirnov (KS) test, which was applied to both the binned and the unbinned distributions. KS test compares the cumulative distribution functions (CDF) obtained from the PDF and the data. The maximum difference between data and models CDFs (KS distance) is used as a test statistics. The KS distance can then be compared to a standard table to find the probability that the data sample is comparable with the model. Since the table is no longer valid if either of the parameters of the model is determined from the data itself, ~ 1000 toy Monte Carlos were used instead.

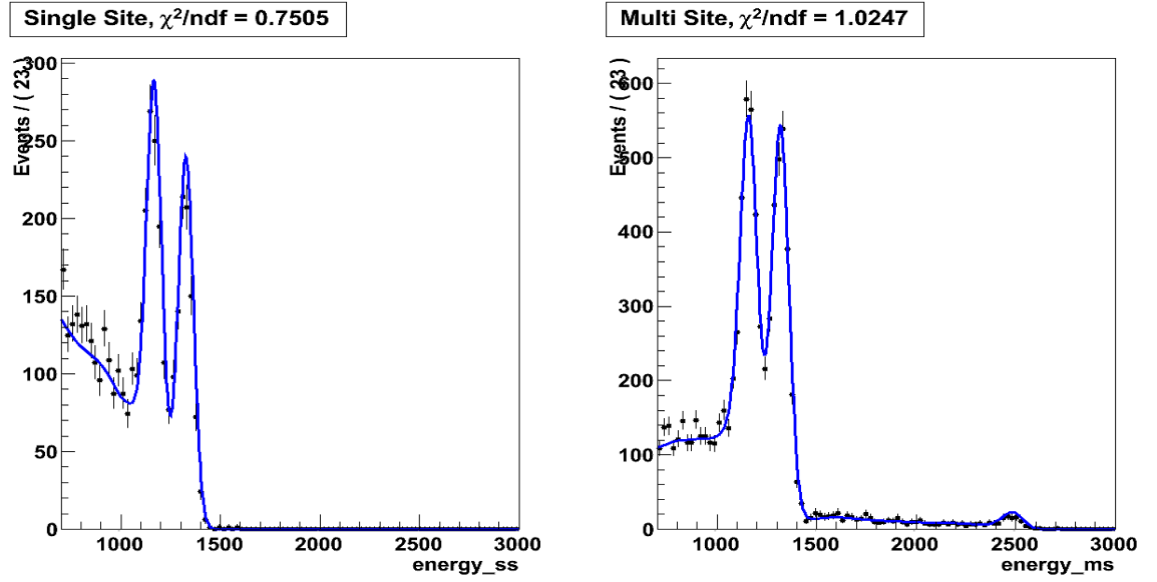


Figure 7.13: Calibration source data (black) vs. best-fit PDFs (blue) for Co source at position S5. Figure taken from [7].

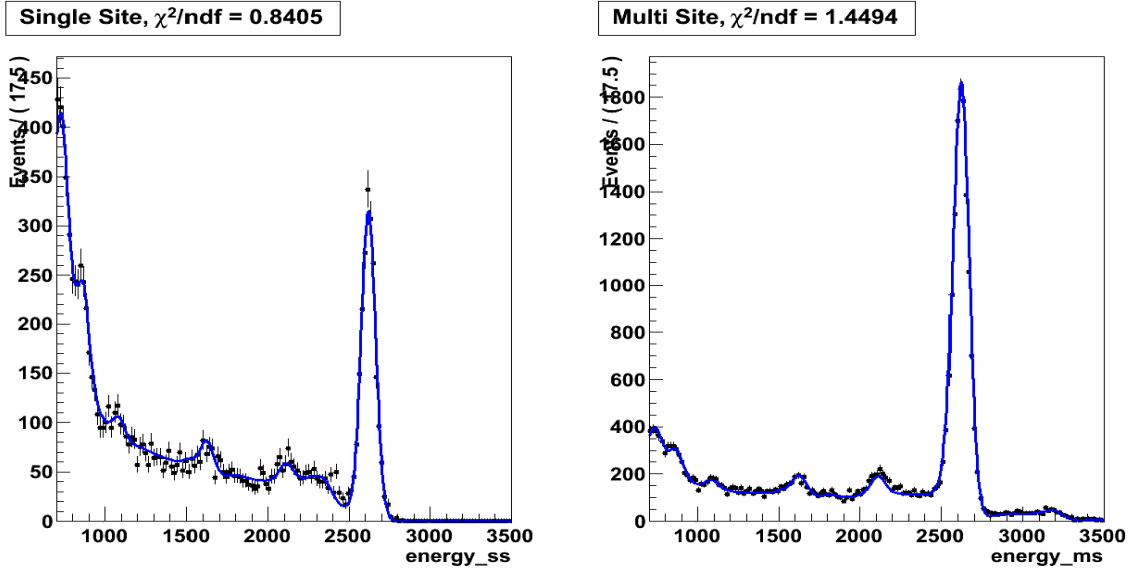


Figure 7.14: Calibration source data (black) vs. best-fit PDFs (blue) for Th source at position S5. Figure taken from [7].

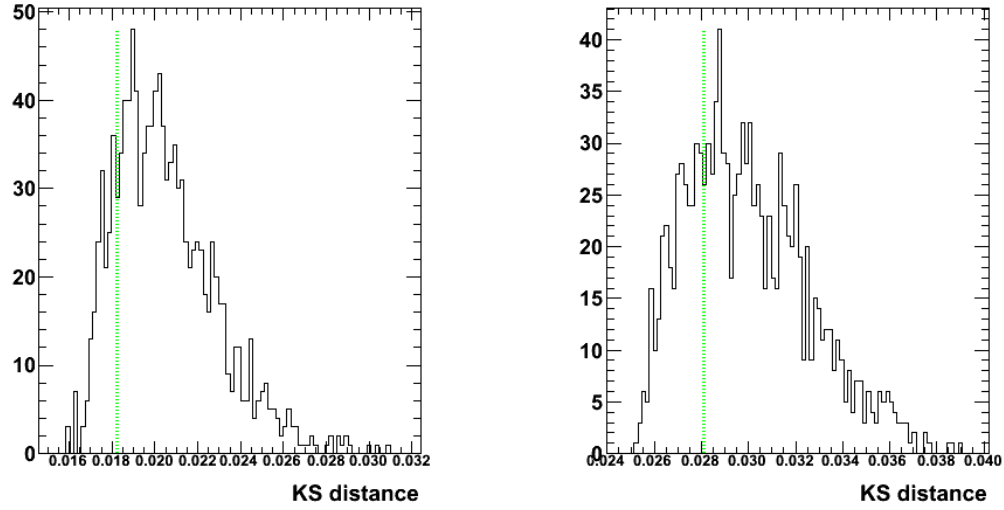


Figure 7.15: KS distance plot for SS (left) and MS (right) for the Th source agreement. 85% probability for the SS fit. 73% probability for the MS fit. Figure taken from [7].

The result of the KS test is that there is 85% (73%) probability that the single site (multiple site) ^{228}Th calibration data is comparable with the Monte Carlo PDF, see Figure 7.15. For the ^{60}Co data, the probability is lower (2.2% for SS, and 3.6% for MS), but the agreement is still within 2-3 σ 's, see Figure 7.16. Between this reasonable result and the reduced χ^2 , the source shape agreement was deemed to be satisfactory.

7.5.2 Source Rate Agreement

Another important crosscheck of the analysis is the comparison of the source rate measured from the data analysis and the expected known rate from external measurement. Large discrepancy may point to some unknown systematics. The

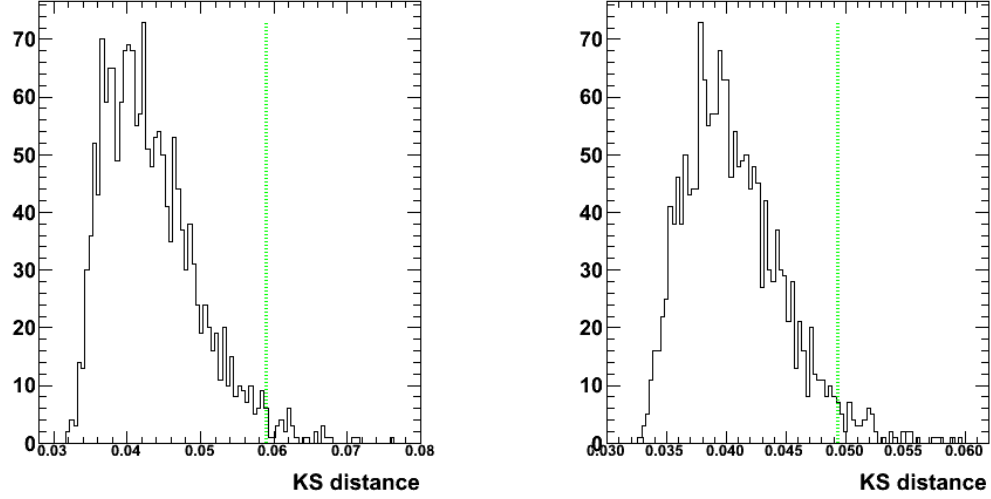


Figure 7.16: KS distance plot for SS (left) and MS (right) for the Co source agreement. 2.2% probability for the SS fit. 3.6% probability for the MS fit. Figure taken from [7].

source activity, γ , is calculated from the data analysis using the formula

$$\gamma = \alpha \frac{N}{\epsilon T}, \quad (7.8)$$

where N is the number of events in the data set above threshold, α is a correction to account for pileup, ϵ is the detection efficiency from Monte Carlo, and T is the livetime of the calibration run. These runs use the random trigger, so the livetime is the number of triggers times the effective time length of the waveform trace (2048 μs). A pileup correction factor is needed due to the cut that removes events with more than one scintillation clusters. α is determined from the total number of scintillation clusters in a ^{228}Th run divided by the number of single scintillation cluster only events; it was measured to be 1.135.

The known activity, factoring in the amount of time since the external mea-

surement, are 643.71 Bq for ^{228}Th and 379.11 Bq for ^{60}Co . With a lower fit range of 700 keV, the measured source activities from the calibration run fits are 710.6 Bq and 417.56 Bq which corresponds to a disagreement, defined as (measured-expected)/measured, to the known activities of 9.4% for ^{228}Th and 9.2% for ^{60}Co . The source of this discrepancy may come from the uncertainty in the true positions of the source during calibration runs.

7.5.3 SS Fraction Agreement

Since the ability to differentiate between Single Site (typically $\beta\beta$ events) and Multiple Site (typically background) is the main tool used for the main $\beta\beta 0\nu$ and $\beta\beta 2\nu$ search, the multiplicity agreements between the Monte Carlo and the data are also compared. The SS and MS differentiation happened during the clustering step (see section 4.5) of reconstruction with the same algorithm applied to both the data and simulation. To compare the multiplicity, the variable of SS Fraction, defined as $\text{SS} / (\text{SS} + \text{MS})$, is used. The relative difference of SS Fraction between data and simulation, $(\text{Data} - \text{MC}) / \text{Data}$ compared to energy is plotted in Figure 7.17. The bin size is 250 keV for ^{60}Co and 500 keV for ^{228}Th sources, chosen to get good enough statistics. By checking the agreement across different energies, possible cancellation effects may be noticed.

The maximum observed deviation is 8.5%. This number is used to define the strength of the corresponding constraint during the Low-Background fit and as the SS Fraction systematic uncertainty. In the final fit, the SS Fractions are allowed to

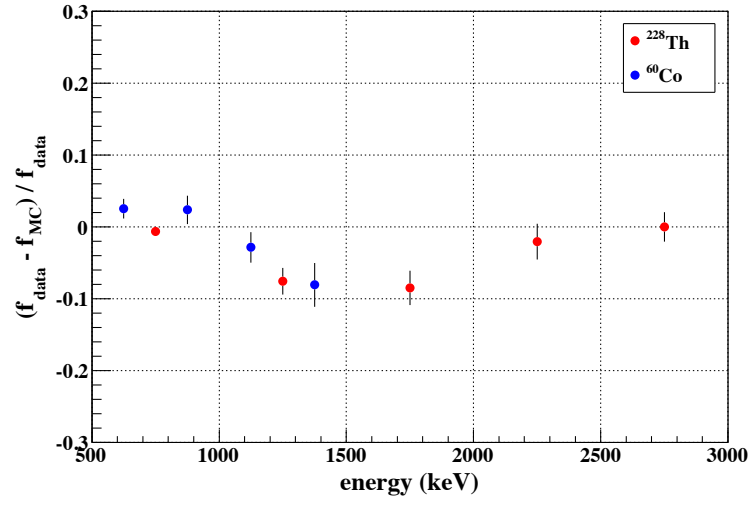


Figure 7.17: Fractional difference of the Single Site Fraction in Monte Carlo to the single site fraction in data for ^{228}Th (red) and ^{60}Co (blue). The largest discrepancy was 8.5 %. Figure taken from [6].

float within 8.5 % independently for each PDF component.

Chapter 8

Fits to Data

Maximum likelihood fits to energy PDFs are performed on the low background data to search for the ^{136}Xe $\beta\beta 2\nu$ decay to the first 0_1^+ excited state of ^{136}Ba . The PDFs used and the background model were generated from MC and described in Chapter 6. The low background data undergo an event selection process before being fitted. For the decay to the excited state, we increase the low total energy analysis threshold to eliminate the possible unwanted effects from the excited decay from the inactive liquid xenon. Uncertainties on the fit results are estimated by taking profiles of the final likelihood function.

8.1 Event Selection

After the raw data are processed through the event reconstruction step, each event corresponding to a physics trigger contains a number of scintillation clusters and their associated charge clusters. The event selection algorithm next loops over all the events to apply numerous cuts, prior to the fitting of the data.

8.1.1 Low background data set

The low-background data used for this analysis were taken in the period between September 22, 2011 and April 15, 2012, when the TPC was filled with enriched

xenon. These dates correspond to runs 2379-3563 and were selected for detector stability. The detector was operated with a 0.1 Hz forced trigger for the duration of these runs; the livetime, then, can be determined by counting the number of triggers, and was found to be 2896.6 hours. The actual average trigger rate was ~ 0.2 Hz. Furthermore, only the highest quality low-background runs were used. Certain runs or parts of runs are thrown out, if they have very high event rates due to microphonic effects caused by fire alarm tests or certain types of work inside the clean room.

8.1.2 Veto Cuts

If an event is tagged as noise, it is rejected entirely. If an event is tagged as a muon, it is not discarded but its event time is recorded. This timing information allows for a posteriori muon veto cut to be applied to vetoed events. These veto cuts are determined by comparing the time since the last muon event to the timing of events. More specifically, the three veto coincidence cuts (total in a dead time of 8.6%.) are:

- Events within 25 ms of a veto panel hit are removed from the data, which has an associated dead time of 0.58%.
- If any two detector events occur within 1 s of each other, both events are vetoed. Such coincident events are most likely to be ^{214}Bi to ^{214}Po coincidences in the xenon or be cosmic ray induced, where some cosmogenically activated isotope is undergoing multiple short half-life decays. This cut incurs a dead

time of 3.3%.

- The position reconstruction of the detector allows for reconstruction of muons traversing the TPC. After such an event, there are some risks of exotic cosmogenically activated isotopes. Events within 60 s after a muon traversing the detector are vetoed, leading to a 5.0% dead time.

8.1.3 Diagonal Cut

After surviving the veto cuts, these non-muon events are next required to have one and only one scintillation cluster. This cut removes ^{214}Bi - ^{214}Po coincidence at an efficiency of 96% given the half-life of ^{214}Po of $164.3\ \mu\text{s}$ [6].

Next, the event energies are transformed into the anti-correlated “rotated energy” space, as discussed in 7.4.1. After this switch, a *diagonal cut* is made to reject events with high scintillation energy but low ionization energy (and fewer events of the opposite variety). These events are most likely α ’s in origin. The poor charge collection may also indicate that the events came from a position near the dead region on the outskirts of the detector. In either case, they are culled by this cut. The diagonal cut is indicated by the red lines in Figure 8.1.

8.1.4 Fiducial Volume Cut

Furthermore, all charge clusters are required to be within the fiducial volume. The fiducial volume for this analysis is a hexagonal geometry with an inner radius of $R=163\ \text{mm}$ and $5\ \text{mm} < |z| < 182\ \text{mm}$. The cross sectional view of this region

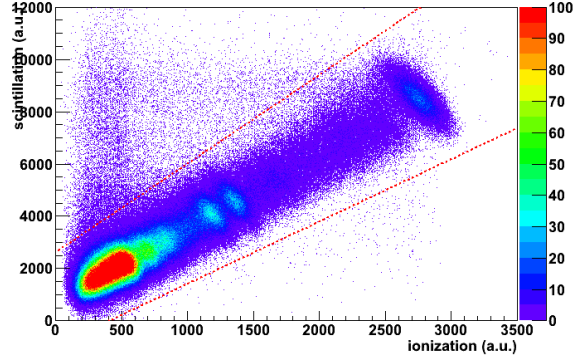


Figure 8.1: Anticorrelated spectrum with the diagonal cut plotted from a Th Source Calibration run at position S5.

is shown back in Figure 3.8. Uncertainty about the actual fiducial volume is the largest source of uncertainty in this analysis and will be discussed in more detail in section 8.5.7.

Fiducial events are also required to have a full three dimensional positional reconstruction, basically requiring both a scintillation signal and a V-wire signal to be associated with every charge cluster. The scintillation detection is fully efficient above 700 keV, but a multiple site event with very high total energy may still contain a low energy charge cluster below the V-wire reconstruction threshold.

The sum effects of the veto cuts (veto panel, coincidence, TPC), “diagonal cut” (labelled as scintillation/ionization ratio), and fiducial volume on all the raw data events are shown in Figure 8.2.

