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*Facilis descensus Averni;
Noctes atque dies patet atri janua Ditis;
Sed revocare gradum, superasque evadere ad auras,
Hoc opus, hic labor est.* Virgil (from Don's thesis!)

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A BU THESIS LATEX TEMPLATE

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ABSTRACT

Have you ever wondered why this is called an *abstract*? Weird thing is that its legal to cite the abstract of a dissertation alone, apart from the rest of the manuscript.

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List of Abbreviations

As per BU library instructions, the list of abbreviations must be in alphabetical order by the **abbreviation**, not by the explanation, or it will be returned to you for re-ordering. **This comment must be removed in the final document.**

CAD	Computer-Aided Design
CO	Cytochrome Oxidase
DOG	Difference Of Gaussian (distributions)
FWHM	Full-Width at Half Maximum
LGN	Lateral Geniculate Nucleus
ODC	Ocular Dominance Column
PDF	Probability Distribution Function
\mathbb{R}^2	the Real plane

Chapter 1

Theory of $0\nu\beta\beta$, Neutrinoless Double-Beta Decay

1.1 Neutrinos in the Standard Model

Neutrinos remain the least understood component of the Standard Model (SM) of Particle Physics[24]. Their elusive nature and extremely weak interactions make them challenging to study, yet they play a crucial role in both particle physics and cosmology. The story of the neutrino began in 1914, when James Chadwick used magnetic spectrometry to resolve the continuous energy spectrum of beta decay, revealing an apparent violation of energy conservation.

To resolve this, Wolfgang Pauli postulated in 1930 the existence of a neutral, light particle that carried away the missing energy[30]. He announced this in his famous letter to the "Radioactive Ladies and Gentlemen." Enrico Fermi later named this particle the "neutrino" ("little neutral one") and incorporated it into his theory of beta decay. The neutrino was finally detected in 1956 by Cowan and Reines[12], confirming its existence. Since then, the SM has been extended to include three flavors of neutrinos, each associated with a charged lepton.

The Standard Model is a gauge theory based on the symmetry group $SU(3)_C \times SU(2)_L \times U(1)_Y$ [24]. Neutrinos participate only in the weak interaction, mediated by the W^\pm and Z^0 bosons, and are electrically neutral. Their extremely small cross-sections make them difficult to detect, but also allow them to traverse vast distances

unimpeded, making them unique cosmic messengers.

1.1.1 Neutrino Interactions

The SM unifies the strong, weak, and electromagnetic interactions under the $SU(3)_C \times SU(2)_L \times U(1)_Y$ gauge symmetry. The $SU(2)_L \times U(1)_Y$ sector describes the electroweak interaction, with the W^\pm and Z^0 bosons mediating the weak force. Neutrinos are part of the left-handed lepton doublets, transforming as weak isospin doublets under $SU(2)_L$:

$$L_\ell = \begin{pmatrix} \nu_{\ell L} \\ \ell_L \end{pmatrix}, \quad \ell = e, \mu, \tau \quad (1.1)$$

where $\nu_{\ell L}$ and ℓ_L are the left-handed neutrino and charged lepton fields, respectively. The left-handed projection operator is $P_L = \frac{1-\gamma_5}{2}$, with $\gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3$ built from the Dirac matrices.

The electroweak quantum numbers are **weak isospin** I and **weak hypercharge** Y . The electric charge operator is:

$$Q = I_3 + \frac{Y}{2} \quad (1.2)$$

where I_3 is the third component of isospin. For the lepton doublet, $I = 1/2$, $Y = -1$, so $Q(\nu_{\ell L}) = 0$ and $Q(\ell_L) = -1$.

			I	I_3	Y	Q
lepton doublet	$L_L \equiv$	$\begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix}$	1/2	1/2	-1	0
lepton singlet	e_R		1/2	-1/2	-1	-1
quark doublet	$Q_L \equiv$	$\begin{pmatrix} u_L \\ d_L \end{pmatrix}$	1/2	1/2	1/3	2/3
quark singlets	u_R		1/2	-1/2	1/3	-1/3
	d_R		0	0	4/3	2/3
			0	0	-2/3	-1/3

Table 1.1: Eigenvalues of the weak isospin I , of its third component I_3 , of the hypercharge Y , and of the charge $Q = I_3 + Y/2$ of the fermion doublets and singlets.

The neutrino components of lepton doublets are called "active" neutrinos, in contrast to hypothetical sterile neutrinos. Right-handed fermions are singlets under $SU(2)_L$ and do not participate in weak interactions. The SM contains one active neutrino per charged lepton (e, μ, τ).

$SU(2)_L$ gauge invariance dictates the form of the weak charged current (CC) and neutral current (NC) interactions:

$$-\mathcal{L}_{\text{CC}} = \frac{g}{\sqrt{2}} \sum_{\ell} \bar{\nu}_{\ell L} \gamma^{\mu} \ell_L W_{\mu}^{+} + \text{h.c.} \quad (1.3)$$

$$-\mathcal{L}_{\text{NC}} = \frac{g}{2 \cos \theta_W} \sum_{\ell} \bar{\nu}_{\ell L} \gamma^{\mu} \nu_{\ell L} Z_{\mu}^0 \quad (1.4)$$

where g is the weak coupling constant and θ_W is the Weinberg angle. The Z^0 decay width into neutrinos constrains the number of light, active neutrinos to $N_{\nu} = 2.984 \pm 0.008$ [24], consistent with three generations.

1.1.2 Fermion Masses in the Standard Model

In the SM, fermion masses arise from Yukawa couplings to the Higgs doublet Φ :

$$-\mathcal{L}_{\text{Yukawa,lep}} = Y_{ij}^{\ell} \bar{L}_{Li} \Phi E_{Rj} + \text{h.c.} \quad (1.5)$$

After spontaneous symmetry breaking ($\langle \Phi \rangle = (0, v/\sqrt{2})^T$), this yields charged lepton masses:

$$m_{ij}^{\ell} = Y_{ij}^{\ell} \frac{v}{\sqrt{2}} \quad (1.6)$$

where $v \approx 246$ GeV is the Higgs vacuum expectation value. In the absence of right-handed neutrinos, no analogous Yukawa term exists for neutrinos, so they are massless at tree level in the SM.

1.2 Neutrino Mass

The discovery of neutrino oscillations[1] demonstrates that neutrinos have nonzero masses and that flavor eigenstates are mixtures of mass eigenstates. The exact mechanism by which neutrinos acquire mass is unknown. Several extensions to the SM have been proposed, as discussed below.