8.1.5 Cluster Cull

In the actual TPC, there are regions inside the active liquid xenon volume where the applied electric field may be zero or very small. Charge deposits that

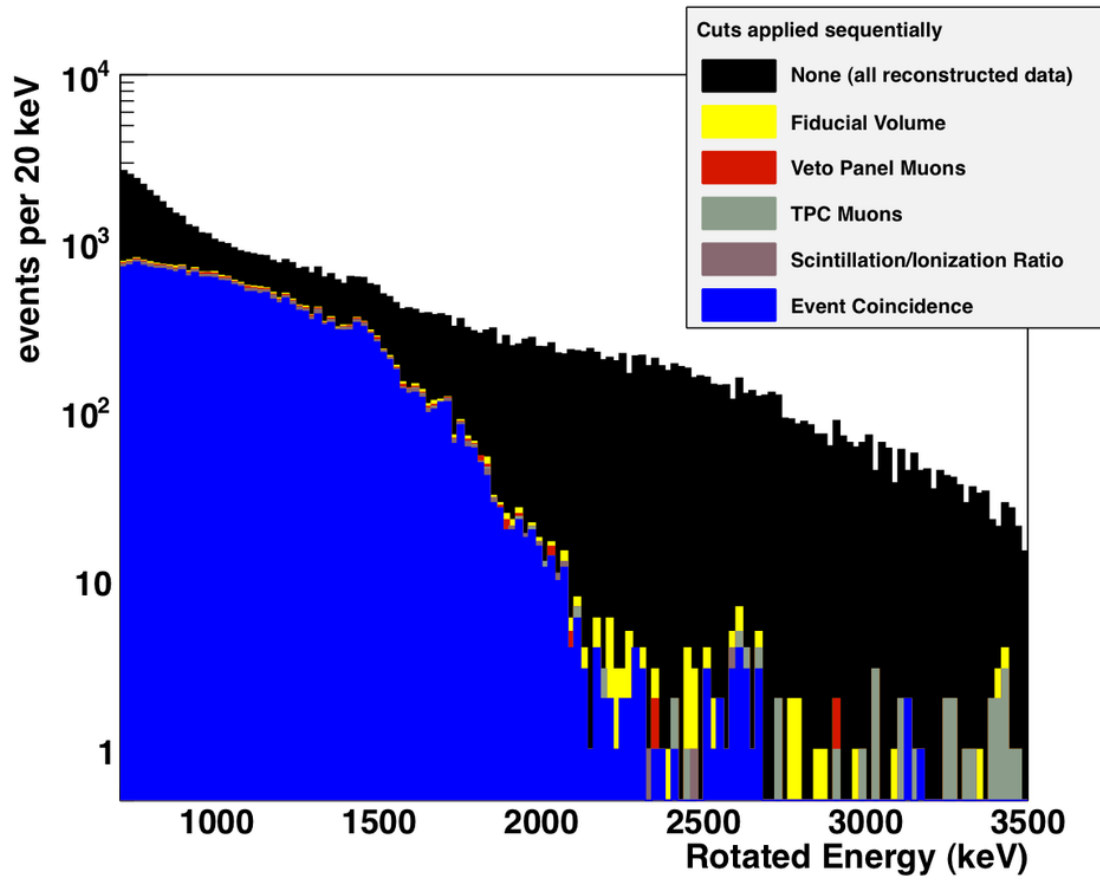


Figure 8.2: Event selection of the single site energy spectrum showing the effects of various cuts. The spectrum with all of the cuts applied (in blue) is used for fits. Figure is taken from [1].

originate in these region may not be collected by the detector. These regions are called “dead regions”. To simulate the effect of “dead region”, a *cluster cull* procedure is implemented to cull any charge deposits outside a defined volume of the active liquid xenon. For the most part, cluster cull affects only the Monte Carlo simulation events to make them more realistic. For consistency, cluster cull is also applied to the low background data. The culled charge deposits are the PCDs from the MC before they are turn into PDFs and the reconstructed charge clusters from the data.

For multi-site events, only the charge clusters that exist in the dead region are culled. The other charge clusters that are reconstructed outside the dead region are unaffected. Culled charge clusters do not contribute to the total energy of that event. For this analysis, clusters at a larger radius than the Teflon reflectors ($r > 183$ mm) are culled. Figure 3.8 indicate the region outside the teflon and how this region does not perfectly correspond with the hexagonal fiducial volume defined, as there are some charge clusters that can exist outside the fiducial hexagon (a little bit smaller than the hexagon formed by the collection wires) but still inside the teflon reflector. An attempt to cull clusters based on the hexagonal fiducial volume resulted in a poorer source agreement.

Unlike the event cuts described before, even if an event is altered by the cluster cull, it is still kept in the low background data and used for the fit. Only parts of the said event, mainly the reconstructed charge clusters deemed to be in the dead region, are thrown away. The definition of the cluster cull algorithm was driven by the source agreement.

8.2 Fitting Technique

The low background data is divided into single site (SS) and multiple site (MS) where both are simultaneously fitted via binned maximum likelihood to a series of PDFs. For this analysis, the total livetime was 120.7 days at 98.5 kg fiducial mass of active enriched xenon (80.6% of it being ^{136}Xe), for a total exposure of 32.6 kg-yrs. of exposure.

8.2.1 Maximum likelihood fitting

The maximum likelihood method, which is the preferred method for low statistic samples, is used to fit the low background data as well as the source runs shown earlier. It is applicable on both binned and unbinned data. For a data sample $\mathbf{x} = (x_0, x_1, \dots, x_n)$ of n independent measurements, the likelihood function is the probability of observing this result. The likelihood is described by the PDF $p(x|\theta)$ of unknown parameters θ 's. The full definition of the likelihood function is

$$L(p|\theta) = \prod_{i=0}^n p(x_i|\theta). \quad (8.1)$$

The maximum likelihood method is the procedure to find the set of θ that maximize this likelihood function. While this can be achieved by taking the partial derivative of L with respect to each of the parameters θ , the more common use is to define the

negative log-likelihood (NLL):

$$-\ln L(x|\theta) = -\sum_{i=0}^n \ln p(x|\theta). \quad (8.2)$$

which is then minimized with respect to θ .

In the low background fit, $p(x|\theta)$ is the normalized sum of all the signal and background PDFs, and θ is the fractional contribution of each signal and background PDFs. For both the single site and multiple site data set, separate log-likelihood functions are built; the two are summed up to perform the fit simultaneously of both data. The negative log-likelihood function is minimized with MINUIT [82] package built into ROOT [83]. It is a generalized program that searches for the local minima of any function and performs error analysis on the parameters and their correlations. For each PDF, two parameters are fitted (representing the single site fraction and the total number of events of SS and MS combined). Additionally, for SS and MS individually, one parameter is used for the energy scale offset and two parameters for the energy resolution.

8.2.2 Profile Likelihood

One can evaluate the likelihood function with one parameter fixed. A comparison of the negative log-likelihood (NLL) to the minimum can give a better uncertainty than the fit result. The 1σ error corresponds to the $-\ln L$ increasing by $1/2$. In order to account for systematic errors due to parameter correlations, the profile likelihood is built over the parameter of interest. The error obtained this way,

including parameter correlations, is often larger than the naive error from assuming a χ^2 distribution.

8.3 Excited State Energy Spectrum

The excited state energy spectrum (from MC with no energy resolution applied) is shown in Figure 8.4 as energy deposited inside the active liquid xenon region, with the events generated from inside the active liquid xenon. The two possible γ energies form peaks at 760.5 keV and 818.5 keV which is effectively just one peak ~ 800 keV. There is a third peak at 1590 keV where the only energy deposited is due to the two γ s alone with no contribution from the $\beta\beta$. These γ peaks correspond to cases where the primary $\beta\beta$ energy deposit is either just outside the fiducial volume or is nearly zero.

Three distinct regions can be defined. The energy less than 800 keV region is the double escape (where both of the γ 's has escaped the active liquid xenon region). For energy between 800 keV and 1590 keV, that region is the single escape (only one of the γ has escaped the active xenon region). The region above 1590 keV is the fully contained (almost all of the energy from the two γ 's and the $\beta\beta$ are recorded). Using the knowledge from the main $\beta\beta 0\nu$ analysis that searches mostly in the single site only spectrum, the $\beta\beta$ is expected to not travel very far and remain as a single cluster.

$\beta\beta 2\nu$ Xe136 to excited PDFs

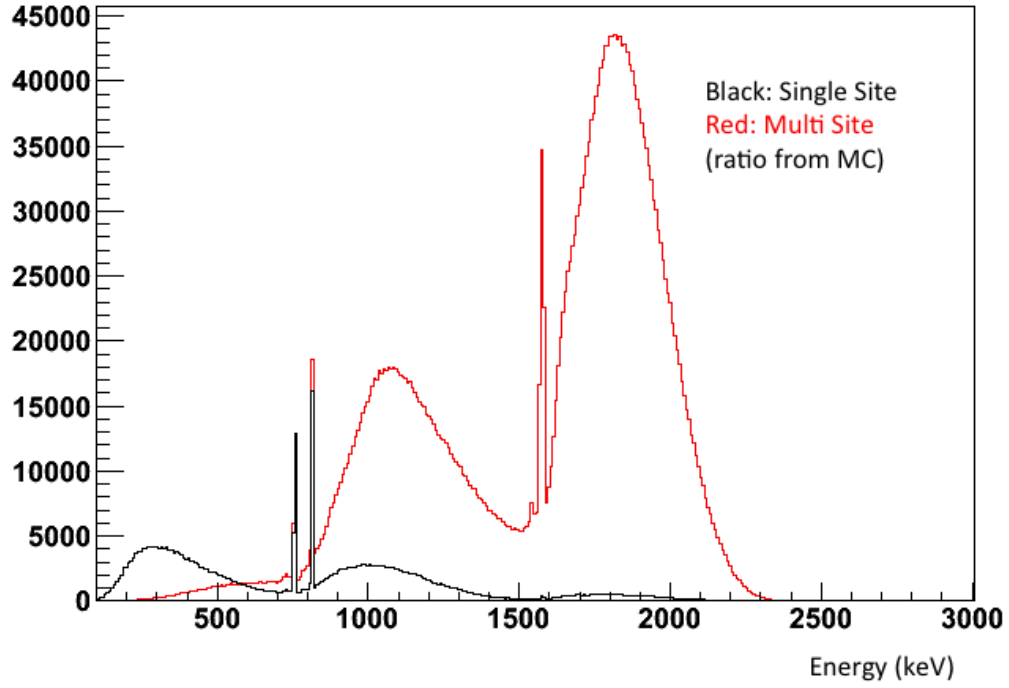


Figure 8.3: Energy spectrum from the decay to the excited state divided into SS and MS. No energy resolution is applied.

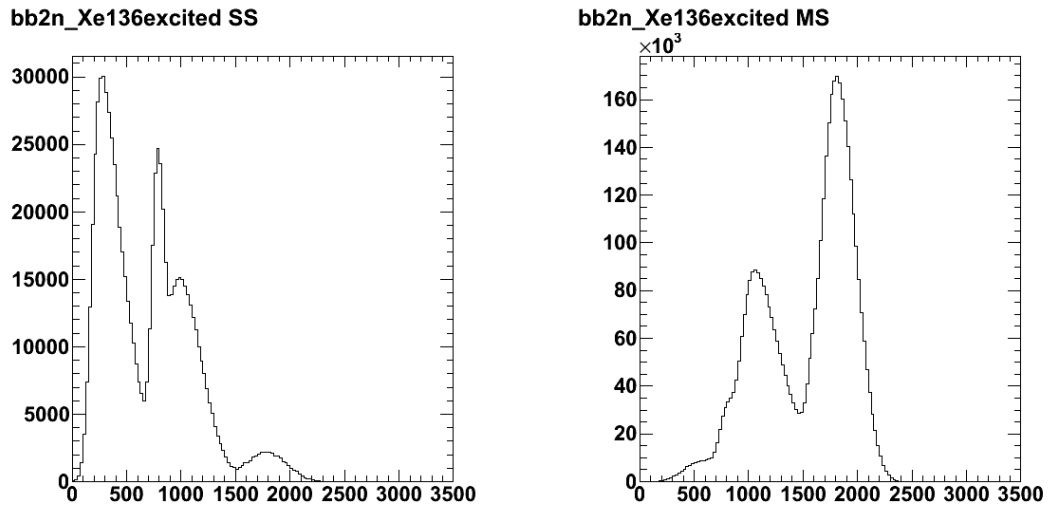


Figure 8.4: The SS and MS PDF used for fitting of the $\beta\beta 2\nu$ decay to the excited state. True energy deposit in the fiducial volume as simulated is convolved with the energy resolution curve (see Figure 7.10) from the rotated energy space.

8.4 Fit Energy Range

In the standard EXO-200 analysis, the fit energy range spans from 700 keV to 3500 keV. For the excited state decay, we have two ~ 800 keV γ 's with fairly good penetrating power (attenuation length is ~ 5 cm for a 800 keV γ [12]). While the primary decay that occurred outside the teflon in the inactive xenon region is unlikely to trigger the detector nor survive the diagonal cut without an associated clear scintillation signal, the γ 's could still contribute energy in the non-fully contained cases. An even bigger concern is those events that originated inside the teflon but originated in the not fully efficient “dead region”. To mitigate potential inaccuracy in the Monte Carlo and to not have to worry about energy depositions that are due to the γ 's originating from non-fiducial decays to the excited state, a higher low energy threshold of 1700 keV is used for the excited state fit. Since the γ energies are fixed but the remaining $\beta\beta 2\nu$ can range anywhere from 0 to 822 keV, the total energy for the fully contained events are at least 1590 keV. Factoring in the energy resolution, 1700 keV was chosen as the lower threshold. The full energy range fitted in this analysis is 1700 keV to 3500 keV.

8.5 Fit Results

8.5.1 Constraints

A few parameters in the PDFs are represented by measurable quantities, and can be constrained by measurements. This is done with multiplicative Gaussian

constraint like the following:

$$C_q = e^{-(q-q_0)^2/2(\delta q)^2}, \quad (8.3)$$

where the multiplicative constraint factor, C_q , for a parameter q has the typical Gaussian form with q_0 being the measured value. This constraint is a multiplicative factor in the likelihood and a term in the NLL.

The list of included constraints is the following:

1. Magnitudes of ^{214}Bi in the air gap between lead wall and cryostat and ^{222}Rn content of the LXe
2. Single-site/multi-site ratio
3. Energy scale (single-site and multi-site)
4. Energy resolution (single-site and multi-site)

The ^{214}Bi in the air gap is constrained by the Rad7 measurement, with an upper limit of 42 ± 6.5 Bq/kg set.

The single-site/multiple-site ratio is constrained separately for each component of the fit. The central value is found from the MC by taking the ratio of events in each spectrum above threshold (the standard 700 keV rather than the higher 1700 keV). The relative uncertainty used on the ratio for all component is taken as the maximum discrepancy found from the studies of the calibration source multiplicity. That maximum difference is 7.52%. This discrepancy comes from the largest single site fraction difference from the calibration data: 1500-2000 keV range from ^{228}Th .

The energy scale and energy resolution constraints are applied using the values and uncertainties listed in Figure 7.9 and Table 7.4, respectively.

8.5.1.1 ^{222}Rn in LXe

A small amount of ^{222}Rn is expected to be present in the liquid xenon from the outgassing within the xenon handling system. Since radon is a noble gas, it is not removed by the purifiers. Three PDFs describe ^{222}Rn in LXe. They are ^{222}Rn in active LXe, ^{222}Rn in inactive LXe, and ^{214}Bi on the cathode.

A detailed α -spectroscopy study of the low background data to set limits on the amount of ^{222}Rn in EXO-200 can be found in [6]. The radon content was measured from three separate ways:

- ^{214}Bi - ^{214}Po coincidence: after the β decay of ^{214}Bi , the following α decay has a half-life of 237 μs . Since a full 1 ms of data following the initial β -decay is recorded in data, 98.5% of ^{214}Po decays are expected to be measurable if one looks for a β event followed by an α event. The α event can be found by their lower charge to light ratio in liquid xenon.
- α -spectroscopy: since the α events have very low charge/light ratio (<0.05), many of the corresponding charge signal may be too low in energy to produce a V-wire signal. A scintillation only study that looks for 5.59 MeV and 6.11 MeV α 's for the ^{222}Rn and ^{218}Po decays in the xenon is expected to have lower systematic uncertainty.
- α - α coincidence: looking across multiple events, one can look for the ^{222}Rn

and ^{218}Po α -decays where the second decay has the half-life of 3.05 minutes.

A consistent result was found from all three methods. The LXe ^{222}Rn content was measured to be $(3.69 \pm 0.39) \mu\text{Bq/kg}$.

With the ^{222}Rn being mobile in the liquid xenon, we would like to categorize the decays by their location. ^{222}Rn decays in the bulk of the TPC leaves behind positively charged daughter ions that drifts toward the cathode under the influence of the electric field. As the decay rate (3.8 days) is significantly longer than the ion drift time (an ion drift velocity of 0.83 mm/s in LXe means the maximum drift time is ~ 4 minutes), most of the daughter ions are expected to reach the cathode and decay there. 70% of measured Bi-Po coincidences came from the cathode surface. When accounting for losses for decays from the cathode, it is estimated that 83% of the ^{222}Rn decays originate from the cathode. The other 17% of decays occur in the bulk, active LXe. These decays are categorized by two PDFs, one for Rn in the bulk, and one for Rn daughters on the cathode. Since the other decays are too low in energy to travel far from the cathode and to simplify the simulation, only the ^{214}Bi decay and its 2448 keV gamma are simulated to represent the ^{222}Rn in the cathode. A third PDF is the ^{222}Rn in the inactive LXe, outside the teflon tiles. There are 30.2 kg of inactive xenon, so $111.4 \pm 11.8 \mu\text{Bq}$ of activity is expected from this contribution.

8.5.2 β -scale

Given how the β -like pair production peak has a energy scale residual that is outside the uncertainty band for the γ peaks (see Figure 7.12), it is a strong hint that β events may require a slightly different energy scale than the γ 's from which the energy scale is set. A β -scale of 0.995 was chosen based on the profile likelihood study where the beta scale, a multiplicative factor applied to the β like events only, is fixed and everything else is left to float to determine the β -scale with the smallest NLL. While this β -scale is chosen from the $\beta\beta 2\nu$ to ground state study, the profile likelihood of changing the β -scale for fits including $\beta\beta 2\nu$ to the 0_1^+ excited state is shown in Figure 8.7. The β -scale is applied to $\beta\beta 2\nu$ and $\beta\beta 0\nu$ as well as the $\beta\beta 0\nu$ decay to excited state (even though 2/3 of the energy for the decay to excited state ends up as γ 's). From the best fit curve of the β -scale profile, the difference in NLL between the default 0.995 and 1 is about 0.5 which is 1σ .

Table 8.2 shows the fit results with and without β -scale applied for both of the $\beta\beta 2\nu$ PDFs. For the number of $\beta\beta 2\nu$ to the ground state events, the inclusion of the 0.995 β -scale changed the total fit result by only 0.8%. For the $\beta\beta 2\nu$ decay to the 0_1^+ excited state, the effect of the β -scale was found to be larger at around 11%.

8.5.3 Vogel vs. Kotila/Iachello $\beta\beta 2\nu$ Spectra Fit Comparison

As mentioned in section 5.2.2, two different $\beta\beta 2\nu$ spectra were considered in this analysis. The default $\beta\beta 2\nu$ spectra comes from the calculation of Petr Vogel

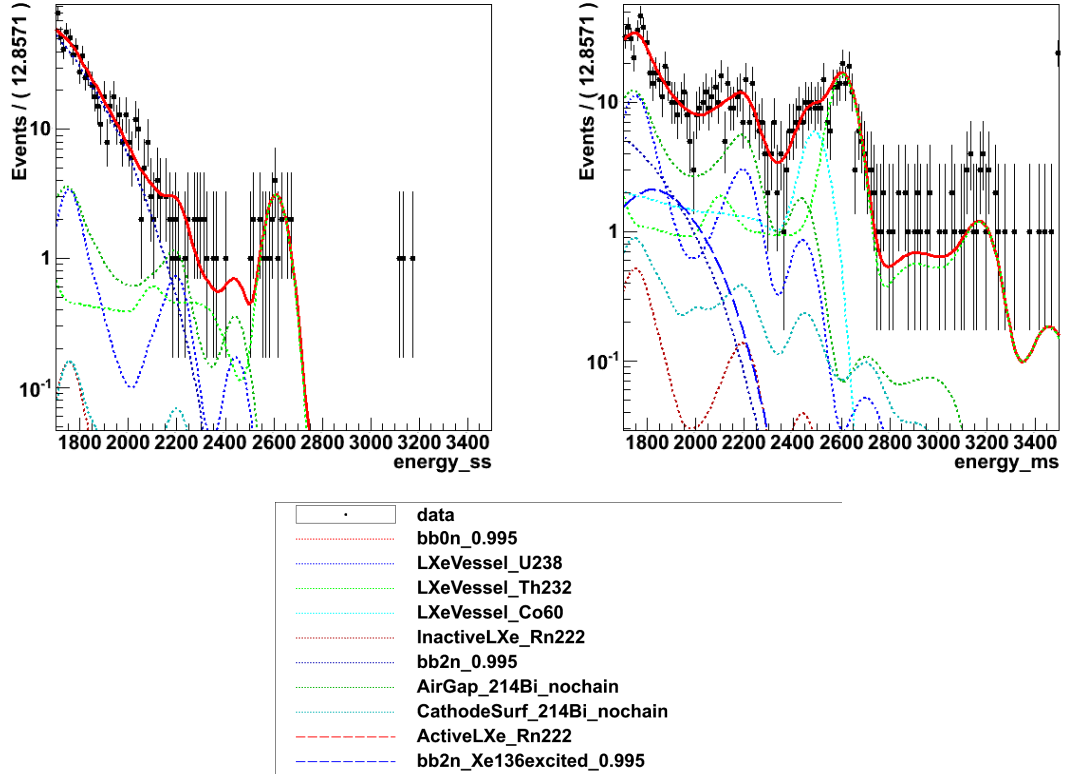
using the usual phase space consideration and the Schenter-Vogel approximation for Fermi function. A different method was used by Kotila and Iachello [11] to calculate the $\beta\beta 2\nu$ spectra. $\beta\beta 2\nu$ using both methods were turn into PDFs and used separately in fits with no applied β -scale. Other than the lack of β -scale and the differences in the $\beta\beta 2\nu$ PDF used, everything else is the same (same fit energy range of 1700 keV to 3500 keV) as the best excited state fit result to be discussed next. The relevant fit results for $\beta\beta 2\nu$ and $\beta\beta 2\nu$ to the 0_1^+ excited state are shown in Table 8.2. The change in the number of $\beta\beta 2\nu$ event is $< 0.1\%$. For the decay to the excited state, the change in the number of events is $\sim 4\%$. While the reason for this larger uncertainty for the excited state due to the $\beta\beta 2\nu$ theory is not fully understood, the $\sim 4\%$ uncertainty is still small compare to a couple of the other considered.

8.5.4 Results

With the smaller fit energy range due to the higher energy threshold of 1700 keV, the 11 backgrounds considered in the background model can be reduced down to 7. ^{54}Mn , ^{65}Zn , and ^{40}K in the liquid xenon vessel and ^{135}Xe in the active liquid xenon are now omitted due to their contributions being below the new energy threshold.

Table 8.1 and Figure 8.5 show the results of the fit. Other than the $\beta\beta 2\nu$, the largest backgrounds were the PDFs for the liquid xenon vessel. The fit indicates 51.9 total signal events (combined SS and MS, although it is mostly from the MS given the SS Fraction of 0.011) of the $\beta\beta 2\nu$ decay to the 0_1^+ excited state with a fit error

Figure 8.5: Fit result with fit range energy of 1700 to 3500 keV.
 Single Site, $\chi^2/\text{ndf} = 0.391$ Multi Site, $\chi^2/\text{ndf} = 0.869$



of 31.2. A more accurate profile likelihood adjusting the number of excited state event is shown in Figure 8.6. From the best quadratic fit of the profile likelihood over the number of $\beta\beta 2\nu$ to 0_1^+ events, a minimum at 53.4 events is found with the one σ upper bound (0.5 in NLL) of 101.9 and the lower bound of 4.8. The number excited state events found from the profile likelihood is $53.4^{+48.5}_{-48.6}$. This fit results is just a little over one σ away from zero $\beta\beta 2\nu$ decays to the excited state.

8.5.5 Efficiency

Detection efficiencies for the signal and background processes are determined from the MC spectra. The Monte Carlo efficiency for events generated inside the

Figure 8.6: Profile likelihood over the number of $\beta\beta 2\nu$ decay to the excited state events. Each data point comes from comparing the negative log-likelihood (NLL) result from a separate fit where the number of excited state events is fixed. Only the fully converged fit results are included. A quadratic fit to the profile likelihood is also shown. 1σ is taken to be the number of events where the NLL has increased by $1/2$. The number of $\beta\beta 2\nu$ decay to the excited state events found by the profile likelihood is $53.4^{+48.5}_{-48.6}$.

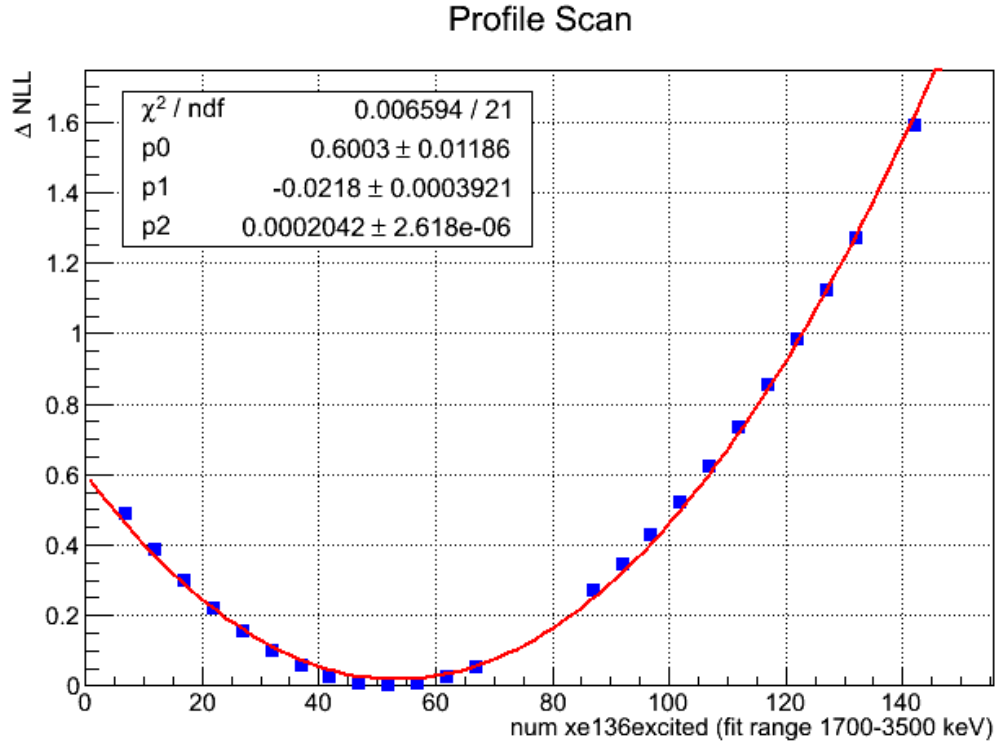


Figure 8.7: Profile likelihood over the β -scale. 1σ is taken to be the number of events where the NLL has increased by $1/2$.

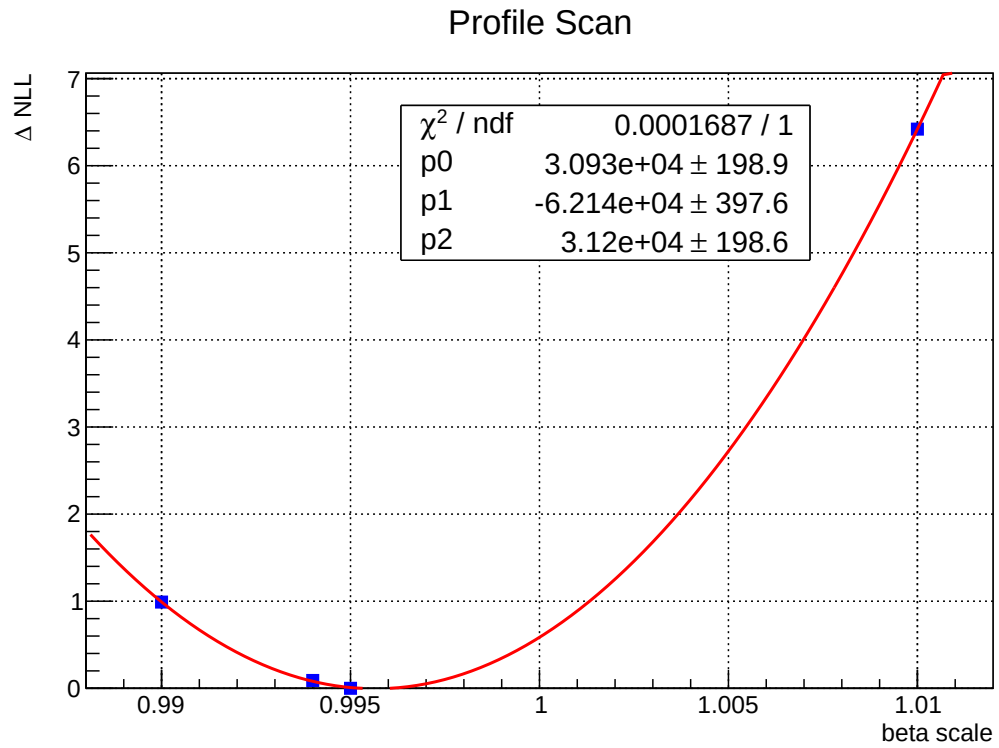


Table 8.1: Best fit values for all observables that are represented by a PDF.

Parameter Type	Location	Source	Fit Result	Error
SS frac	ActiveLXe	Rn222	1.4907e-01	2.17e-04
SS frac	AirGap	214Bi nochain	1.9581e-01	1.73e-02
SS frac	CathodeSurf	214Bi nochain	1.1554e-01	2.24e-04
SS frac	InactiveLXe	Rn222	2.0198e-01	2.18e-04
SS frac	LXeVessel	Co60	3.3109e-03	2.81e-04
SS frac	LXeVessel	Th232	1.6405e-01	1.27e-02
SS frac	LXeVessel	U238	2.0088e-01	1.69e-02
SS frac	Active LXe	bb0n	8.2753e-01	7.02e-02
SS frac	Active LXe	bb2n	8.9304e-01	2.35e-02
SS frac	Active LXe	bb2n Xe136excited	1.1114e-02	9.45e-04
num	ActiveLXe	Rn222	1.1806e+00	1.72e-03
num	AirGap	214Bi nochain	3.2887e+02	2.98e+01
num	CathodeSurf	214Bi nochain	2.6574e+01	5.12e-02
num	InactiveLXe	Rn222	9.2282e+00	9.98e-03
num	LXeVessel	Co60	1.3836e+02	2.70e+01
num	LXeVessel	Th232	3.1671e+02	2.34e+01
num	LXeVessel	U238	2.0196e+02	4.76e+01
num	Active LXe	bb0n	7.9462e-07	1.01e+00
num	Active LXe	bb2n	6.8487e+02	2.76e+01
num	Active LXe	bb2n Xe136excited	5.1899e+01	3.12e+01
Parameter	Label	Multiplicity	Best fit value	Error
Energy scale offset	b_0	MS	11.872	2.94
Energy scale offset	b_0	SS	8.6283	3.22
Energy res. (noise)	r_1	MS	39.711	2.04e-1
Energy res. (noise)	r_1	SS	35.234	3.35e-1
Energy res. (drift)	r_2	MS	1.0347e-2	1.76e-4
Energy res. (drift)	r_2	SS	9.0412e-3	3.71e-4

Table 8.2: Fit Results Comparison for β -scale and different $\beta\beta 2\nu$ theoretical spectra

Fit Type	best (β -scale 0.995)	no β -scale regular bb2n	no β -scale Kotila/Iachello bb2n
num bb2n	684.87	678.51	685.12
SS frac bb2n	0.89304	0.89734	0.89002
num bb2n Xe136excited	51.899	57.717	55.258
SS frac bb2n Xe136excited	1.1114e-02	6.9769e-02	6.9803e-02
NLL	0	0.1	0.5

fiducial volume that passes all the cuts was found to be 22.4%. The effects of the individual cuts are show in Table 8.3. This number is obtained by calculating the fraction of events that deposited more than 1700 keV inside the fiducial volume out of all events that originated inside the fiducial liquid xenon volume. The lowest efficiency number is due to the combined effect of the energy threshold of 1700 keV as well as the escape probabilities of the two ~ 800 keV γ 's.

Table 8.3: Efficiency of various cuts applied. The three applied cuts are the 1700 keV threshold on the total event energy, requirement that the event occur in the fiducial volume, and that the events is fully reconstructed in three dimensions (no missing V-wire signal).

Cut Applied	Efficiency (%)
1700 keV threshold	40.7
1700 keV and fiducial	32.2
1700 keV and full 3D reconstructed	27.8
1700 keV, fiducial, and full 3D reconstructed	22.4

8.5.6 $\beta\beta 2\nu$ to the Excited State Half-life Limit

From the profile likelihood, the central value for the number of $\beta\beta 2\nu$ decays to the excited state is found to be $53.4^{+48.5}_{-48.6}$. For the one side upper limit at the 90% confidence level, the number of excited state decay events is $53.4 + 48.5 \times 1.65$ or 133.2. We assume an additional 15.0% increase due to the systematic uncertainties (discuss in more details in section 8.5.7) to arrive at $n_{\beta\beta 2\nu^*} < 153.2$ at the 90% C.L.

We can then convert this to a limit on the $\beta\beta 2\nu$ to the excited state half-life, $T_{1/2}$, with the formula

$$T_{1/2} = \ln(2) \frac{N(^{136}\text{Xe})T\epsilon}{n_{\beta\beta 2\nu^*}}, \quad (8.4)$$

where $N(^{136}\text{Xe})$ is the number of ^{136}Xe atoms in the fiducial volume, $T = 2896.6$ hours is the livetime of the experiment, and $\epsilon = 22.3\%$ is the efficiency for excited state detection. From the fiducial mass of ^{136}Xe , $M_{Xe} = 79.4$ kg, we can find

$$N(^{136}\text{Xe}) = \frac{M_{Xe}N_A}{M}, \quad (8.5)$$

where $M = 135.6$ g/mol is the molar mass of the enriched Xe, and N_A is Avogadro's number. Thus $N(^{136}\text{Xe}) = 3.53 \cdot 10^{26}$ atoms. This corresponds to a lower limit on the half-life of the $\beta\beta 2\nu$ decay of ^{136}Xe to the first excited state (0_1^+) of ^{136}Ba of

$$1.2 \cdot 10^{23} \text{ years at 90\% C.L.} \quad (8.6)$$

Table 8.4: Table of systematic uncertainties considered. The total is obtained from adding all the considered systematics in quadrature.

Systematic	% Increase in $T_{1/2}$
Fiducial Volume	9.4%
β -scale	11%
$\beta\beta 2\nu$ theory	4%
SS Fraction	0.93%
Total	15.0%

8.5.7 Systematic Uncertainties

While most of the systematic uncertainties can be determined by taking profile likelihood scans over the relevant fit parameters, we will just take a conservative estimate based on the systematic uncertainty study for the EXO-200 $\beta\beta 0\nu$ analysis. The primary source of the systematic uncertainties is the fiducial volume, based upon the source rate agreement. The expected source rate in the TPC from MC depends on both the given source activity and the fiducial volume. Attributing the source rate agreement to the fiducial volume uncertainty, 9.4% was determined as the systematic uncertainties on the fiducial volume. Particularly for the decay to the excited state, the potential contributions from the “dead layer” region of the active xenon volume may be even more problematic given the propensity of the γ ’s to travel more than the β ’s; thus, the true volume of xenon that contributes to the spectrum is a bit uncertain. Other sources of systematics considered in the $\beta\beta 0\nu$ analysis were the β -scale, the difference in $\beta\beta 2\nu$ model, SS Fraction, energy scale, and energy calibration. The difference in the fit with and without the β -scale for

the decay to the excited state is at 11%. This systematic due to the β -scale is a bit larger than the 9.32% used by the $\beta\beta 0\nu$ analysis. By using the Iachello/Kotila $\beta\beta 2\nu$ spectrum with no β -scale, the fit result differs by 4% with the default Vogel $\beta\beta 2\nu$ spectrum with no β -scale. Swapping out the Vogel $\beta\beta 2\nu$ spectrum for the Iachello/Kotila has a negligible effect on the $\beta\beta 0\nu$ analysis. While the the rest of the floating fit parameters of SS Fraction, energy scale, and energy calibration all contribute only slightly with the SS Fraction being 0.93% and the energy scale and energy calibration both being negligible. Adding all these systematics together in quadrature, we end up with a total systematic uncertainty of 15.0%.

Chapter 9

Developing Analyses for the Decay to Excited State Search

The energy spectral shape of the $\beta\beta 2\nu$ decay to the first 0_1^+ excited state, as shown in Figure 8.5, is not distinctly different from that of the background. It would be difficult to claim a positive result without a complete understanding of all the backgrounds. A new energy variable may allow the decays to the excited state to stand out. Toward achieving this new goal, we hope to exploit the uniqueness of the decay to the excited state: the two γ 's with very specific energies.

In this chapter, we will discuss two developing analyses that may give a better sensitivity for the decay to the excited state. The first analysis is a position dependent two-dimensional fit. This analysis is similar to the next main $\beta\beta 0\nu$ EXO-200 data analysis. The second analysis is excited state specific, where a special new energy variable called “reduced energy” is being developed that should result in a large signal for the decay to the excited state only.

9.1 Position Dependent Fits

The result presented in Chapter 8 is fitting the low background data to energy dependent PDFs only. PDFs of other variables can also be produced and fitted. Multi-dimensional fits can be done by fitting PDFs of multiple variables together.

9.1.1 2D PDF

Given how the desired physics process would come from the bulk of the liquid xenon detector while the backgrounds are closer to the outside, 2 dimensional PDFs are made with energy and a positional variable - “standoff distance”. Standoff distance is defined as the difference between either event’s radial location and radius of the Teflon reflector or events’ Z coordinate and V-wire plane, whichever is smaller. Typically, this is the distance to the side of the cylinder but for some events it is the distance in the Z-direction. For multiple site events the shortest of the cluster’s standoff distances is used.

An example of a 2D PDF is shown as a heatmap in Figure 9.1.1. This is the PDF for the decay to the excited state. While all the standoff distribution has a peak around low standoff distance and slowly falls (partially due to there being more volume closer to the edge of the cylinder), the rate of fall is different for events originated from within the active liquid xenon and those who came from the outside.

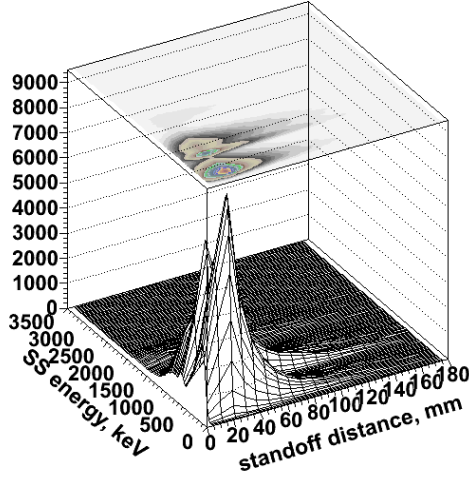
9.1.2 Analysis Improvements

A few improvements have been made for the generation of the 2D PDFs above compared the method discussed in the first 8 chapters of this thesis. These changes represent the overall progress in the EXO-200 analysis. They will be quickly summarized here.