Here we follow the derivation in [17]. Landau, Lee and Yang, and Salam showed that a massless fermion can be described by a chiral field via their two-component theory of massless neutrinos. Let us begin that derivation with the Dirac Equation:

$$(i\gamma^\mu \partial_\mu - m)\psi = 0 \quad (1.7)$$

given a fermion field, $\psi = \psi_L + \psi_R$, the Dirac equation is equivalent to the system of equations:

$$i\gamma^\mu \partial_\mu \psi_L = m\psi_R \quad (1.8)$$

$$i\gamma^\mu \partial_\mu \psi_R = m\psi_L \quad (1.9)$$

for the chiral fields, ψ_L and ψ_R , whose space-time evolutions are coupled by the mass m .

If the fermion is massless, the two equations, 1.8 and 1.9, are decoupled:

$$i\gamma^\mu \partial_\mu \psi_L = 0 \quad (1.10)$$

$$i\gamma^\mu \partial_\mu \psi_R = 0 \quad (1.11)$$

Thus, a massless fermion can be completely described by a single chiral field (either left-handed or right-handed) which has only two independent components. The equations, 1.8 and 1.9 are known as the Weyl equations and the spinors ψ_L and ψ_R are the Weyl spinors.

The simplest form of the SM incorporates what is known as the two-component theory of massless neutrinos. Whereby the neutrino is entirely described by the left-handed Weyl spinor which participates in the weak interaction, ν_L , and there are no ν_R fields.

1.2.1 Dirac Masses

If right-handed neutrino fields ν_R exist, a Dirac mass term, just like the one for the charged leptons, can be written:

$$-\mathcal{L}_{\text{Dirac}} = Y_{ij}^\nu \bar{L}_{Li} \tilde{\Phi} \nu_{Rj} + \text{h.c.} \quad (1.12)$$

where $\tilde{\Phi} = i\sigma_2 \Phi^*$. This yields Dirac masses $m_{ij}^\nu = Y_{ij}^\nu v / \sqrt{2}$. However, the tiny observed neutrino masses ($m_\nu < 1$ eV) would require $Y_{ij}^\nu < 10^{-12}$. The huge discrepancy between the neutrino masses and the other fermions imply the existence of some underlying mechanism which suppresses the neutrino masses. In the absence of such explanation, the light neutrino masses bring up a naturalness problem. Many neutrino mass models have been proposed that produce light neutrino masses via a more natural mechanism.

1.2.2 Majorana Neutrino Mass

Since neutrinos have indeed been shown to have mass, the two-component theory is insufficient. In 1937, Ettore Majorana proposed a new solution to the Dirac equation. His insight was that a massive fermion could be described with a single spinor instead of the two, $\psi = \psi_L + \psi_R$. Majorana made the assumption that the two spinors are not independent, but rather:

$$\psi_R = C \bar{\psi}_L^T \quad (1.13)$$

where C is the charge conjugation operator. By observing that C and the left-handed projection operator P_L have the following relationship,

$$P_L(C\psi_L^T) = 0 \quad (1.14)$$

one can clearly see that $C\psi_L^T$ is a right-handed field. Charge conjugating a left-handed Weyl spinor converts the spinor to its right-handed form. Modifying the Dirac equation, we now obtain the Majorana equation for the chiral field:

$$i\gamma^\mu \partial_\mu \psi = m\psi^C \quad (1.15)$$

ψ^C represents the charge conjugated Majorana field. This implies that, $\psi = \psi_L + \psi_L^C$, which finally leads to the Majorana relation:

$$\psi = \psi^C \quad (1.16)$$

Equation 1.16 implies that the particle ψ is its own antiparticle. Since neutrinos interact only through weak interactions, and are electrically neutral, the charge parity of the neutrino field has no physical meaning and can be chosen arbitrarily. Among the elementary fermions, only the neutrinos are neutral and have the potential to be Majorana particles.

Should the neutrino be Majorana, the neutrino and antineutrino would only be distinguishable by their helicities. It is customary to refer to negative helicity neutrinos as "neutrinos" and positive helicity neutrinos as "antineutrinos".

With majorana neutrinos, the simplest mass term one could construct with SM fields and respecting SM symmetries is the lepton number violating term:

$$\mathcal{L}_5 = \frac{Z_{ij}^\nu}{\Lambda} (\bar{L}_L^i \bar{\Phi})(\bar{\Phi}^T L_L^j) + h.c. \quad (1.17)$$

Here, Z_{ij}^ν is a 3x3 matrix which controls the mixing between the neutrino masses for each flavor combination, along with the Yukawa coupling strengths. Finally, Λ is the high energy scale at which we should expect new physics, which suppresses the neutrino masses. This lagrangian extension generates the Majorana neutrino mass term:

$$\mathcal{L}_{M_\nu} = \frac{Z_{ij}^\nu}{2} \frac{v^2}{\Lambda} \bar{\nu}_{L_i} \nu_{L_j}^C + h.c. \quad (1.18)$$

With the majorana neutrino mass matrix:

$$\mathcal{M}_\nu = Z_{ij}^\nu \frac{v^2}{\Lambda} \quad (1.19)$$

Comparing the effective lagrangian, equation 1.17, to the charged lepton mass terms, equation 1.5, our new effective Lagrangian term has two Higgs fields to couple to the extra L_L field. This raises the dimension of this operator to 5, rendering the term non-renormalizable while following the SM gauge transformations. This term hints at new physics beyond the Standard Model at the mass scale Λ . Also, note that this term is the only possible dimension-5 Lagrangian term to generate neutrino mass. The new physics mass scale, Λ , suppresses the neutrino masses by $\frac{v^2}{\Lambda}$. This suppression of the neutrino masses has the same structure as the masses produced by the seesaw mechanism that will be discussed in the next section.

1.2.3 Seesaw Mechanism

We will now discuss one interesting extension of the Standard Model which produces light active neutrinos, the addition of one or more heavy sterile neutrinos. Adding m new sterile neutrinos, ν_{si} ($i = 1, \dots, m$), leads to two types of mass terms.

$$-\mathcal{L}_{M_\nu} = M_{D_{ij}} \bar{\nu}_{si} \nu_{L_j} + \frac{1}{2} M_{N_{ij}} \bar{\nu}_{si} \nu_{sj}^C + h.c. \quad (1.20)$$

Here, M_D is a complex matrix of dimension $m \times 3$ and M_N is a symmetric $m \times m$ matrix.

The first term is often referred to as a Dirac mass term, after spontaneous symmetry breaking, the neutrinos acquire a mass through Yukawa couplings, similar to the charged fermions and as discussed in an earlier section.

$$Y_{ij}^\nu \bar{\nu}_{si} \tilde{\phi}^\dagger L_{Lj} \Rightarrow M_{D_{ij}} = Y_{ij}^\nu \frac{v}{\sqrt{2}}, \quad (1.21)$$

The second term is a lepton number violating Majorana mass term.