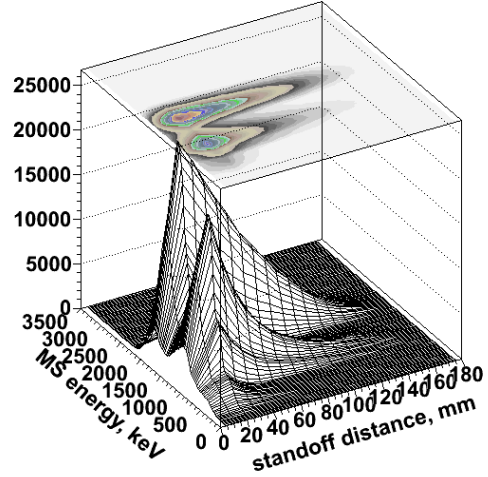
- Monte Carlo: More details have been added to the Monte Carlo code, particularly for the copper LXe vessel. See Figure 9.3 for all the new details in the

Figure 9.1: 2D (Standoff distance and energy) PDFs for the single site (SS) and multiple site (MS) of $\beta\beta 2\nu$ to excited state (a) and ground state (b).

bb2n_Xe136excited SS

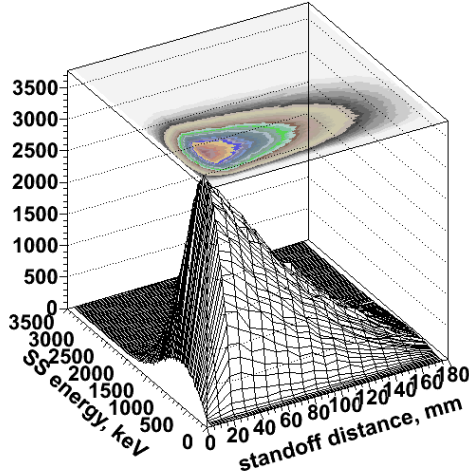


bb2n_Xe136excited MS

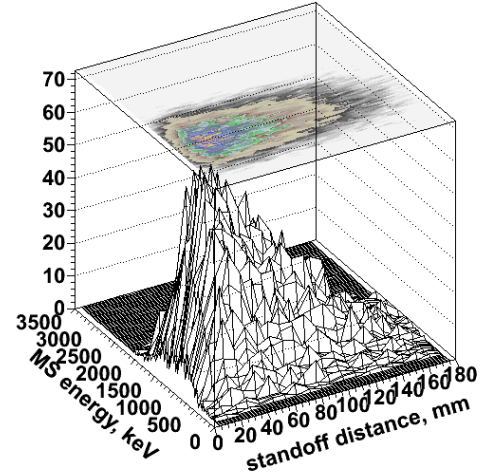


(a) SS and MS 2D PDF for the ^{136}Xe $\beta\beta 2\nu$ decay to the excited state

bb2n SS



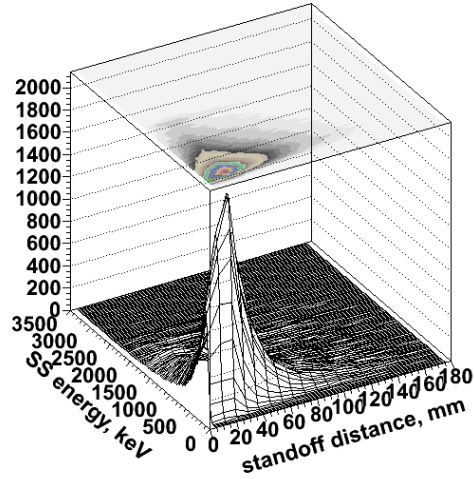
bb2n MS



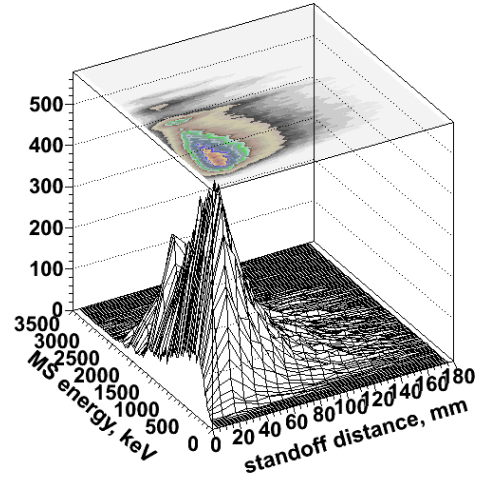
(b) SS and MS 2D PDF for the ^{136}Xe $\beta\beta 2\nu$ decay to the ground state

Figure 9.2: 2D (Standoff distance and energy) PDFs for the single site (SS) and multiple site (MS) of ^{214}Bi in the aIr gap (a) and ^{222}Rn in the inactive xenon volume.

AirGap_214_Bi_nochain SS

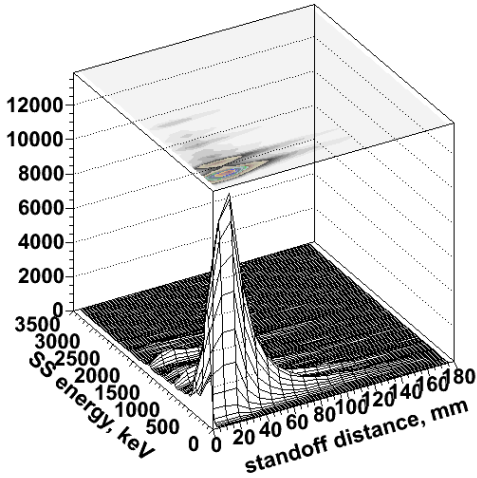


AirGap_214_Bi_nochain MS

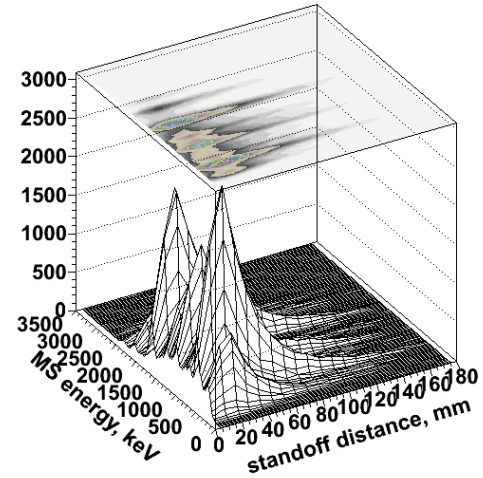


(a) SS and MS 2D PDF for the ^{214}Bi in the aIr gap

InactiveLXe_Rn222 SS



InactiveLXe_Rn222 MS



(b) SS and MS 2D PDF for the ^{222}Rn in the inactive xenon volume

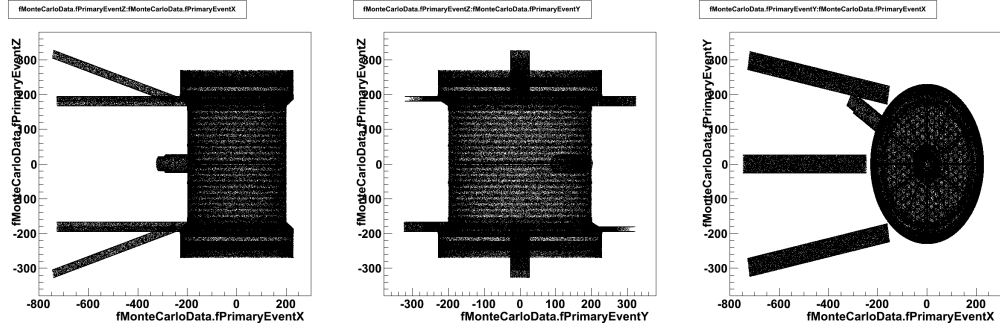


Figure 9.3: All of the copper component being simulated in the new MC, as plotted by GEANT4. TPC legs and the cathode feedthrough are all visible here, along with details in the APD platter frame.

copper component being considered as the “Vessel”.

- Clustering: A new clustering algorithm is implemented in the reconstruction step. The main difference is in the assignment of V-wire signals to the U-wire signals by considering more of the timing differences between signals. By getting better coordinates to the wire-signals, charge clusters size and location are more reliable. This improvement would be particularly important for the development of the second new analysis technique discussed in this Chapter, which require better knowledge of detector events on a cluster-by-cluster basis.
- Energy calibrations: Improvements have been made to understand and correct the differences in the channel-by-channel U-wire gains, as well as the grid wire shielding effects. Possible time-dependent energy calibration effects have also been looked at, although it is not applied to the 2D fit result shown here.

9.1.3 2D Fit Result

Fit result with the standoff distance are shown in Table 9.1 and Figure 9.1.3. There were 25 fit parameters considered, SS Fraction and the total number of events for each PDF and an overall normalization factor. The fit found 27.1 events (SS and MS, although it is still most definitely from the MS only, with the SS Fraction of 0.011) for the $\beta\beta 2\nu$ decay to the excited state with a fit error of 8.1. This result is 3.3σ away from zero, although a profile likelihood would need to be done for a more statistical robust measure of the uncertainty.

9.1.4 Even Higher Dimensional PDF Fit

This same concept of a multi-dimensional simultaneous fit can be applied to other variables than the “standoff distance”. In principle, more variables can be simultaneously fitted to optimize the search for a signal, although the computational time increases with every additional variable. The correlation between the variables considered would also need to be carefully studied.

9.2 Reduced Energy

The new variable designed to identify the decays to the excited state is an energy variable that we call *reduced energy*. The name stem from the variable being the total energy *reduced* by the one charge cluster that we think is the $\beta\beta$ cluster. From the $\beta\beta 2\nu$ and $\beta\beta 0\nu$ analyses, we know that $\beta\beta$ events are mostly single-sited and identified as a single charge cluster. If we can measure all of the rest of the

Figure 9.4: Two-dimensional fit result with fit range energy of 1700 to 3500 keV and standoff distance.

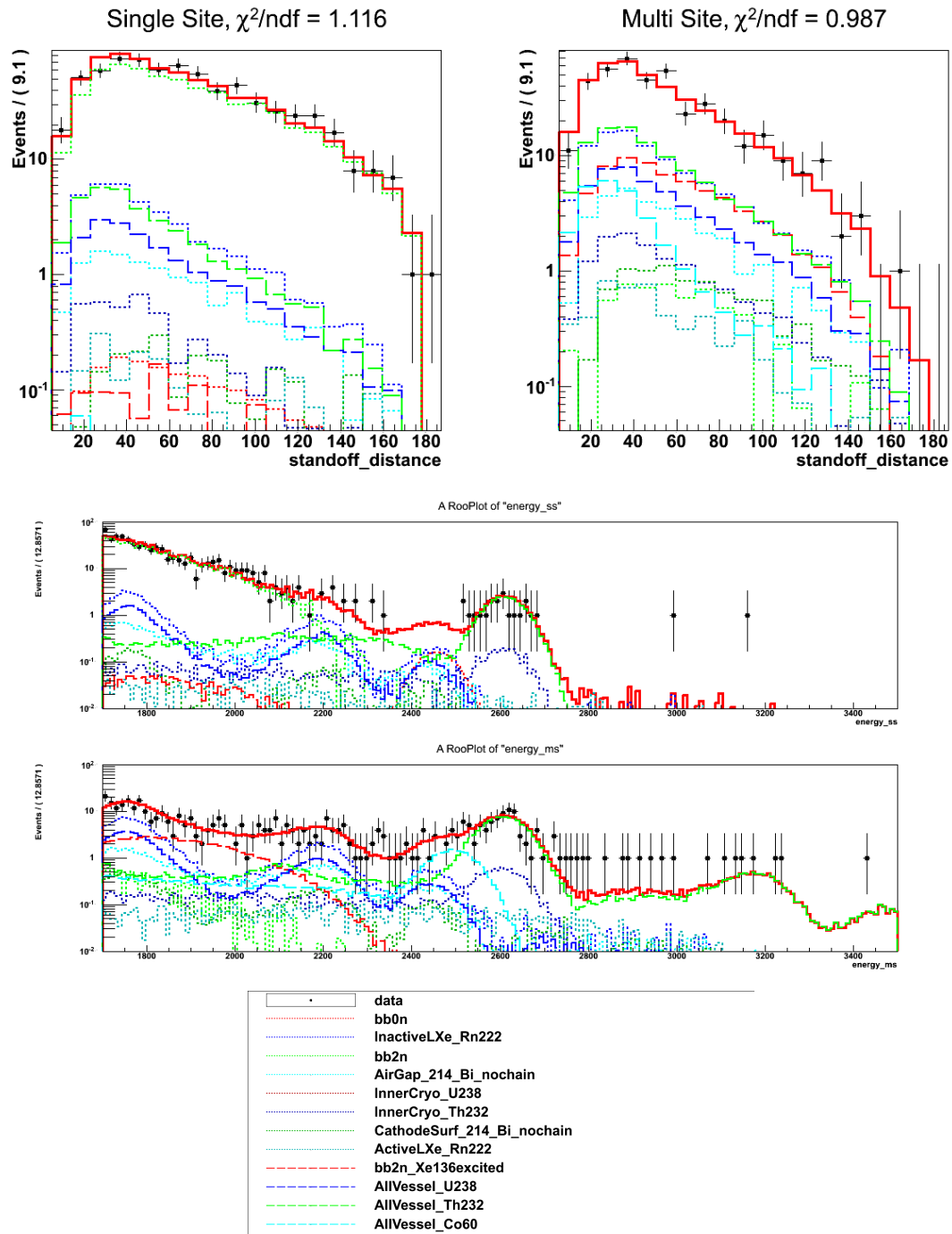


Table 9.1: Best fit values for all observables represented by a 2D PDF.

Parameter Type	Location	Source	Fit Result	Error
SS frac	ActiveLXe	Rn222	2.2438e-01	1.91e-02
SS frac	AirGap	214Bi nochain	2.7651e-01	2.38e-02
SS frac	CathodeSurf	214Bi nochain	2.0685e-01	1.76e-02
SS frac	InactiveLXe	Rn222	2.7755e-01	2.30e-02
SS frac	LXeVessel	Co60	2.5923e-03	2.20e-04
SS frac	LXeVessel	Th232	2.5022e-01	2.11e-02
SS frac	LXeVessel	U238	2.7593e-01	2.33e-02
SS frac	InnerCryo	Th232	2.6009e-01	2.18e-02
SS frac	InnerCryo	U238	2.7351e-01	2.34e-02
SS frac	Active LXe	bb0n	9.4214e-01	8.19e-02
SS frac	Active LXe	bb2n	9.8901e-01	1.26e-02
SS frac	Active LXe	bb2n Xe136excited	1.4863e-02	1.27e-03
num	ActiveLXe	Rn222	6.9450e+00	7.04e-01
num	AirGap	214Bi nochain	1.8395e+01	5.28e+00
num	CathodeSurf	214Bi nochain	1.0997e+01	1.12e+00
num	InactiveLXe	Rn222	5.6052e+01	5.73e+00
num	LXeVessel	Co60	1.0671e+01	4.58e+00
num	LXeVessel	Th232	5.7340e+01	8.96e+00
num	LXeVessel	U238	2.7308e+01	1.08e+01
num	InnerCryo	Th232	7.5547e+00	3.98e+00
num	InnerCryo	U238	5.8843e-04	1.25e+01
num	Active LXe	bb0n	1.2739e+00	1.26e+00
num	Active LXe	bb2n	6.1762e+02	6.73e+01
num	Active LXe	bb2n Xe136excited	2.7099e+01	8.10e+00
norm			9.4057e-01	8.70e-02

energy from the decay to the excited state except for the $\beta\beta$, we would effectively be measuring just the energies of the two γ 's (for the cases where the γ 's are fully contained), which would be about 1579 keV for the ^{136}Xe decay to the 0_1^+ state of ^{136}Ba . Of course, we have no idea which of the many charge clusters is the $\beta\beta$ cluster. Consequently, we need to come up with an algorithm that can identify the correct $\beta\beta$ cluster, most of the time.

Even in the EXOsim Monte Carlo, the reconstructed clusters are not explicitly associated with the source of the energy deposition. From the Monte Carlo, however, we do know the true position of the source decay where the $\beta\beta 2\nu$ to the excited state is generated. Since the $\beta\beta$ is not expected to travel far inside liquid xenon compare to the γ 's, we can assume that the $\beta\beta$ charge cluster is the one closest to the primary event location. Figure 9.5 shows the distance between the closest charge cluster to the primary decay location for the simulated $\beta\beta 2\nu$ to the excited state. As expected, bulk of this minimum distance is within 1 cm of the primary decay, followed by a long tail for special cases where the $\beta\beta$ may have been generated in the “dead layer” and the nearest cluster is due to a γ . With this expected distribution, we claim that the nearest cluster (within 1 cm) is indeed the $\beta\beta$ cluster.

The next step is to figure out an algorithm where we can pick the $\beta\beta$ cluster among all of the clusters in an event. One possibility is to look for the energy ranking of the clusters. The $\beta\beta$ cluster is at most 822 keV while the γ 's are both ~ 800 keV. For the cases where all three particles each result in an single cluster, the 3rd lowest energy cluster would be the $\beta\beta$. In reality, the γ is likely to Compton scatter and be observed as multiple clusters. However, we can still look at the energy rank,

from the highest to the lowest, of the nearest cluster to the primary decay location that we believe to be the $\beta\beta$ cluster. Figure 9.6 shows the energy rank of the $\beta\beta$ candidate cluster separately for simulated events with 3, 4, and 5 fiducial charge clusters (only charge clusters that are reconstructed inside the fiducial volume is considered in the energy ranking). An addition cut on the total energy of at least 1700 keV is also applied. Clearly, the most probable energy ranking for the $\beta\beta$ candidate cluster is the 3rd.

With the desire to increase the efficiency of this new variable, we have also decided to include the events where there are only two fiducial clusters. In these cases, the energies would most likely be split between a cluster containing one of the γ and the $\beta\beta$ while the other cluster would be the other γ (with the minimum total energy requirement of 1700 keV, only the fully contained events are considered). For these two cluster cases, by subtracting the higher energy cluster, we should be left with a cluster representing one of the γ energy alone, which would be ~ 800 keV.

So the reduced energy definition is the following:

For all two event with the multiplicity of two, the energy of the *LARGER* charge cluster is the reduced energy. For all events with three or more charge clusters, the reduced energy is the *SUM* of all charge clusters *OTHER THAN THE THIRD HIGHEST ENERGY* charge cluster.

The spectrum of what reduced energy for the $\beta\beta 2\nu$ decay to the excited state signal is shown in Figure 9.7. The smaller peak ~ 800 keV corresponds to the two cluster

event while the larger peak ~ 1570 keV corresponds to the events with three or more charge clusters.

Among the excited state events generated that passes the required cuts of being inside the fiducial volume and being fully reconstructed in 3-dimensions with at least two fiducial clusters ($\sim 46\%$ of all generated events), the choice of the third highest energy cluster selects the nearest cluster to the primary event location (candidate $\beta\beta 2\nu$ charge cluster) $\sim 21\%$ of the the time out of all of the 3 or more fiducial clusters events ($\sim 37\%$ all generated signal events). The addition of the two fiducial cluster events ($\sim 9\%$ all generated signal events) allow 52% of the $\beta\beta 2\nu$ cluster to be correctly identified. All together, 12.4% of the generated signal events (or 27% of all events pass the standard cuts) are correctly identified by our definition of reduced energy.

9.2.0.1 Signal vs. Background

The important advantage of the reduced energy variable is in its unique spectrum for the $\beta\beta 2\nu$ decay to the excited state signal. Figure 9.8 compares the reduced energy for the signal against all of the other considered backgrounds. While the main peak centered around 1570 keV of the $\beta\beta 2\nu$ decay to the excited state is sitting on top of a wider but similarly shaped background from the ^{214}Bi events of the ^{238}U chain (including ^{222}Rn), the secondary peak at ~ 800 keV from the two cluster signal events make the signal spectrum distinguishable. A realistic charge-only calibration of at best 3.5% at 2500 keV is applied in this plot, otherwise the 1570 keV would

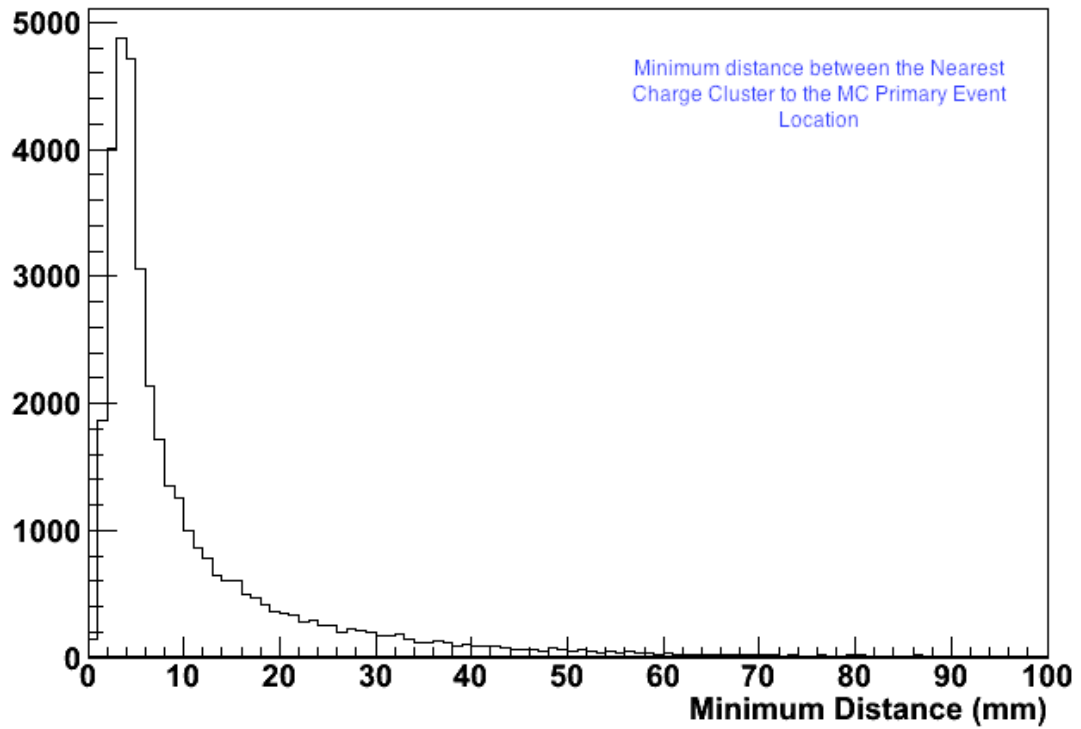


Figure 9.5: Plot of the distance between the nearest charge cluster to the primary event location from the MC. Bulk of the clusters are within 1 cm of the primary event and are believed to be the $\beta\beta$ cluster.

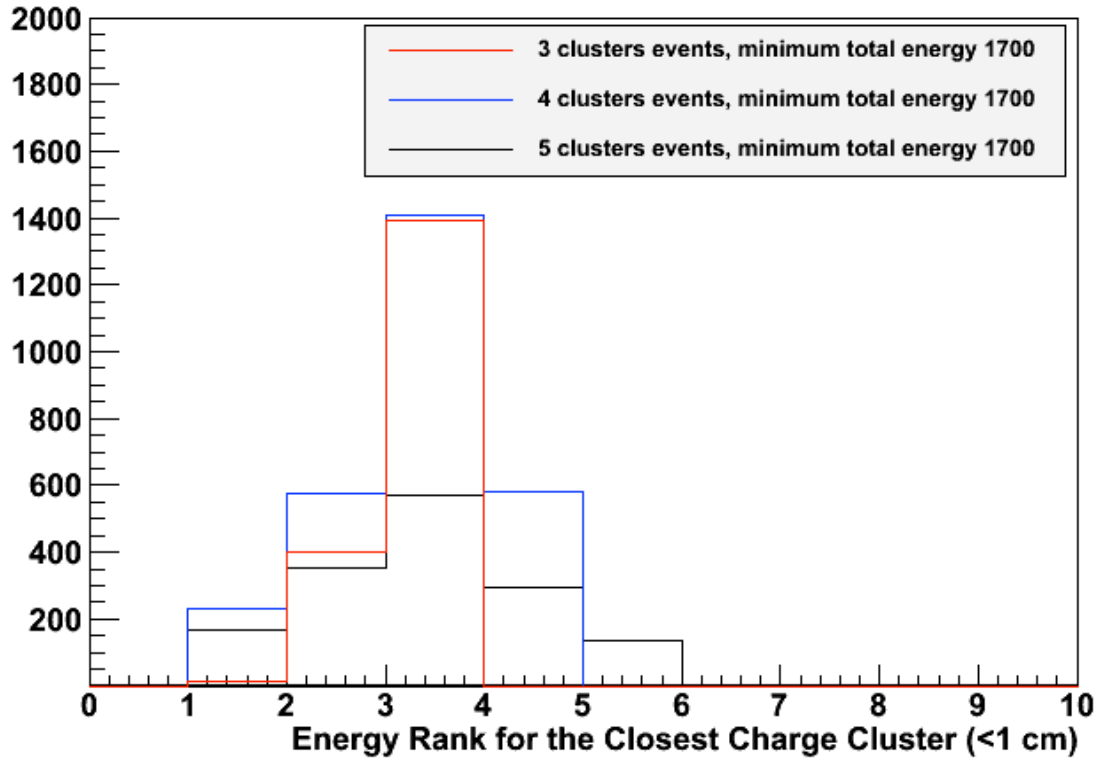


Figure 9.6: For the charge cluster believed to be the $\beta\beta$ cluster due to it being the nearest charge cluster to the primary event location and $<$ than 1 cm away, the energy ranking (from the highest to the lowest) of that cluster is plotted here for events with 3 (blue), 4 (red), and 5 (black) clusters. The choice of the 3rd highest energy cluster is particularly good for events with the minimum total energy of 1700 keV. That restriction was eventually loosened up to down to 1000 keV to both incorporate more data and to look for the secondary reduced energy peak from two cluster events.

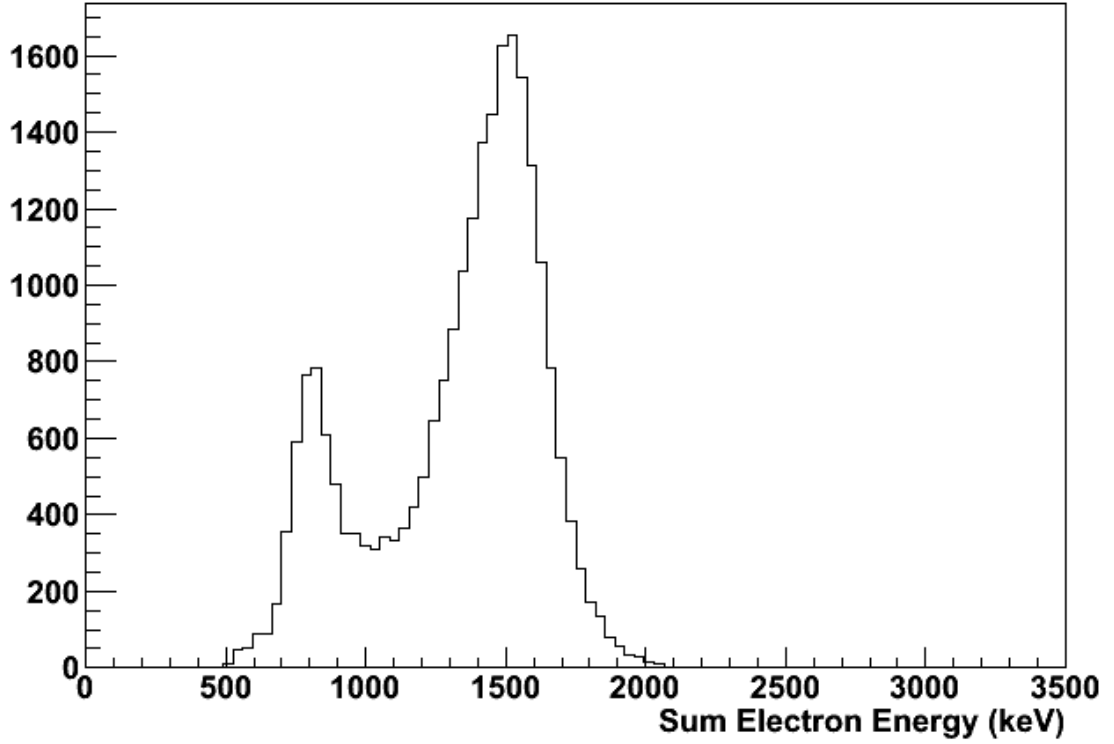


Figure 9.7: “Reduced energy” histogram for the simulated $\beta\beta 2\nu$ decay of Xe^{136} to the excited state, with the requirement that total energy is at least 1000 keV (to encompass the fully contained and single escape events). The two peaks of the histogram come from the case of just two clusters (first peak at around 800 keV) and the cases with three or more clusters (second peak at around 1570 keV).

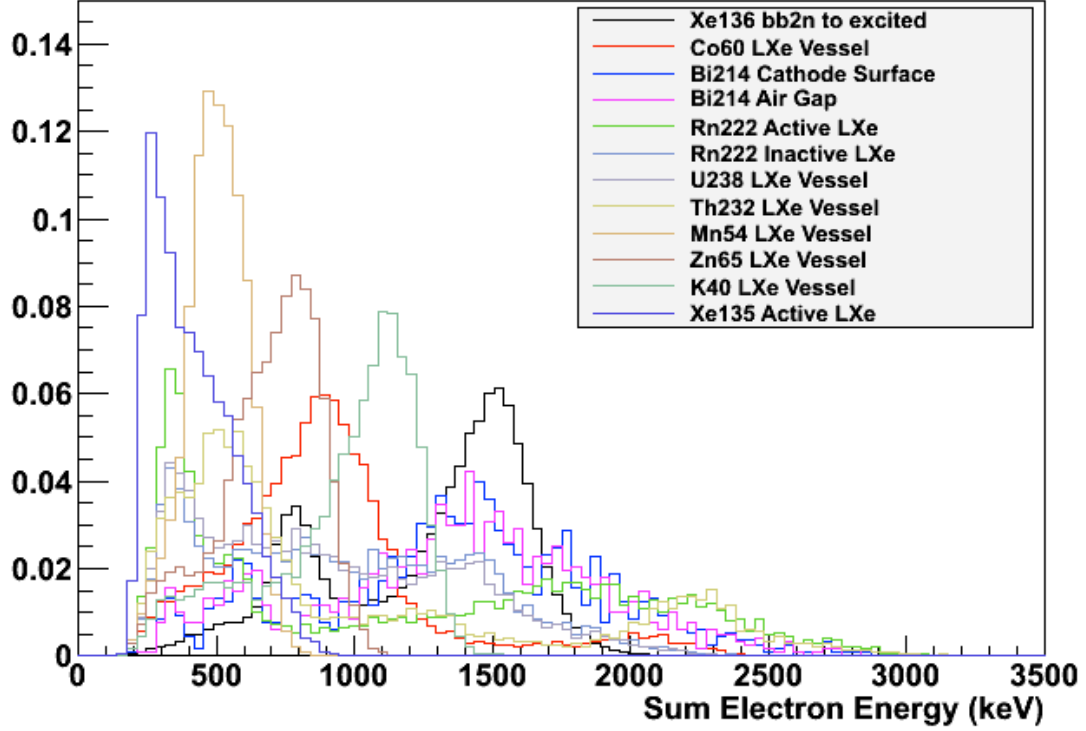


Figure 9.8: “Reduced energy” for the $\beta\beta 2\nu$ decay to the excited state signal (black) and the common backgrounds. Reduced energy is defined as the sum of all charge clusters except for specially chosen one which is either the the second highest energy charge cluster for two cluster events or the third highest energy cluster for events with three or more charge clusters. Charge only energy resolution was applied to all of these simulations. No minimum total energy is required. All of the histograms have been normalized to 1.

be a lot more prominent. All of these spectra in the Figure are normalized to 1. In reality, the background rates would be much higher in comparison to the decay to the excited state signal rate.

9.2.1 Charge Only Calibration

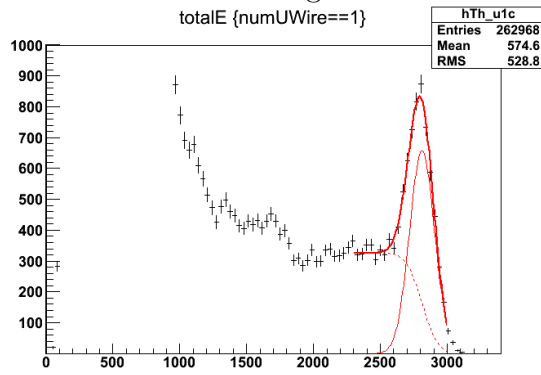
Looking at the multiple site data and manipulating the charge clusters individuals to define reduced energy, we cannot apply the usual rotated energy technique since there is only one scintillation cluster associated with all of the charge clus-

ters. Consequently, reduced energy means that we only have the charge only energy resolution, $\sim 3.5\%$ at 2500 keV compare to the rotated energy energy resolution of $\sim 0.5\%$.

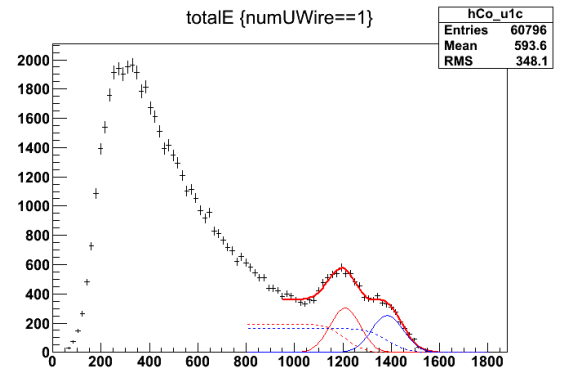
Different from the original analysis where all of the multiple site events are lumped together with one energy calibration, we are interested in the events by the number of charge clusters level, separating the two cluster events from the three cluster events and the four cluster events. While calibration by the number of fiducial charge clusters was considered, we ultimately decided that the truest result would be to use the calibration of events separated by the number of U-wires.

From the single U-wire calibration events, we do the fits for the three calibration sources (^{60}Co , ^{137}Cs , and ^{228}Th) to fit for the four peaks and use the location and the width of those four peaks to set energy scale and energy resolution calibration, respectively. Figure 9.9 shows the fit results for the single U-wire cases. The energy resolution calibration for the single U-wire events is shown in Figure 9.10. The result of Figure 9.10 is actually the energy calibration curve used to smear all charge clusters (discussed in more detail in the next section), rather than an energy calibration being applied to the total energy as in the original analysis. For the two and three U-wire events, the fit results are shown in Figure 9.11 and Figure 9.12. We apply the energy scale from these fits to the corresponding data with the same number of U-wire signals.

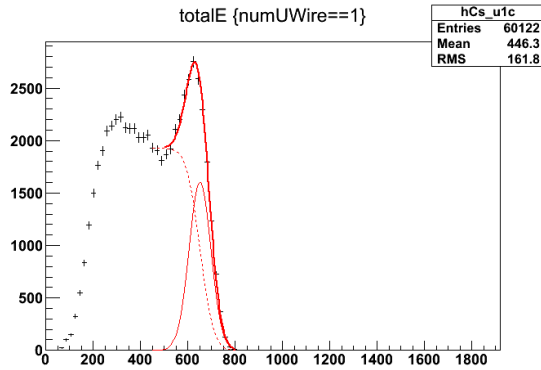
Figure 9.9: Source calibration fits for single U-wire. The energy resolution function fit used came from fitting these results.



(a) Single U-wire Th Fit



(b) Single U-wire Co Fit



(c) Single U-wire Cs Fit

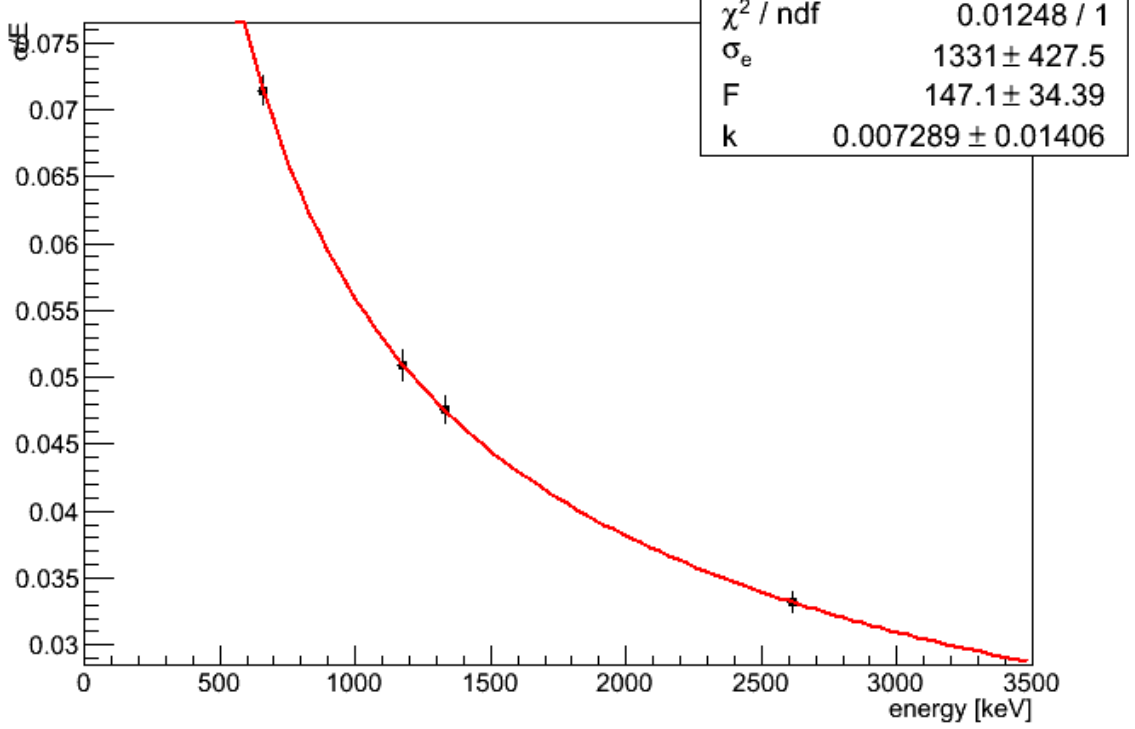
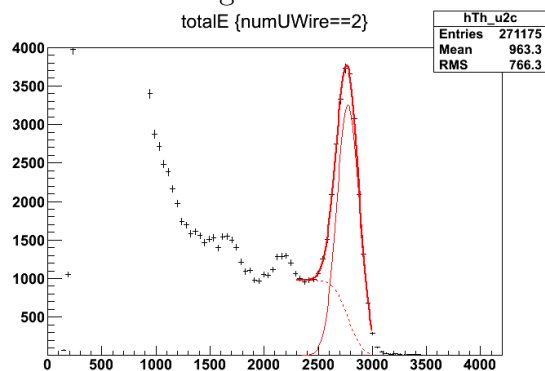


Figure 9.10: Energy resolution fit for the charge only calibration used. Only calibration events with signal on just one single U-wire are used to make this calibration.