Eq. 1.20 can be rewritten as:

$$-\mathcal{L}_{M_\nu} = \frac{1}{2} (\bar{\nu}_L \quad \bar{\nu}_s) \begin{pmatrix} 0 & M_D^T \\ M_D & M_N \end{pmatrix} \begin{pmatrix} \nu_L^c \\ \nu_s^c \end{pmatrix} + \text{h.c.} \equiv \bar{\nu} M_\nu \nu + \text{h.c.} \quad (1.22)$$

where $\vec{\nu} = (\bar{\nu}_L, \bar{\nu}_s^c)^T$ is a $(3+m)$ -dimensional vector. The matrix M_ν is complex and symmetric, and can be diagonalized producing mass eigenstates:

$$(V^\nu)^T M_\nu V^\nu = \text{diag}(m_1, m_2, \dots, M_{3+m}) \quad (1.23)$$

$$\vec{\nu}_{\text{mass}} = (V^\nu)^\dagger \vec{\nu} \quad (1.24)$$

Eq. 1.22 can be rewritten in terms of the mass eigenstates:

$$-\mathcal{L}_{M_\nu} = \frac{1}{2} \sum_{k=1}^{3+m} m_k (\bar{\nu}_{\text{mass},k}^c \nu_{\text{mass},k} + \bar{\nu}_{\text{mass},k} \nu_{\text{mass},k}^c) \quad (1.25)$$

$$= \frac{1}{2} \sum_{k=1}^{3+m} m_k \bar{\nu}_{Mk} \nu_{Mk}, \quad (1.26)$$

where $\nu_{Mk} = \nu_{\text{mass},k} + \nu_{\text{mass},k}^c$. Thus, the Majorana condition is satisfied, $\nu_M = \nu_M^c$, and are referred to as Majorana neutrinos.

In this new neutrino mass basis, the original weak-interacting neutrino fields are:

$$\nu_{Li} = P_L \sum_{j=1}^{3+m} V_{ij}^\nu \nu_{M_j}, \quad i = 1, 2, 3 \quad (1.27)$$

In the specific case, where the M_N mass eigenvalues are much higher than the scale of electroweak symmetry breaking, v , the diagonalization of M_ν leads to three light neutrinos, ν_l , and m heavy neutrinos N :

$$-\mathcal{L}_{M_\nu} = \frac{1}{2} \bar{\nu}_l M^l \nu_l + \frac{1}{2} \bar{N} M^h N \quad (1.28)$$

where

$$M^l \simeq -V_l^T M_D^T M_N^{-1} M_D V_l, \quad (1.29)$$

$$M^h \simeq V_h^T M_N V_h, \quad (1.30)$$

$$V^\nu \simeq \begin{bmatrix} \left(1 - \frac{1}{2} M_D^\dagger M_N^{*-1} M_N^{-1} M_D\right) V_l & M_D^\dagger M_N^{*-1} V_h \\ -M_N^{-1} M_D V_l & \left(1 - \frac{1}{2} M_N^{-1} M_D M_D^\dagger M_N^{*-1}\right) V_h \end{bmatrix}, \quad (1.31)$$

where V_l and V_h are 3×3 and $m \times m$ matrices respectively that parameterize neutrino mixing between the light nad heavy states. V_l could be thought of as the PMNS, Pontecorve-Maki-Nakagawa-Sakata, matrix which we will discuss in a later section in more detail. We can see that the heavier mass states are proportional to M_N , while the lighter mass states are proportional to M_N^{-1} . This behavior is where the seesaw mechanism gets its name. This seesaw mechanism is of Type I specifically, where new sterile neutrinos are added. The seesaw mechanism also produces heavy states that are mostly right-handed, while the light states are mostly left-handed.

Thus, the Type I seesaw mechanism is a promising extension to the SM that produces light, weakly interacting, left-handed neutrinos and heavy, sterile, right-handed neutrinos, while providing a more natural suppression of the active neutrino masses.

Not to mention that these heavy, right-handed steriles could also be candidates for dark matter.

1.2.4 Lepton Number Violation and Leptogenesis

A key consequence of Majorana neutrinos is lepton number violation. Lepton number violation is what is known as an accidental global symmetry in the Standard Model. Where the symmetry is not enforced when constructing the model, but comes about simply because no terms that violate it were included. Many beyond the Standard Model theories include lepton number violation.

Lepton number violation also plays a key role in leptogenesis. Leptogenesis is a proposed solution to one of the most fundamental questions in elementary physics: Why is there more matter than antimatter?

A thorough review of the phenomenology of matter-antimatter asymmetry is beyond the scope of this chapter. In lieu of that, here is a highly condensed description of the matter-antimatter asymmetry of our universe.

The value of the baryon asymmetry of the Universe is inferred from two independent observations. The first is of the abundances of light elements, D , 3He , 4He , and 7Li , after big bang nucleosynthesis. These abundances depend on the asymmetry parameter, η , measured to be [13]:

$$\eta^{BBN} \equiv \frac{n_B - n_{\bar{B}}}{n_\gamma}|_0 = 4.7 - 6.5 \times 10^{-10} \quad (1.32)$$

The second observation is of the cosmic microwave background (CMB) anisotropies [20]. A key CMB observable is c_s , the speed of sound in the photon-baryon fluid. Measuring the temperature fluctuations in the CMB constrain the baryon energy density, ρ_B , which is related to η by:

$$\Omega_B = \frac{\rho_B}{\rho_{crit}} \quad (1.33)$$

$$\eta^{CMB} = 2.74 \times 10^{-8} \Omega_B h^2 = 6.1_{-0.2}^{+0.3} \times 10^{-10} \quad (1.34)$$

where $h = H_0/100 \text{ km s}^{-1} \text{ Mpc}^{-1} = 0.682 \pm 0.0028$ is the present Hubble parameter[2]. The impressive consistency between the nucleosynthesis and CMB constraints on the baryon density of the Universe is a triumph of hot big-bang cosmology.

Sakharov outlined three conditions for generating a dynamic baryon asymmetry, now referred to as the Sakharov conditions.

1. Baryon number violation
2. C and CP violation
3. Out of equilibrium dynamics

While the Standard Model features all three ingredients, no SM mechanism generates a large enough baryon asymmetry. Leptogenesis is a beyond the Standard Model theory that introduces the previously discussed singlet neutrinos. Along with new sphaleron processes that can convert lepton number violation into baryon number violation, The Type I seesaw sterile neutrions play a pivotal role in Leptogenesis.

1.2.5 Neutrino Mass Hierarchy

We've discussed open questions relating to neutrino nature; whether they are dirac or majorana, what is the absolute neutrino mass scale, and their potential role in resolving matter-antimatter asymmetry in the Universe. Another open question has to do with the relative ordering of the light neutrino masses.