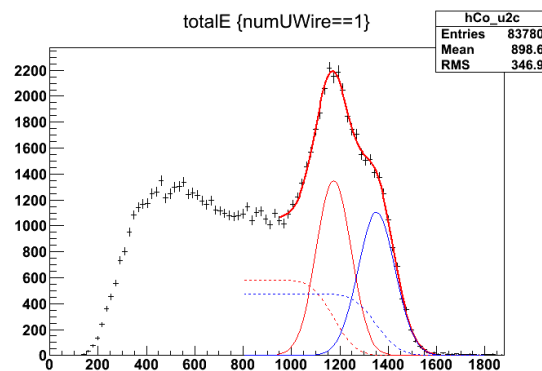
9.2.2 Applying the Calibration

PDFs are constructed from smearing the true pixilated charges from the MC simulations like before. However, there is a major difference between how this was done in the original analysis and here; the smearing was applied to the *total energy* in the original analysis while the smearing is now done to the *cluster energies* before they are summed up to get the total energy. Looking at the energy resolution curve (see Figure 9.10), the energy resolution is clearly not linear with energy. Consequently, the energy resolutions applied is different from the two methods.

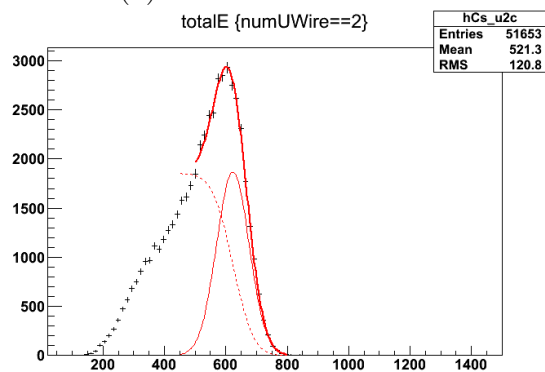
Figure 9.11: Source calibration fits for two U-wires.



(a) Two U-wire Th Fit

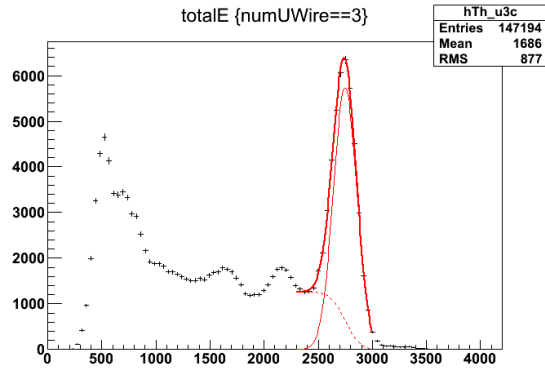


(b) Two U-wire Co Fit

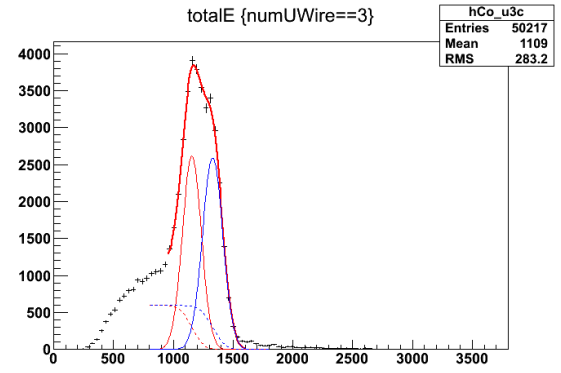


(c) Two U-wire Cs Fit

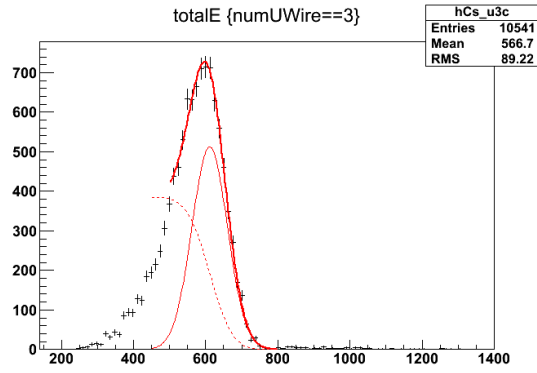
Figure 9.12: Source calibration fits for three U-wires.



(a) Three U-wire Th Fit



(b) Three U-wire Co Fit



(c) Three U-wire Cs Fit

9.2.3 Source Agreement

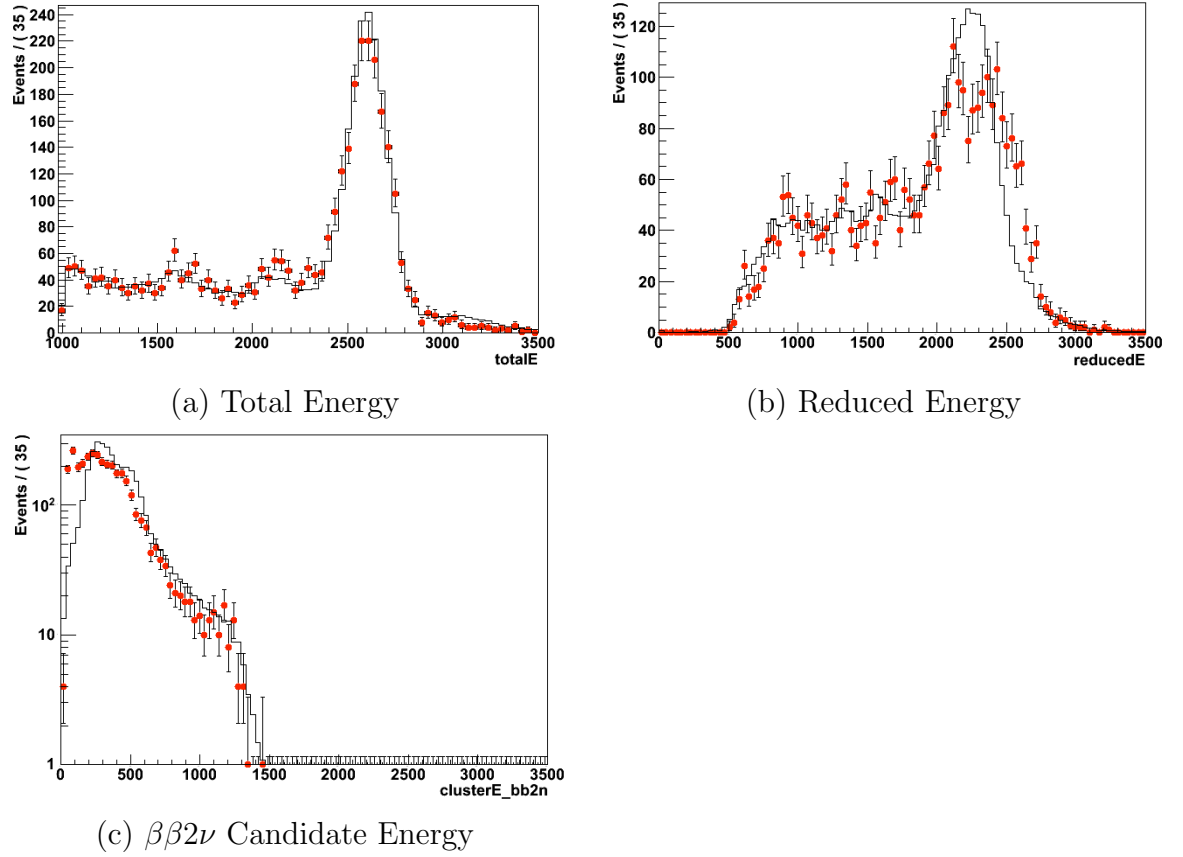
Figure 9.2.3 shows the source agreement plots for Total Energy, Reduced Energy, and the complement $\beta\beta 2\nu$ Candidate Energy with the charge only calibration. The $\beta\beta 2\nu$ Candidate Energy is the energy of the single cluster that was subtracted from the Total Energy. For each event, its entry for Reduced Energy and $\beta\beta 2\nu$ Candidate Energy should add up to equal its entry in Total Energy.

While the source agreement is quite good for the Total Energy (Figure 9.2.3a) despite the change in energy resolution smearing technique, the source agreements for Reduced Energy and $\beta\beta 2\nu$ Candidate Energy (Figure 9.2.3b and Figure 9.2.3c) are not nearly as good. On the individual charge cluster basis, the source agreement still needs to be improved. Differences in the threshold between MC and data is evident in the $\beta\beta 2\nu$ Candidate Energy plot. The same effect is seen in the disagreement at the higher energy in the complementary variable of Reduced Energy. Better agreement in the low energy threshold between data and simulation is probably the first step toward getting better source agreement. Further advancement in the charge clustering algorithm should also help with this endeavor in the near future.

9.3 Future Considerations

Since this is essentially the first attempt at studying individual charge clusters in multiple-site events in the EXO-200 data, plenty of improvements may be possible in the future. Given that the energy is more spread out in the multiple site event, the

Figure 9.13: Source agreement plots of a Th calibration run with charge-only single U-wire calibration applied. A Total Energy cut of 1000 keV is applied and only the multiple site events are considered. The same normalization, taken from the Total Energy fit, is used in all three plots.



signal-to-noise ratio of each charge cluster is smaller. Both hardware and software improvements may increase the ability of EXO-200 to observe low energy clusters as well as distinguish spatially between multiple small charge clusters.

The source disagreement for the Reduced Energy and other variables, which do depend on individual cluster energy, may be improved by upgrading the way clustering is done in reconstruction. Smarter grouping of measured charge deposits into clusters, particularly at the low energy, could help with the source agreements at the individual cluster energy level. The low energy threshold disagreement may be solved this way. Having a fundamental agreement of the individual charge cluster energies would be the first step toward the viability of these new variables, such as the reduced energy or its complement the $\beta\beta$ candidate energy, that are the combination of individual charge cluster energies.

As the study and understanding of the multiple site spectrum increase, so should the ability of EXO-200 to distinguish the various multiple-site signals and backgrounds. The current problem of not having as good of source agreements for the multiple-site spectra is how “multiple site” encompass events of various origins (different number of charge clusters). As more source calibration runs are taken, maybe there is enough statistical prowess to have event differentiation beyond single and multiple site, but based on the actual number of charge clusters. Improvement on the analysis technique in addition to more data accumulated should lead to the testing of the theoretical half-life for $\beta\beta 2\nu$ decay to the 0_1^+ excited state before the conclusion of EXO-200.

Chapter 10

Conclusions

A search for the two neutrino double beta ($\beta\beta 2\nu$) decay of ^{136}Xe to the first 0_1^+ excited state is presented in this thesis. Based upon 2896.6 hour of EXO-200 data, representing $3.53 \cdot 10^{26}$ ^{136}Xe atoms, the number of $\beta\beta 2\nu$ decays to the excited state is found from the profile likelihood of the fit results to be $53.4^{+48.5}_{-48.6}$. This result is 1.1σ away from zero, which is not statistically significant. Including a conservative estimate of 15% uncertainty to account for the systematics, we have set a half-life lower limit on this decay of $1.2 \cdot 10^{23}$ year at 90% C.L. This limit is still a couple of order of magnitude away from the expected theoretical rate of $2.5 \cdot 10^{25}$ year, calculated from applying theoretical suppressions of the known $\beta\beta 2\nu$ decay rate to the ground state.

The method used in this first search for the decay to the excited state has not been fine-tuned to take advantage of the unique characteristics of the decay to the excited state, mainly the presence of two γ 's with very specific energy. Next generation of analysis could have a better discrimination of the backgrounds with new variables that require better understandings of the data on an individual charge cluster level. Given the theoretical expectations of this decay, there may be dozens or so signal events in the data by the time EXO-200 is done collecting data. A discovery of the decay to the excited state can shed some light on the validities

of the various nuclear physics models, which may assist in the extraction of the effective neutrino mass limit from limits on the neutrinoless double beta decay rate.

Appendix A

Development of a single-ion Barium source from ^{137}Cs

A.1 Motivation

As described in previous chapters, the main strategy for double beta decay experiments to potentially discover neutrinoless double beta decay ($\beta\beta 0\nu$) is to very carefully measure the sum electron energy spectrum. The presence of radioactive backgrounds may result in energy deposition in the target narrow energy window of interest, however. To achieve the necessary low background, the EXO collaboration is developing the technology of “barium tagging”. Since natural backgrounds that may mimic the signal of the decay in energy deposition inside the detector do not produce a corresponding barium ion, the identification of a barium ion from a candidate event surely indicates the presence of a xenon double beta decay.

To test the capability and efficiency of barium tagging, a single ion barium source is needed as the rate of the desired nuclear decay is akin to finding “a needle in a haystack”, a single ion in $5 \cdot 10^{24}$ atoms for a ton scale xenon experiment. Bulk creation of barium ion is easily achievable by the use of a barium oven, often a hot barium wire (getter), or by laser spallation on a piece of barium metal. However, ions are expected to have vastly different behaviors, such as mobility and lifetime before neutralization, in bulk compared to as a single particle. Furthermore, determinations of the method efficiencies require situations where ideally each barium

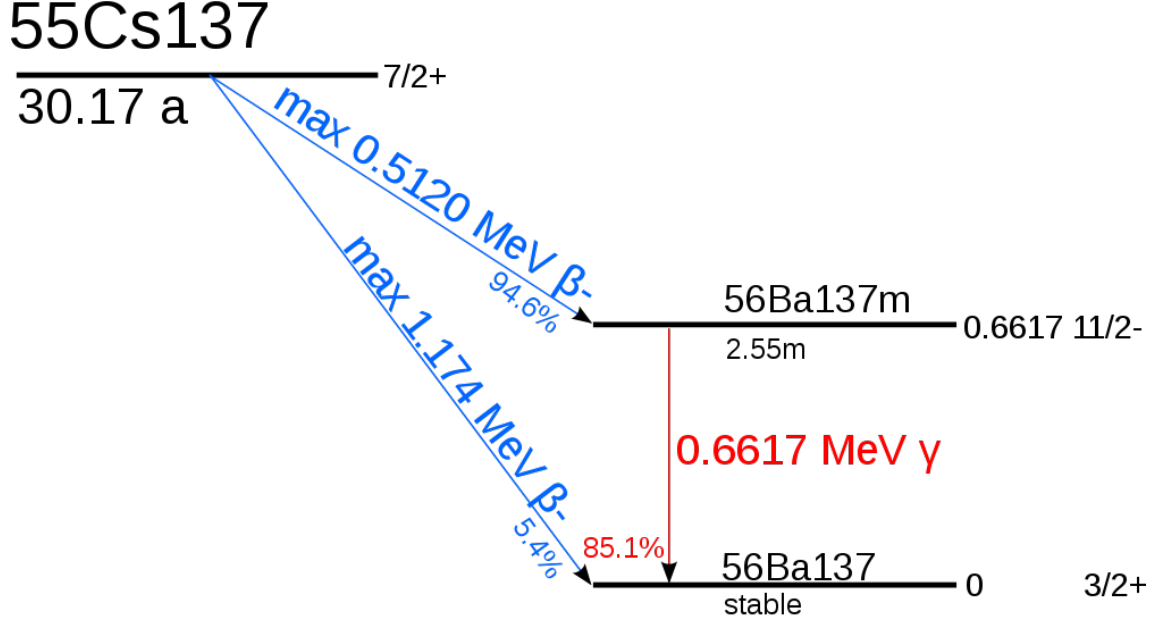


Figure A.1: Energy diagram indicating the ^{137}Cs decay scheme. Figure is taken from [15].

ion production can be accounted for in some way.

In this appendix, we describe the development of a single barium source via ^{137}Cs . By utilizing its well known beta decay (see decay diagram in Fig A.1), each ^{137}Cs (half-life of 30.07 year) creates a barium ion with the added benefits of a coincident beta and a briefly delayed (2.55 minute) 662 keV gamma that can be used to tag that ion. With the barium being produced by a beta decay, which is physically similar in many ways to the double beta decay that is the primary goal of EXO, the behavior of the barium ions should be similar. The ^{137}Cs method described here have one of the best potential for creating a very realistic barium atom/ion test given the ability to tag individual ion, when compared to some of the other ideas also developed in EXO.

A.1.1 Other EXO Barium Sources

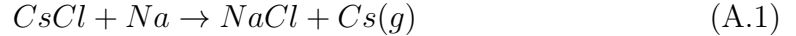
EXO have also developed other means of creating a single-ion barium source such as the radionuclide-driven [84] and the vacuum only electron impact ion source with varying successes. Both of these methods have been tested using the time of flight method, where a mass spectrometer is used to record the time of flight of the various species produced by the source.

The radionuclide-driven source utilizes the recoil energy of an alpha decay (^{148}Gd , with a half life of 74.6 year) product (the resultant ^{144}Sm rather than the alpha particle) to knock barium ion off a thin layer of barium fluoride (BaF_2) that has been vapor deposited over the gadolinium. The source is fabricated by electroplating the ^{148}Gd directly on an alpha counter (a p-doped Si surface barrier detector), follow by the thin layer of barium fluoride. While the individual alpha decays are recorded by the counter, only in a fraction of the time would the recoil ion be in the correct direction. The time of flight measurements of the source products indicate that a further fraction of those created are other types of ion (barium fluoride, contaminants, etc.) in addition to the desired barium ion.

The electron impact ion source is basically a barium ion source (electron gun on a barium getter) with a beam chopper. The beam chopper is an electrostatic gate (Bradbury-Neilson gate) which consists of layer of parallel wire grids. On adjacent wires, opposite voltages can be applied when the gate is in the “off” position as the electric field in this configuration will divert an incoming ion beam. This method has the drawback of only being able to work in a vacuum environment.

A.1.2 ^{137}Cs Cesium

^{137}Cs is a commonly used beta source in nuclear physics. Commercial radioactive ^{137}Cs comes in the form of $^{137}\text{CsCl}$ salt, used in nuclear medicine. For EXO purposes, the goal is the production of single barium ion at the end, rather than the barium chloride molecule. To chemically create atomic cesium from CsCl salt, the following chemical reaction [85][86], traditionally used in atomic physics experiments to create cesium beams, is attempted to separate the cesium from the chlorine:



when heated to 200°C . By comparison, cesium chloride does not evaporate until about 550°C .

Atoms stick to wall via either physisorption, sticking to the wall only for some time, or chemisorption, chemically reacting with the wall and being permanently stuck. Cesium likes to stick to walls, permanently bonding to the wall chemically [87]. This behavior poses a potential challenge down the line of mixing the cesium in the xenon medium. Bare metal is expected to bond with cesium easily, with the image charge of the cesium attracting the atom to the wall via Van der Waal force. Additionally, many wall coatings are found to react chemically with cesium at room temperature, and the reaction rate increases at elevated temperatures [87]. Ideally, if the cesium isolating reaction can be conducted in xenon gas directly over a liquid xenon bath, some of the ^{137}Cs may mix with the liquid xenon. rather than directly sticking to the walls of the vessel.

One difference between the cesium beta decay and the desired Xe double beta decay is that the barium ion created by the ^{137}Cs decay is $^{137}\text{Ba}^+$, but the actual daughter ion created by the double beta decay of ^{136}Xe is $^{136}\text{Ba}^{++}$. However, the barium ion is expected to prefer the $^{136}\text{Ba}^+$ state. The confirmation of this behavior is one of the many goal that is hope to be studied once a single barium ion source can be integrated into a xenon detector.

A.2 Experimental Setup

The cesium chloride and sodium chemical reaction was conducted inside a large, approximately 6 liter, customized vacuum chamber as displayed in Fig A.2. The radioactive CsCl salt was first dissolved in deionized water. A small droplet of the dyed radioactive solution then was deposited on a 0.75 inch by 0.5 inch tantalum foil, with a thickness of 0.02 mm, and placed in a fume hood until the water had evaporated. Six CsCl deposited foils with activity of about 1 microcurie each were made for this project. Tantalum, a commonly used metal substrate in surface science experiments, was chosen due to its resistivity to corrosion. The tantalum foils and the deposits on it could be heated by applying current across the foil using a power supply (EICO 1064S, capable of achieving up to 12V and 10A). A SAES Getter AMD (alkaline metal dispenser) Na wire was used to provide the sodium. The sodium wire was activated by running current through it, using the same EICO power supply. Although its datasheet stated that the start of evaporation would begin at around 6A, a current of closer to 9A was needed to start the evaporation,

particularly on the first batch of sodium wires used in this study which had exceeded its expiration date. Brand new sodium wires were found to have lower turned-on currents that were within the specification listed. To minimize the contamination of radioactivity of the vacuum chamber, the inside of the vacuum chamber was initially lined with thin sheets of Kapton to absorb the stray CsCl and Cs. These Kapton sheets, potential sources of outgassing, were eventually removed and not replaced in an effort to conduct experiments with clean xenon gas. The vacuum chamber was primarily pumped down by a Pfeiffer turbo pump station. Once the pressure became low enough, the ultra high vacuum was maintained by a Varian ion pump. This ion pump also served the purpose of containing the released radioactive ^{137}Cs , instead of exhausting directly to the room like the typical setup of the turbo pump with the diaphragm backing pump. A pair of ultra thin, fast response aluminal and chromal thermocouple wires was used on various occasions to calibrate the temperature of similar sized tantalum foils with respect to the amount of current passed through it. In later experiments, a pair of thermocouple was spot welded directly onto the CsCl foil to get an accurate reading on the foil temperature.

The cylindrical shaped vacuum tank consisted of six Conflat Flange (CF) feedthroughs: two 8 inch flanges found along the two end caps of the cylinder while four 2.75 inch flanges were positioned symmetrically on the sides. Two sets of translators were available to move the foils in a linear manner. A custom made feedthrough including 6 copper wire leads and 3 sets of aluminal and chromal thermocouples was the mean to connect up to 3 sets of separate foils or sodium wire to be heated by the applying current. A Kimball coupler with the Kimball groove

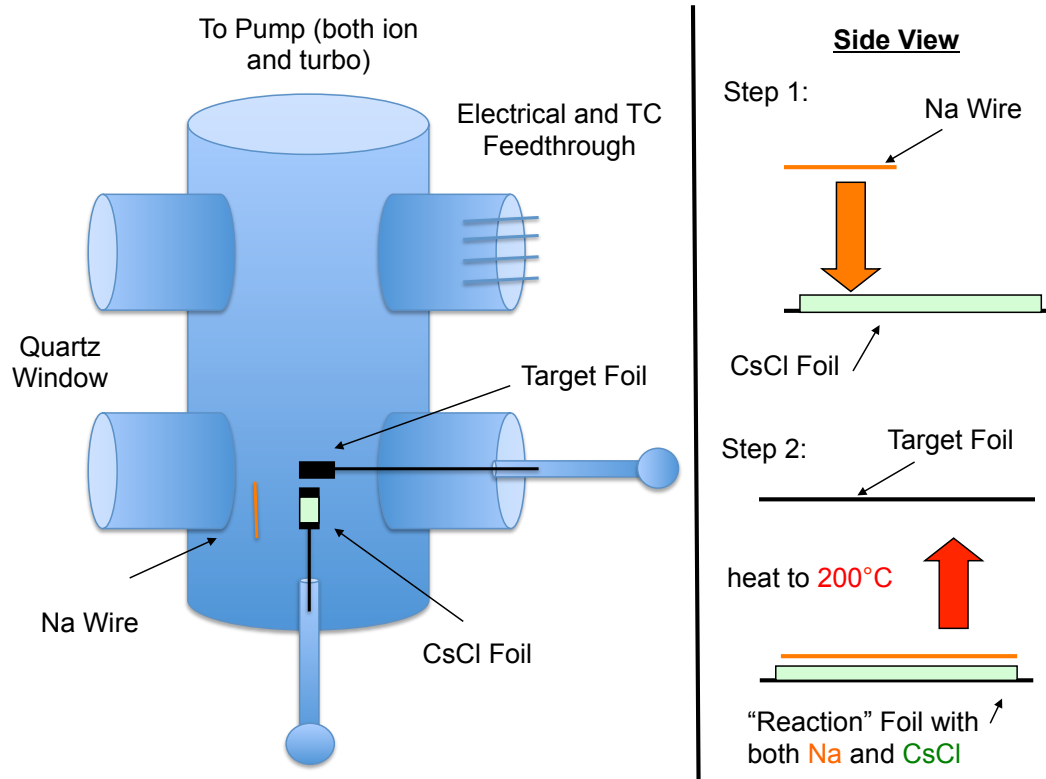


Figure A.2: Schematic of the experimental setup and the steps to chemically produce atomic cesium.

grabber technology was used on one of the 2.75 CF flange to allow for the mounting of a fixed positioned internal component. Tantalum foils were mounted on specially fabricated macor holder, chosen to withstood the high heating temperature, with threaded holes for set screws to hold the tantalum foil lead wires (nickel wire spot welded to the tantalum foils) in place. Internal lead wires were initially insulated with Kapton tape but latter switched to be insulated by alumina beads to minimize outgassing and possible contamination. Due to their lightness, however, Kapton tape was still the insulator used for the super thin fast responding thermocouple wires.

To indicate the presence and the amount of ^{137}Cs , a thallium-doped sodium

iodide detector was used to measure the associated 662 keV gamma emission from the cesium beta decay. The NaI detector was powered by a power supply (Ortec 556 High Voltage Power Supply) set to 1.5 kV. The resulting pulse was then sent to an amplifier (Canberra Spectroscopy Amplifier) which both amplified and reshaped the signal before sending the output to a multichannel analyzer (Ortec TRUMP-PCI-MCA board). A lead brick structures consisting of 10 regular sized lead bricks was used to shield the NaI detector from the external background radiation of the room during the measurement of the foils.

The rigid lead wires and the fragile thermocouple wires on the translator posed problems when the translator was moving. To simplify the task and minimize the failure rate due to lead wire breaking/shortening inside the vacuum chamber, translator use was minimized in practice.

The *reaction foil*, where the reaction took place, started as a CsCl foil mounted on the main translator inside the vacuum chamber. The reaction foil could then be moved to be positioned just opposite the sodium wire for sodium deposition. After a brief outgassing, sodium was directly deposited on the surface of the CsCl foil, which may have some surface contaminants. A second Ta foil (later, target of copper foil for biased test and glass slide for non-biased tests were used) of the same size was mounted on a secondary location away from the Na deposition but reachable by the reaction foil. The reaction foil was then moved to a second position that was roughly 1.5 inch away from the target foil. When the reaction foil was heated at this second position, the target foil was expected to possibly capture some of the evaporated cesium or cesium chloride coming off the the reaction foil. While this

method was quicker to setup and less complicated, the external measurement of the foil requires the breaking of the vacuum when a foil was to be counted.

For each experiment described below (non-radioactive, vacuum, xenon gas), a control experiment was conducted where no sodium was deposited. The goal was to show that the cesium transference from the reaction to the target can only occur with the deposition of sodium when the reaction foil is heated to about 200°C.

A.2.1 Systematic Errors

A couple of systematic errors for this reaction experiment were the amount of reactants (more specifically, the amount of reactants that are deposited in the same location that a reaction is possible) and the geometry (the distance, the solid angle, and the amount obscured by other items inside the vacuum chamber such as the wire leads, thermocouples, etc.). Additionally, the possible chemical effects of the surface contaminants and the contaminants in the xenon gas could not be quantified.

A.2.1.1 Temperature

Temperature of the foil was primarily determined through the measurement of a set of Omega Precision fine gage Aluminal-Chromal (Type K) thermocouple. These thin (0.075 mm wire diameter) wires were designed to be fast responding without disturbing the base temperature of the material which they are measuring. The bared thermocouple wire pairs were insulated by Kapton tapes, except for the

last inch or so by the junction. Integrity of the thermocouple connection could be checked by shining the heavy duty flash light on the foil (even across the quartz window). A noticeable and quick rise in temperature was observed if the thermocouple was installed properly and not shorting out at the feedthrough.

For the majority of the tests, the actual temperature of the radioactive foil was inferred rather than directly measured. A similar sized, non-radioactive foil was used to calibrate the temperature response of the foil relative to the applied heating current. Based on the temperature calibration curves (Figure A.3), the actual radioactive CsCl foil, which does not have the thermocouple attached, was heated to the desired current. Eventually (such as the case for all the tests for xenon gas pressure less than one atmosphere), a set of thermocouple is specially spot weld directly onto the tantalum foil. This step ensures that the temperature of the foil was precise without having to worry about duplicating the same condition (foil size, lead wire connection to the foil, pressure, etc.) for the various tests to that of the temperature calibrations.

Attempts to use an inexpensive IR pyrometer (Traceable® IR thermometer made by Control Company) to measure the foil temperature through a quartz window ultimately failed as the window absorbed too much of the IR given out by the foil despite the high IR transmission through quartz. Even had the quartz window been transparent, the reflectivity of the tantalum foil could also pose a problem to the IR pyrometer. The Traceable IR thermometer did allow the user the freedom to change the emissivity based on the material being measured. For tantalum foil, the emissivity would have to be lowered to 0.05 from the default setting of 0.95 (for

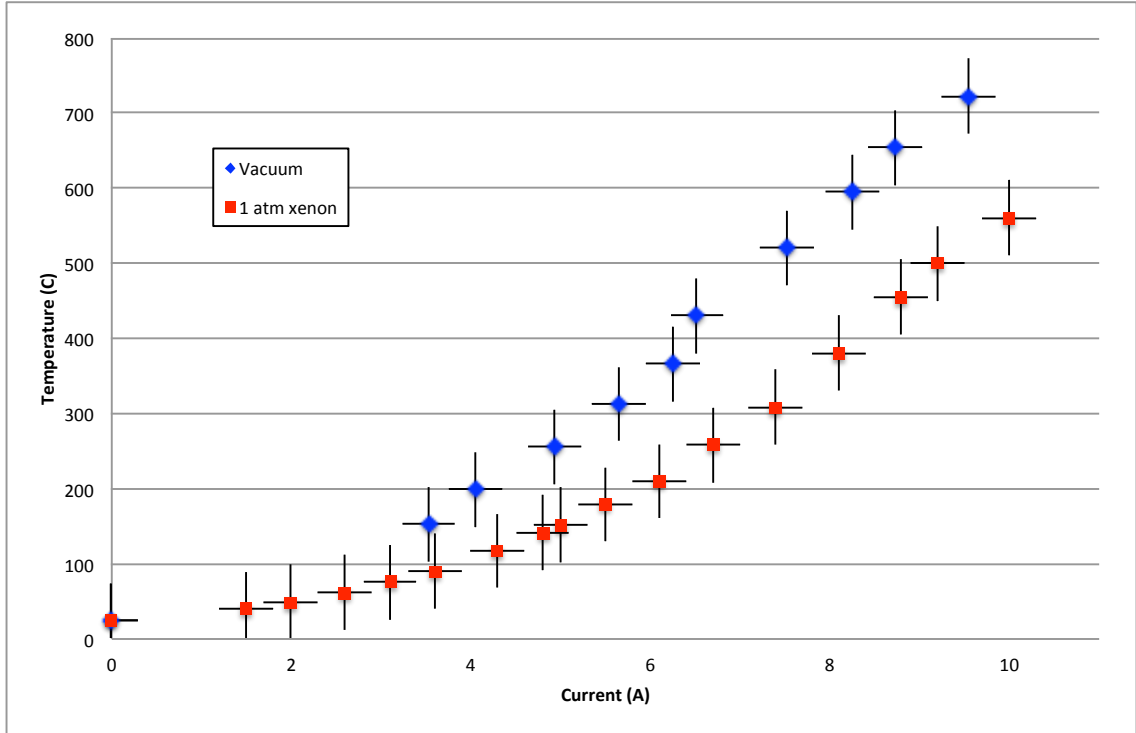


Figure A.3: Calibration curves of the input heating current and the corresponding tantalum foil temperature for both vacuum and 1 atmosphere of xenon gas. The input current is the value measured with an inline Fluke ammeter, rather than the reading on the power supply which is typically lower by 25%.

black coatings).

The amount of inserted xenon gas into the chamber was determined roughly by the analog Swagelok pressure gauge (Part number: PGU-50-PC30-L-4FSE), capable of reading pressures from -30 in Hg to 30 psi. For this pressure gauge at around 0 psig (1 atmosphere), the error on the pressure reading could possibly be off by as much as 5 psi (about 250 Torr). The imprecision in the pressure might have an effect on the temperature calibration. To alleviate the error on the temperature based on the inferred method, thermocouples were spot welded directly onto the foil for better understanding of the temperature in the xenon gas experiments.

A.2.1.2 Internal Geometry

Distance and solid angle (obscuration by lead wires, TC wires, etc.) were not known very well. Most importantly, these changes from run to run making meaningless the determination of efficiency based on the amount of cesium transferred. Between the various target used, larger copper and glass targets were used in the latter experiments to increase the possibility of cesium capturing on the target.

While cares have been taken to ensure that the foils were mounted in the correct position relative to each other and the Na wire, a large source of error came from the lack of precision in the foils distance and positions, as well as the potential obscuring of the foil by lead wires and thermocouples. The thin reaction foil could potentially be folded from the collision with internal vacuum chamber parts. Typically, the distance between the reaction foil and the target was designed to be around 1-2 inch. The geometrical uncertainties, between the deposited coverage of the sodium on the CsCl foil and the relative location of the target to the CsCl foil at reaction position, presented such a large uncertainties that no reasonable efficiency of the reaction can be estimated.

To improve the geometric acceptance of the target, glass microscope slides of dimensions 1 inch by 3 inch were used as targets for the non-biased target tests. This is a 1.3 time increase in the width over the old target (0.75 inch wide) and a more comprehensive coverage in the length side of the target. Since the target needed to be slightly raised to avoid hitting the reaction foil, the glass slide is tilted up at a small angle. With the longer length of the slide, there were a few instances

where the glass slide solid angle coverage was improved but the distance between the target and the reaction foil had in fact increased by roughly 50%.

A.2.1.3 Chemical Contamination

External counting method required that the reaction foil, often already with both CsCl and Na deposited on the surface already, be exposed to air. During the long hiatuses between experiments, the foils were merely kept in a cool environment rather than a dessicator that can ensure dryness. Sodium, for example, is known to react with water.

The SAES sodium wires came packaged in a vacuum sealed can. After opening the can, the sodium wires were stored without a dessicator. The first set of sodium wires used were also past the listed expiration date. Compare to the new batch of the same SAES sodium wire, a clearly highly activation current (9A as opposed to the listed 6A) as well as smaller yield was clearly evident for the old set of wires.

Set of test between November 2010 until February 2011, when the xenon was recovered, post-test xenon gas purity study via the cold trap spectrometer method [88] indicated that the xenon gas had been contaminated (40 ppm O₂, 125 ppm N₂). The initial xenon purity was 20 parts-per-billion (ppb) N₂ and an unmeasurable amount of O₂. This contamination could have been made during the xenon recovery process, where cryopumping is known to possibly open up a leak on the recovery bottle valve (particularly when the bottle was made of aluminum). Another possibility may be that the xenon is seriously contaminated by the outgassing of the

Kapton electrical wire insulation, particularly the long duration heating to 550°C in 1 atmosphere of xenon. In early test when Kapton tapes were used as the electrical insulation of the lead wires, noticeably blackened Kapton tape could be observed when $\sim 8\text{A}$ of current was applied. It was unknown whether this “burning” of the Kapton tape caused deposition onto the reaction foil.

While the spot welding done to attach the tantalum foils to nickel leads were done prior to the deposition of the CsCl, additional spot welds were required to repair the nickel lead as well as to add a aluminal-chromal (type K) thermocouple onto the foil. With the spot welding taking place on the edge of the foil, while the ^{137}Cs deposits were located in the center of the foil, the chemical contamination concern from the brief heating of the foil during the spot-weld were minimal. Only about 2 joules of energy was expected to be dumped uniformly on the Tantalum foil (about 0.08g of Tantalum), corresponding to a calculated temperature rise of only about 80°C. Nevertheless, the actual spot welding process did cause the spot welder tip to come in contact with the cesium chloride. On a few occasions, a small but detectable amount of radioactivity was transferred to the spot welder tip.

A.3 Results

A.3.1 Non-radioactive Test

A non-radioactive CsCl with Na reaction was conducted first. Three foils were sent for surface analysis by X-ray Photoelectron Spectroscopy (XPS) which determines the elemental surface composition of the foils. Since the foils were exposed to

air for days, plenty of contaminants, such as C and O, were both expected and found by XPS. The elements of interest, Cs and Cl, are usually not a part of the surface contaminants. Figure A.4 shows the results of the XPS of the three samples. With the XPS procedure having different sensitivity to different elements (a property of the differences in the work functions), the relative ratio of the different elements on a sample is not as important as how the relative percentage of the same element changed across the different samples. The summary table showed that the beside the abundance of the usual surface contaminants, cesium was only observed in the reaction foil, as expected, and the target foil. The control for this measurement was a blank tantalum foil that showed no measurable amount of cesium. Additionally, chlorine was only observed in the reaction foil but not the target foil or the blank foil. Interestingly a trace amount of sodium was found in all three foils, with significantly more in the reaction foil as expected. The actual relative percent composition number is not useful, as it is dominated by the surface contamination (carbon and oxygen).