In the simplified 2-flavor case, the probability of a neutrino "surviving" or being observed in the flavor state in which it was produced, is:

$$P(\nu_e \rightarrow \nu_e) = 1 - \frac{1}{2} \sin^2 2\theta_{12} \sin^2 \left(\frac{\delta m_{21}^2}{4E} L \right) \quad (1.35)$$

Note that while the survival probability or one minus the oscillation probability is dependent on the absolute value of the squared-mass difference, $\delta m_{ij}^2 = m_i^2 - m_j^2$, it is insensitive to its' sign. Solar neutrino oscillation experiments have measured the following squared- mass difference:

$$\delta m_{21}^2 = \delta m_{sol}^2 \approx 7.39_{-0.20}^{+0.21} \times 10^{-5} eV^2 \quad (1.36)$$

while observation of atmospheric oscillation data results in:

$$|\delta m_{13}^2| = |\delta m_{23}^2| = \delta m_{atm}^2 \approx 2.449_{-0.030}^{+0.032} \times 10^{-3} eV^2 \quad (1.37)$$

As mentioned previously, oscillation experiments demonstrated that neutrinos have mass, however these experiments only measure the mass-squared differences.

While observation of neutrino oscilation enhancement in matter determined the sign of δm_{21}^2 , the signs of δm_{13}^2 and $|\delta m_{23}^2|$ are unknown. This leaves two possible orderings of the three neutrino mass eigenstates.

- **Inverted Ordering** with negative δm_{13}^2 and $m_3 < m_1 < m_2$
- **Normal Ordering** with positive δm_{13}^2 and $m_1 < m_2 < m_3$

Where m_1 is the neutrino mass eigenstate with the highest ν_e flavor content. According to combined T2K, Super-K atmospheric analysis, the normal ordering is slightly favored [33].

1.3 Neutrinoless Double Beta Decay

Neutrinoless Double Beta Decay, $0\nu\beta\beta$, is a hypothesized process that has implications for all the open questions about neutrino nature discussed so far. It is the most

sensitive probe into whether neutrinos are Dirac or Majorana.

$$(A, Z) \rightarrow (A, Z + 2) + 2e^- \quad (1.38)$$

This lepton number violating process is shown in Fig 1·1.

Double Beta Decay, $2\nu\beta\beta$, is a rare nuclear process by which two neutrons simultaneously undergo beta decay, emitting a neutrino and electron. First studied by Maria Goeppert-Mayer in 1935, $2\nu\beta\beta$ is a Standard Model process that has now been observed in multiple isobaric nuclei, nuclei with even numbers of protons and neutrons.

$$(A, Z) \rightarrow (A, Z + 2) + 2e^- + 2\bar{\nu}_e \quad (1.39)$$

In some of these isotopes, single beta decay is energetically forbidden. Because the isotope a single-beta decay step away is at a higher energy level than the isotope two steps away. Figure ?? shows how isobaric nuclei can produce this arrangement of nuclear states. As a second-order weak interaction, $2\nu\beta\beta$, is the slowest process in the universe that has been experimentally observed.

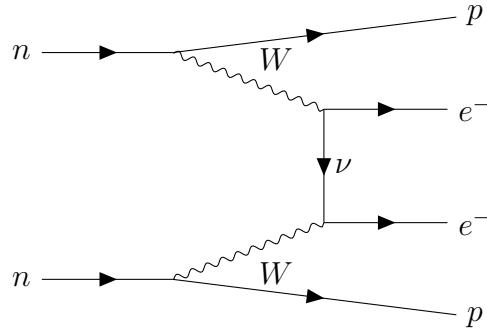


Figure 1·1: Feynman diagram for neutrinoless double beta decay ($0\nu\beta\beta$).

In $0\nu\beta\beta$, the final state electrons carry away almost the entire decay energy, while the energy is split between electrons and neutrinos in $2\nu\beta\beta$. When the easier to observe electron kinetic energies are accumulated, the distribution is as shown

in Figure ???. The sharp peak at the endpoint of the $2\nu\beta\beta$ decay spectrum is the experimental signature of $0\nu\beta\beta$.

The key observable in a $0\nu\beta\beta$ decay experiment is the half-life of $0\nu\beta\beta$. A prediction for the half-life is given by:

$$|T_{1/2}^{0\nu}|^{-1} = G_{0\nu} |M_{0\nu}|^2 \left(\frac{m_{\beta\beta}}{m_e} \right)^2 \quad (1.40)$$

where $G_{0\nu}$ is the phase space integral accounting for the final states of the electrons and daughter atom, $|M_{0\nu}|$ is the nuclear matrix element of the transition, and $m_{\beta\beta}$ is known as the effective Majorana mass of ν_e ,

$$m_{\beta\beta} = \left| \sum_i m_i U_{ei}^2 \right| = \begin{cases} m_0 c_{12}^2 c_{13}^2 + \sqrt{\Delta m_{21}^2 + m_0^2} s_{12}^2 c_{13}^2 e^{2i(\eta - \eta_1)} \\ \quad + \sqrt{\Delta m_{32}^2 + \Delta m_{21}^2 + m_0^2} s_{13}^2 e^{-2i(\delta_{CP} + \eta_1)} & \text{in NO,} \\ m_0 s_{13}^2 + \sqrt{m_0^2 - \Delta m_{32}^2} s_{12}^2 c_{13}^2 e^{2i(\eta_2 + \delta_{CP})} \\ \quad + \sqrt{m_0^2 - \Delta m_{32}^2 - \Delta m_{21}^2} c_{12}^2 c_{13}^2 e^{2i(\eta_1 + \delta_{CP})} & \text{in IO,} \end{cases} \quad (1.41)$$

Thus, the effective majorana mass is sensitive to the PMNS parameters which govern neutrino oscillation, such as the neutrino masses and mixing angles. It is also sensitive to the majorana CP violating phases, η_1 and η_2 , which neutrino oscillations are independent of.

As the Majorana phases are unknown, there is a range of allowed $m_{\beta\beta}$ bounded by the oscillation parameters. Figure 1.6 shows how the allowed regions vary over $m_{lightest}$.

1.3.1 Nuclear Matrix Elements

The determination of the nuclear matrix element $M_{0\nu}$ is a theoretical challenge in connecting the experimental observable, $T_{1/2}^{0\nu}$ to the neutrino mass. There are several nuclear structure methods for calculating NMEs, and there remain significant differences, up to factors of 3, between the NME values calculated with different methods, and sometimes even between NME values calculated with the same methods. Figure

1·2 demonstrate the large theoretical uncertainty in $0\nu\beta\beta$ nuclear matrix elements.

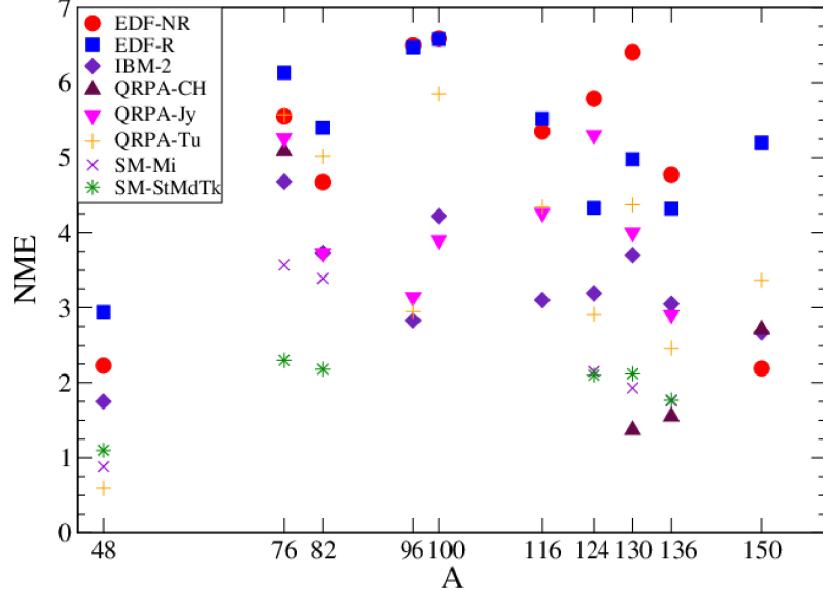


Figure 1·2: Results from various NME calculation of $M_{0\nu}$ on particular $0\nu\beta\beta$ decaying isotopes versus atomic mass. Figure taken from [25]

1.3.2 Black Box Theorem for $0\nu\beta\beta$ Decay

The half-life definition of Eq. 1·40 assumes the light neutrino exchange mechanism for $0\nu\beta\beta$ shown in Figure 1·1. Under this assumption the interaction strength is governed by the effective Majorana mass, $m_{\beta\beta}$. While there are other possible mechanisms that could facilitate $0\nu\beta\beta$, a key insight was given by Schechter and Valle in [31]. In what is now known as the famous Black Box Theorem, they propose that[15]:

- Should $0\nu\beta\beta$ be observed, its Feynman diagram must feature two electrons, two up-quark fields, and two down-quark fields. The process connecting these fields is arbitrary and is referred to as the "black box process". The theorem argues that this "black box process" effectively establishes the dimension-9 operator
- The up and down quarks are contracted by the W boson

- On the other end of the W boson propagators, electron fields are converted into neutrino fields
- The entire diagram can be rotated to turn into a process that converts anti-neutrinos to neutrinos as shown in Figure 1.3
- Finally, the possible cancelation of this process by other diagrams is dismissed by naturalness arguments.

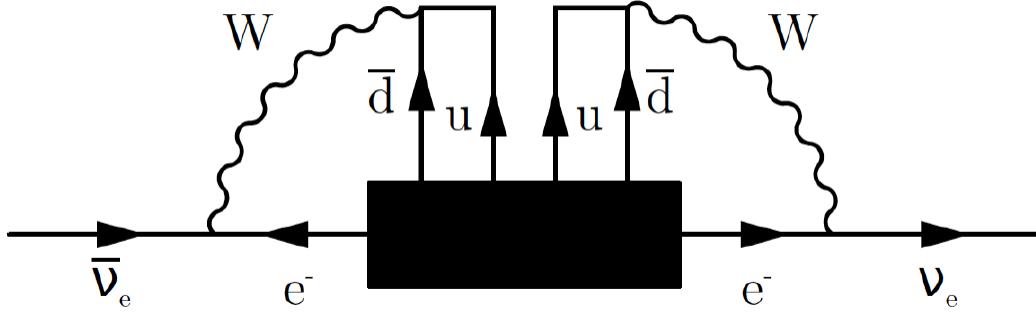


Figure 1.3: Depiction of the $0\nu\beta\beta$ black box theorem, the black box represents an arbitrary $0\nu\beta\beta$ process, which can be used to convert antineutrinos into neutrinos. Figure taken from [15]

The key conclusion of the black-box theorem is that should $0\nu\beta\beta$ be observed, even if the observed mechanism is not light majorana neutrino exchange, the neutrino is a majorana particle. It should be noted that since the theorem's original proposal, counterexamples have been found allowing $0\nu\beta\beta$ without majorana neutrinos, but the theorem still indicates potential links between $0\nu\beta\beta$, Majorana mass, and lepton number violation more broadly.

1.3.3 Double Beta Decay to Excited States

A related physics process can provide further experimental input into the NME calculations, and aid in the interpretation of $0\nu\beta\beta$ experiment results, $2\nu\beta\beta$ to excited

states, or $2\nu\beta\beta^*$. $2\nu\beta\beta^*$ is a SM process in which the parent isotope undergoes double-beta decay but transitions to an excited state of the daughter nucleus instead of the ground state. These decays are suppressed by orders of magnitude compared to decays to ground states because of the reduced phase space from smaller Q values[19]. Mirroring the status of NME calculations, predictions for the decay rates into excited states vary by multiple orders of magnitude, see Figure 1·4. An observation of this decay in Xenon could inform NME calculations and reduce the theoretical uncertainties.

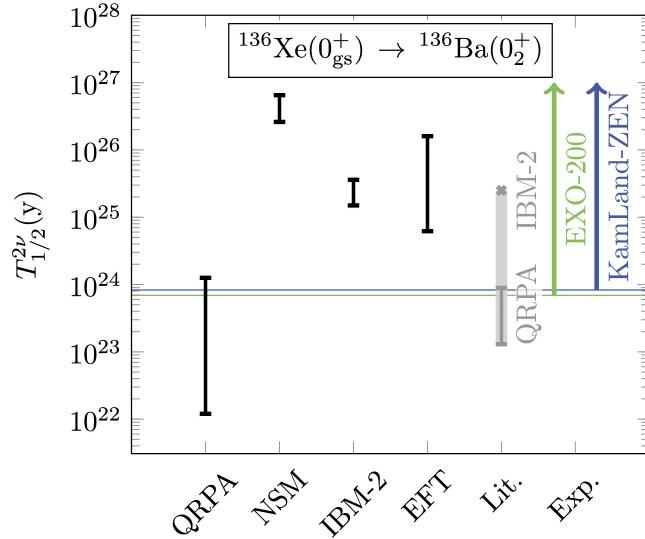


Figure 1·4: Predictions of $T_{1/2}^{2\nu*}$ using various NME calculation methods. Figure taken from [21].