A.3.2 Vacuum Test

With the radioactive cesium chloride, the first experiments were done in vacuum. After pumping down with the turbo pump to 10^{-5} Torr, the ion pump was turned on to transform the vacuum chamber into a closed system. A vacuum of at least $5 \cdot 10^{-7}$ Torr was achieved by the ion pump alone at this point. As indicated in Fig A.5, essentially the 662 keV gamma peak was only observed on the target foils

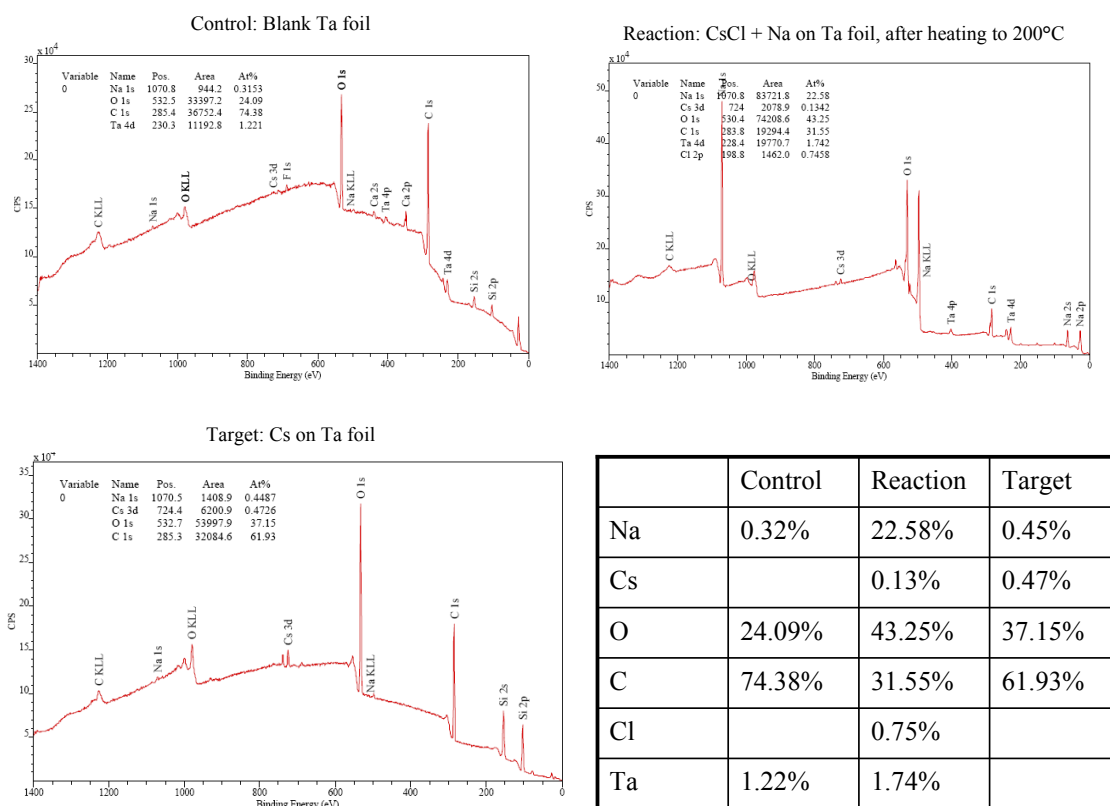


Figure A.4: X-ray Photoelectron Spectroscopy results for Control Foil (upper left), Reaction Foil (upper right), Target Foil (lower left), with a summary chart (lower right).

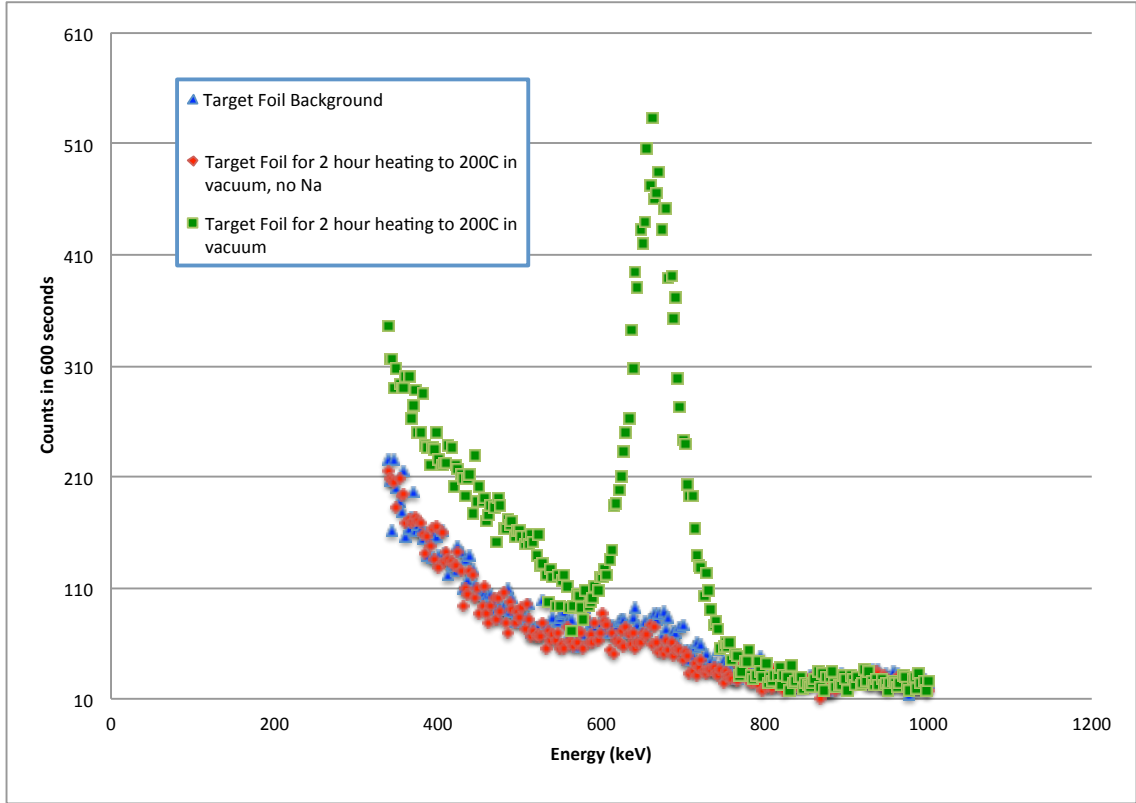


Figure A.5: Target foil measurements by a NaI detector for the background (blue), after 2 hour of 200°C heating in vacuum without Na deposition (red), and 2 hour of 200°C heating in vacuum with Na (green). The counting time was 10 minutes and the energy calibration was done with based on the CsCl foil spectrum.

when sodium has been deposited to the CsCl foil that was heated to about 200°C for 5 minutes. Additionally, the 662 keV peak became more prominent (higher activity) for the case when the target foil had been exposed to some additional cesium from the same reaction in an additional round of heating (up to 110 minutes). This result demonstrated that the reaction did not occur all at once, and the reaction foil could be used to produce cesium in at least two different times. It should be noted that the reaction foil, containing both CsCl and Na, was still capable of producing more cesium after being exposed to air, after the target foil had been extracted and externally measured by the NaI detector.

A.3.3 1 Atmosphere of Xenon Test

Since the heating of the reaction tantalum foil was done by resistive heating, the presence of the xenon gas lower the achievable temperature by the cooling of the xenon gas. The relatively low temperature of 200°C necessary to start the reaction was still easily achievable. Furthermore, this limited the possibility of accidental overheating to the necessary 550°C for the CsCl to evaporate. The xenon gas pressure was determined by an analog rough pressure gauge and the 760 Torr achieved is only known to within 200 Torr.

From the xenon system capable of doing sensitive mass spectroscopy by using a cold trap [88], xenon of purity <20 part-per-billion nitrogen (better than two times factory bottle xenon) was obtained to inject into the vacuum chamber. The xenon was recovered back via cryopumping into a bottle after several tests, and the recovered xenon purity showed purity as bad as >1 parts-per-million nitrogen. Care was taken to minimize the xenon purity contamination by switching the wire electrical insulation from kapton tape to alumina bead, burning a tungsten wire to clean up the oxygen [89], and simplifying the plumbing by not recovering the xenon. Target foil was biased at -100V to increase its attraction to the potentially positively ionized Cs ion that might be formed from the reaction. No ^{137}Cs spectrum was observed on the target. Following the negative result, a follow up vacuum test was performed as a control to determine that the reaction should have been viable.

Indicated in Figure A.7, no ^{137}Cs spectrum was found on the target for the one atmosphere xenon gas. Repeated experiments aimed to improve the tempera-

ture (thermocouple added directly to the reaction foil), xenon purity (by burning a tungsten filament for 12 hours or more), target (both geometrically and by biased the target electrically to -100V), and the combination of these improvements did not ever lead to a positive observation on the target. However, heating a foil to $>600^{\circ}\text{C}$ was found to be capable to moving the ^{137}Cs (probably in the form of CsCl) across to the (unbiased) target foil in an atmosphere of xenon gas.

The much lower amount of ^{137}Cs transference to the target, in the follow up vacuum test to an unsuccessful xenon gas heating, hinted at the occurrence of a reaction on the surface of the reaction foil. One possible explanation may be that the xenon gas suppress the sublimation of the Cs into gas. Additional deposition of sodium onto these gas heated reaction foil had not shown the ability to transfer ^{137}Cs in vacuum heating (despite a still overwhelming presence of ^{137}Cs on the foil as measured by the NaI counter). The crude set up of this experiment cannot differentiate between whether the presence of ^{137}Cs on the reaction foil was still in form of CsCl or another Cs compound (if not atomic Cs itself).

A.3.4 50 Torr Test

With the failure to detect ^{137}Cs in the target foil for the 1 atmosphere test, further tests with an intermediate pressure between one atmosphere and vacuum were performed. 50 Torr was chosen as it was the last pressure reading before vacuum on the pressure gauge. Given the constraint of reusing of CsCl foils, foil histories had to be considered for all the 50 torr xenon gas tests. A positive vacuum

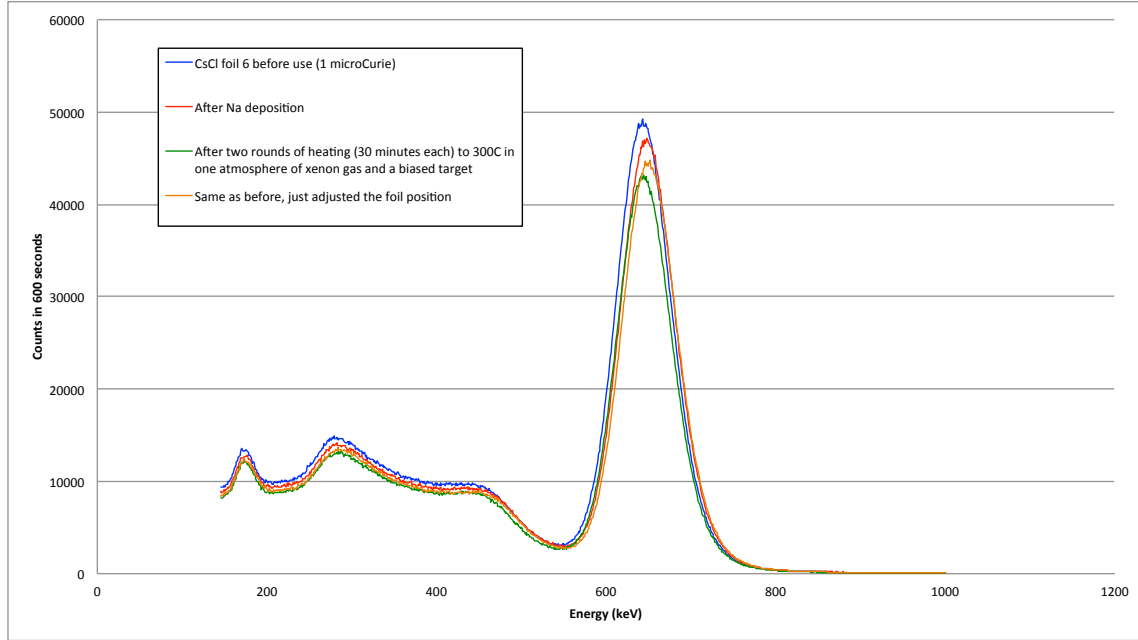


Figure A.6: CsCl foil 6 spectrums over its history - before usage, after Na deposition, after two rounds of heating for a total of 1 hour of heating in 1 atmosphere of (dirty?) xenon gas. Foil activity dropped by 8-10% over its history, even though its target did not pick up detectable amount of radioactivity.

test results after the low pressure xenon gas heating was the control test for the result to be meaningful. In many cases, the vacuum control test did not result in the movement of the radioactivity. Either the foil was not going to react or the foil had already reacted causing the ^{137}Cs to be in a different form of cesium than the original cesium chloride.

The only successful transfer of cesium was the 300°C heating trial where a the glass slide (non-biased but good solid angle coverage) was less than 0.5 cm away from the reaction foil to the point when it might even be touching. However, cesium was positively identified to be deposited on the glass slide as opposed to just a small casual cesium contamination from radioactive macor dust. A repeat experiment with the target being further away (greater than 3 cm away) showed a negative

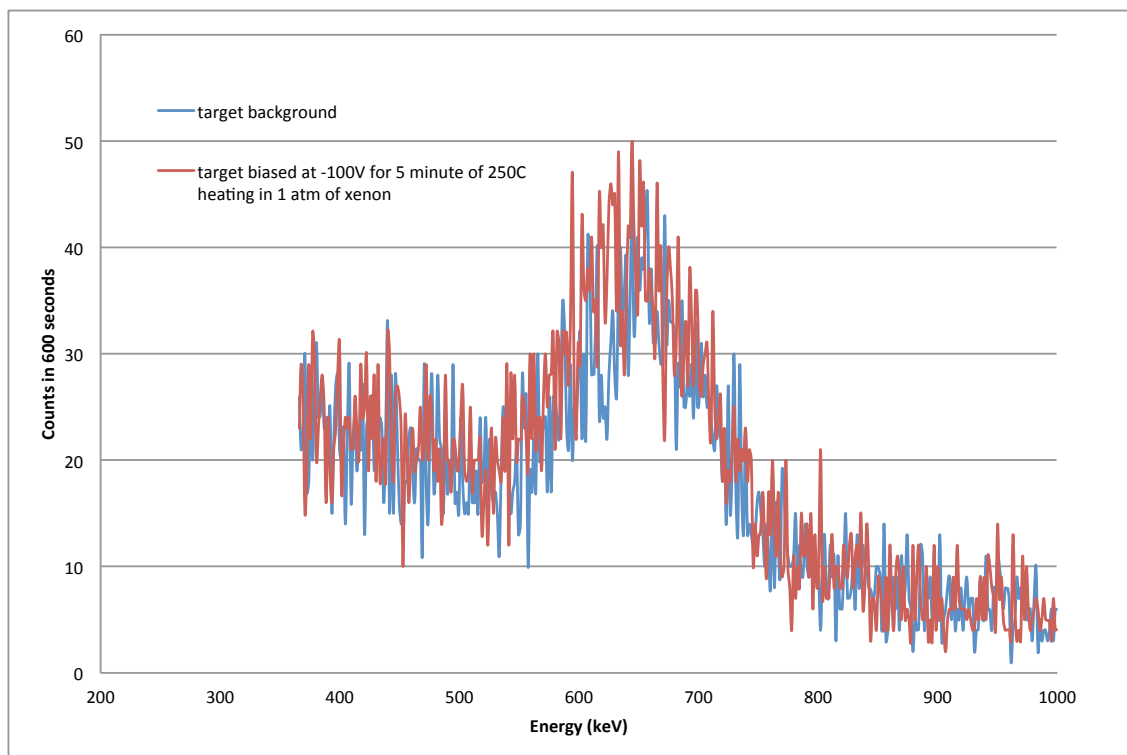


Figure A.7: Target foil measurements by a NaI detector for the copper target background (blue) and after it served as a biased (-100V) target for 5 minutes of 250°C heating of CsCl and Na in 1 atmosphere of xenon gas. The xenon gas had been “cleaned” by burning a tungsten wire in an adjacent elbow for 29 hours. The counting time was 10 minutes and the energy calibration was done with based on the CsCl foil spectrum.

result.

A.3.4.1 Interpretations of Results

Using the standard assumption about ideal gas law, the mean free path of the cesium (atomic diameter of 5.2 angstroms) in one atmosphere at room temperature (300K) is 0.03 micron. Even when the pressure is lowered to 50 torr, the mean free path only improved to 0.5 micron long. By comparison in a mediocre vacuum of 10^{-6} torr, the mean free path is greater than 2.5 meter long. Interaction between the cesium atom and the xenon gas may have caused the cesium to switch direction and stick back on the reaction foil.

If this was indeed the cause and that cesium was isolated during the extended xenon gas heating, then the reaction would have been exhausted from the gas heatings. This hypothesis would explain why some of the vacuum control check also came back negative since all the plausible reaction had already occurred.

A.3.4.2 Foil Resurrections

After all of the foils had been used, further tests were done on the same foils. Redeposition of the sodium was the attempt to either cover part of the CsCl which did not come in contact with sodium in the first sodium deposition or provide fresh sodium in the case that the deposited sodium had chemically reacted with air over time.

The inability for the foils to transfer radioactivity even in vacuum for the

future tests may either indicate that the prolonged (on the scale of over an year) exposure to air have caused some unwanted (but not very surprising) side reaction to have occurred on the foils. The only successful vacuum tests among the resurrected foil experiments required a higher heating temperature (at least 300°C) than before. This difference is either due to a different chemical reaction or more kinetic energy needed for the cesium atom to escape from being produced few atomic layers below the surface.

A.4 Conclusions

The ^{137}Cs as single-ion barium source has some unique advantages. The chemical reaction to isolate atomic cesium from CsCl by heating with Na to 200°C has been shown to work in vacuum from both the XPS method for the non-radioactive test and the detection of the 662 keV gamma by a NaI detector. Reaction efficiency cannot really be determined since the crude setup did not allow a very good check of the sodium deposition coverage to figure out the expected yield.

For the reaction in 1 atm of xenon gas, extremely little to no radioactivity was transferred to the target foil. Even when using xenon gas with extremely good purity (minimizing the presence of O_2) and the usage of a DC bias (-100V) on the target, radioactive cesium was still not observed on the target. When the reaction foil was heat to >600°C, radioactive CsCl (presumably) was found to transverse through the xenon gas to the target. The lack of success of the cesium isolation reaction in xenon gas does significantly limit the potential effectiveness of this type

of source for EXO barium tagging development.

The single successful cesium transfer for the 50 Torr of xenon gas came when the reaction foil was heat to greater than 300°C (but well below 550°C to transfer CsCl) and the target foil being extremely close to the reaction foil (perhaps even coming in contact). Since this test was done with a CsCl foil that has had sodium deposited and heated for an extended period in dirty xenon gas, it cannot be completely ruled out that the cesium had formed some other type of compound or a different chemical reaction than the one desired had occurred at 300°C to cause the transfer of something other than atomic ^{137}Cs .

The ability for the foil to still react and produce cesium despite having been exposed to air mean that the ^{137}Cs source can potentially be made quite compact. Rather than having an extra set of electrical feedthrough to deposit fresh sodium onto the CsCl foil, the sodium deposition can conceivably be done before the ^{137}Cs source is inserted into a system.

If the resultants from the reaction are cesium ions as opposed to just neutral cesium atoms, a time of flight measurements of the product can determine the fraction of possible contaminants as well as the potentially molecular cesium chloride that are ejected from the reaction. Additionally, this measurements (which is limited to only being able to be performed in vacuum) can also measure the ionization state (+ or ++) of the resultant cesium from the reaction.

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