The physical signature of $2\nu\beta\beta^*$ is of a $2\nu\beta\beta$ decay immediately, few pico-second delay, followed by a gamma cascade as the daughter nucleus relaxes into its ground state. The task of detecting this rare process becomes one of either particle identification or resolving a distortion in the much larger decay to ground state background.

While neither $2\nu\beta\beta$ or $2\nu\beta\beta^*$ has had their decay rates successfully predicted, close correlation between the NMEs of $2\nu\beta\beta$ and $0\nu\beta\beta$ have been demonstrated. Figure 1·5 shows the correlations between $2\nu\beta\beta$ and $0\nu\beta\beta$ NME as calculated by two

different methods.

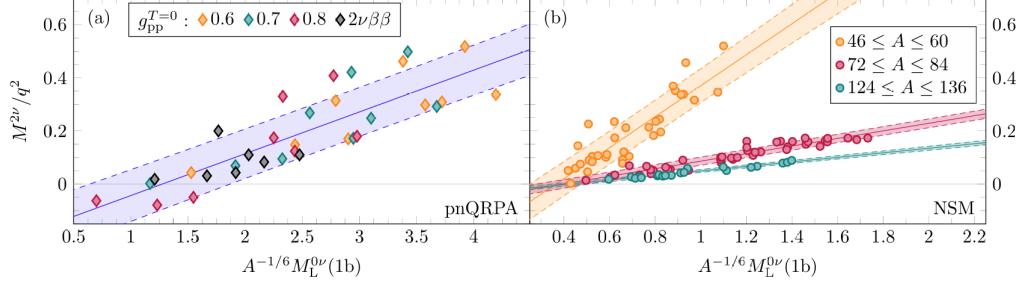


Figure 1.5: Correlation of $2\nu\beta\beta$ and $0\nu\beta\beta$ NME as calculated by NSM (Nuclear Shell Model) and pnQRPA (proton-neutron quasiparticle random-phase approximation) methods. Figure taken from [9].

All this further motivates a better understanding of $2\nu\beta\beta$ and $2\nu\beta\beta^*$ to aid in theoretical calculations of $M^{0\nu}$.

1.4 Double Beta Decay Experiments

$0\nu\beta\beta$ if it exists has an incredibly long half-life greater than 10^{26} years. Should it be discovered, $0\nu\beta\beta$ would be the slowest natural process observed experimentally. To successfully carry out this rare event search, $0\nu\beta\beta$ experiments must be designed with crucial criteria in mind:

- **High Energy Resolution:** Distinguishing the $0\nu\beta\beta$ peak at the $2\nu\beta\beta$ endpoint requires precise energy resolution to reduce ROI (region of interest) contamination from the $2\nu\beta\beta$ decay spectrum. Modern experiments on the forefront of this design criterion are achieving $\frac{\sigma_E}{E} \approx 0.1\%$ resolution, and completely suppressing the $2\nu\beta\beta$ background.
- **High Isotope Loading:** Maximizing the amount of double-beta decaying isotopes in the sensitive regions of the experiment is crucial for achieving sensitivity to long $0\nu\beta\beta$ half-lives in a reasonable timeframe, usually a decade of data-taking. Modern experiments are instrumenting about a metric ton of

double-beta decaying isotope. The limiting factor to this criterion is often budgetary or enrichment capability.

- **Low Unrelated Backgrounds:** Experiments need to be prepared in environments with low incidental radioactivity. This necessarily means deep underground facilities, with the experiments themselves being constructed with the highest standard of radiopure materials.

The current world leading limit on Majorana neutrino mass has been set by KamLAND-ZEN at $m_{\beta\beta} < (28 - 122)$ meV, at 90% C.L. The limits on majorana neutrino mass based on multiple NME calculations can be seen in Figure 1.6. It is readily apparent that the exact values of the NMEs drastically impact the significance of the latest experimental results. For the highest NMEs, the limits placed by KamLAND-ZEN enter the non-degenerate regions of inverted ordering phase space. While for the lower NMEs, the limits remain in the degenerate region. KamLAND-ZEN is the only $0\nu\beta\beta$ experiment to place limits in the inverted ordering region for any NME.

1.4.1 Observations and Current Limits of $2\nu\beta\beta^*$

Double beta decay to excited states has been observed in only two isotopes, a minority of the isotopes known to undergo double-beta decay.

- $^{100}\text{Mo} - ^{100}\text{Ru}(0_1^+) : T_{1/2} = 5.9_{-0.6}^{+0.9} \times 10^{20}$ years
- $^{150}\text{Nd} - ^{150}\text{Sm}(0_1^+) : T_{1/2} = 1.33_{-0.26}^{+0.45} \times 10^{20}$ years

$2\nu\beta\beta^*$ has yet to be observed in ^{136}Xe the double beta decaying isotope of the KamLAND-ZEN experiment and the focus of this thesis. The current world-leading limit on this process is $T_{1/2}^{2\nu}(0^+ \rightarrow 0_1^+) > 1.4 \times 10^{24}$ years at 90% C.L. set by the EXO-200 experiment. This work describes the latest analysis of KamLAND-ZEN 800 data which surpasses this limit.

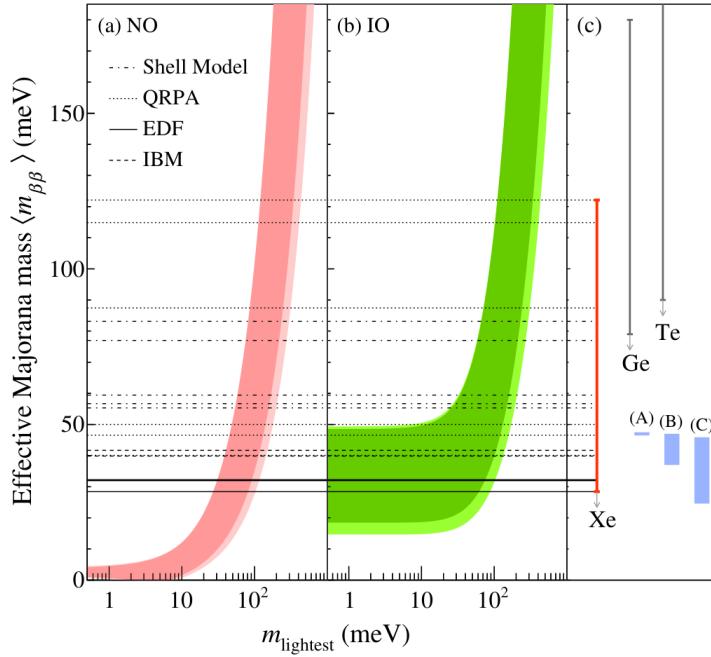


Figure 1.6: Effective Majorana neutrino mass as a function of the lightest neutrino mass state m_{lightest} . The shaded regions are based on best-fit values of neutrino oscillation parameters for (a) the normal ordering (NO) and (b) the inverted ordering (IO), the lighter shaded regions indicate the 3σ ranges based on oscillation parameter uncertainties. The horizontal lines indicate 90% C.L. limits on $m_{\beta\beta}$ considering multiple NME calculations. Figure taken from [3].

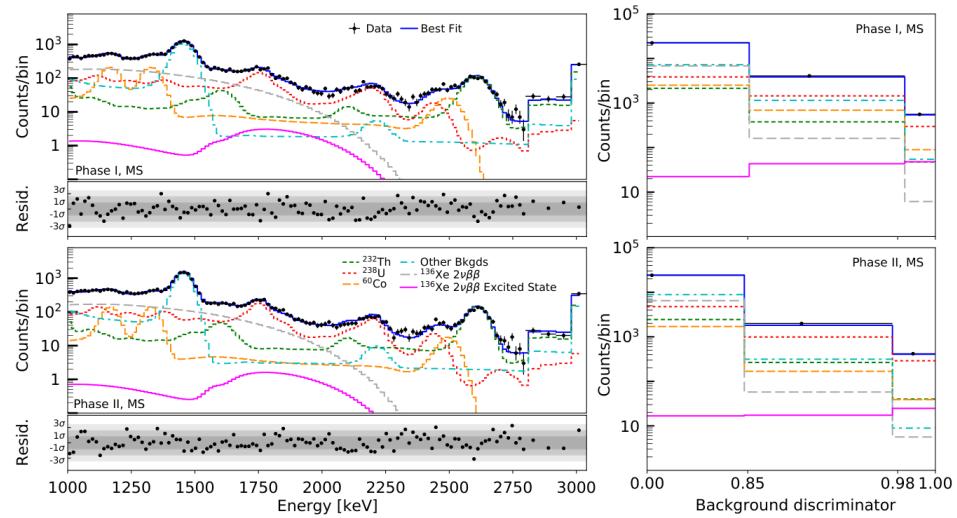


Figure 1.7: EXO-200's fit over energy spectrum (left) and particle ID discriminator spectrum (right) in two data-taking phases of the excited state signal and background. The decay to excited states was not found, and a lower limit was placed. Figure taken from [7].

Chapter 2

The KamLAND-ZEN Experiment

KamLAND, the **K**amioka **L**iquid-scintillator **A**nti **N**eutrino **D**etector, is a large liquid scintillator calorimeter detector situated 1km below mt. Ikenoyama in Gifu prefecture, Japan. I will describe the KamLAND detector's and the corresponding KamLAND experimental area's important components and features in this chapter. I will also explain how each component contributes to the KamLAND's scientific goals and the work of this thesis.

2.1 KamLAND

One can think of KamLAND as an onion made up of many spherical layers, each layer serving the ultimate goal of shielding and observing the central core, the xenon-loaded liquid scintillator.

2.1.1 Detector Infrastructure and Outer Detector

The KamLAND detector is surrounded by the KamLAND experimental area, situated in an old iron mine, multiple caverns and passageways were excavated and set aside for KamLAND experimental use.

The KamLAND site is shown in Figure 2.1. The control room contains networking and monitoring equipment which on-site shifters use to observe real-time detector activity. The first LS purification areas contain liquid-liquid extraction and nitrogen purge purification systems. The second LS purification area contains a distillation

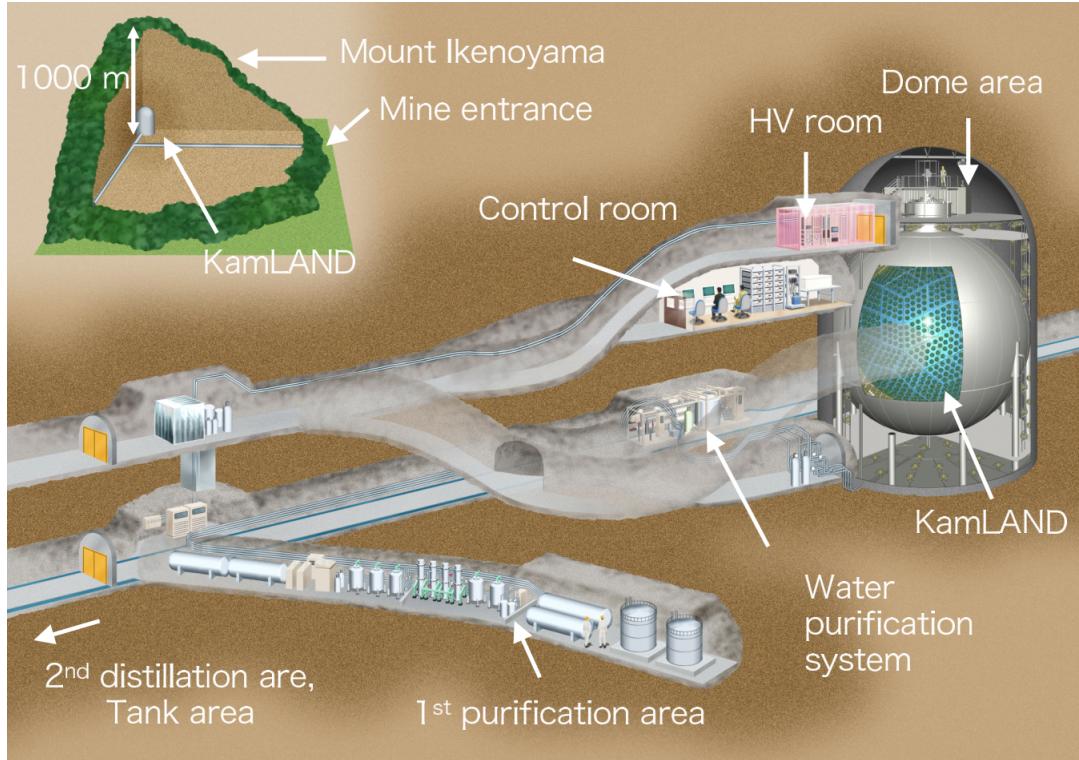


Figure 2.1: KamLAND site

purification system. A new Xenon purification area was built for KamLAND-Zen. The dome area is a class 1,000 clean area atop the detector and includes a calibration source preparation room and electronics enclosure (electronics hut or e-hut). At the center of the dome area, there is a secondary class 100-1000 clean tent covering the KamLAND chimney. The inner balloon installations took place in August 2016 and May 2018 inside this clean tent.

The outer detector (OD) is a cylindrical water tank 20m tall and with 20m diameter and filled with pure water. The OD was refurbished in 2016, and 140 new 20-inch PMTs (R3600) were installed inside the cavity. The inner wall of the outer tank and the outer surface of the inner detector stainless steel spherical tank are covered highly reflective Tyvek sheets (Tyvek 1073B and 1082D) to collect as much of the light generated by crossing cosmic ray muons as possible. The outer detector's role is

to tag cosmic ray muons, shield radioactivity and fast neutrons from the outer rock, and to stabilize the temperature of the ID.

2.1.2 Inner Detector

KamLAND's inner detector (ID) is the main spherical liquid scintillator detector, it is shown in Figure 2·2. The ID is contained in a 18m diameter stainless steel sphere tank. 1,879 PMTs are mounted onto the inner wall of the ID, 1,325 17-inch and 554 20-inch PMTs. The PMTs are submerged in non-scintillating buffer oil (BO). An acrylic panel separates the buffer layer into two shells. This panel prevents the convection of radon out-gassed from PMT glasses into the central parts of the detector.

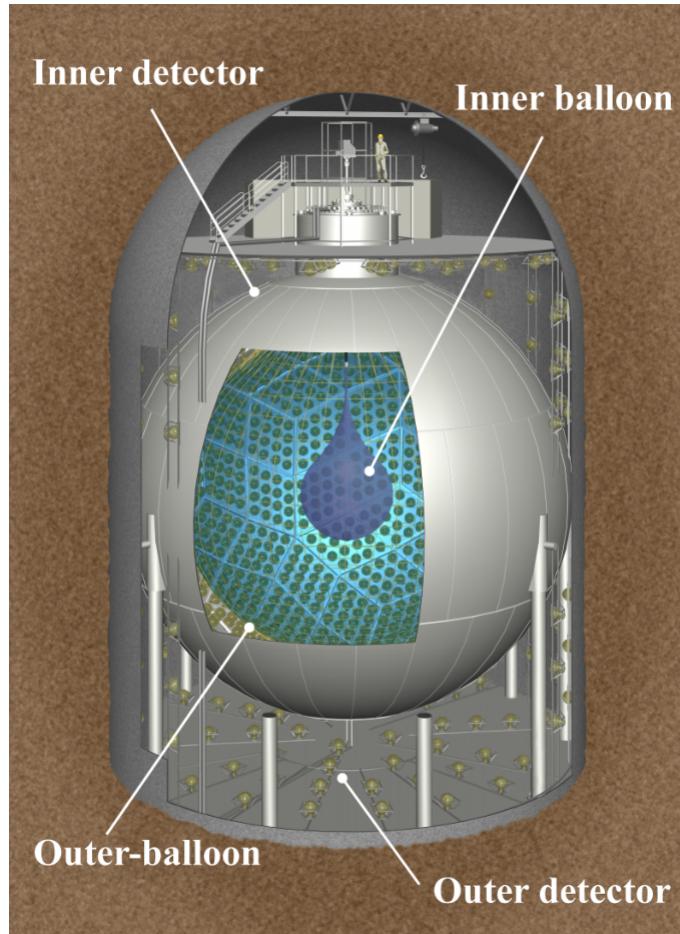


Figure 2·2: KamLAND-ZEN detector

Photomultiplier tubes (PMTs) are KamLAND’s eyes, detecting individual photons of light emitted by the passage of charged particles through the liquid scintillator volumes. Photons that hit PMT photocathodes are converted into a photoelectron. This photoelectron is then guided by electric fields to a series of dynodes. Each dynode multiplies the photoelectrons many times over, until the first photoelectron becomes 10^{6-7} electrons. Should multiple photons hit the photocathode simultaneously, the output voltage increases proportionally. This current is converted to a voltage by a coupling capacitor and read out via long coaxial cables. Figure 2.3 is a diagram of the 17in and 20in PMTs.

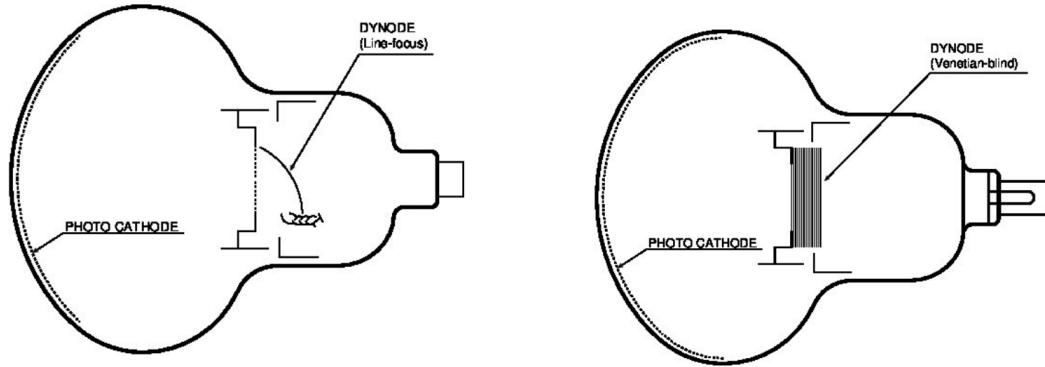


Figure 2.3: 17-inch and 20-inch PMTs, both have the same footprint, but the 17-inch PMT photocathode is masked to a 17-inch diameter.

The 1,325 17-inch PMTs are Hamamatsu R7250s while the 554 20-inch PMTs are Hamamatsu R1449s and R3600s. The 20-inch PMTs were inherited from the Kamiokande experiment to increase our light collection. Both sets of PMTs have a bialkali photocathode sensitive to 300-650nm light which is well-suited for the emission spectrum of the LS. The pmts also differ by dynode design; while the 17-inch PMTs feature "box-and-line" designs, the 20-inch PMTs have "venetian-blind styles". The different dynode designs along with the masking on the 17-inch PMTs, give us 17-in PMTs with better transit time spread (TTS) and 20-inch PMTs with better light collection efficiency. In total, the photocathode coverage of the ID is 34%, with 23%

contributed by the 17-inch PMTs.

Furthermore, the PMT performance can be affected by the earth's magnetic field. To reduce this unwanted effect, the entire KamLAND detector is surrounded by geomagnetic compensation coils to counteract this external magnetic field. The residual magnetic field is less than 50mG, which has negligible effect on the PMT performance.

Another important characteristic of PMTs is their quantum efficiency (QE). The QE quantifies the probability that a photon arriving on the photocathode will produce a photoelectron. A PMT's QE varies over the wavelength of the incoming light. To improve our light collection, KamLAND's LS is doped with PPO to shift the wavelength of the incoming light to where the PMTs are most sensitive. Figure 2.4 shows the PMT QE curve and the PPO reemission spectrum.

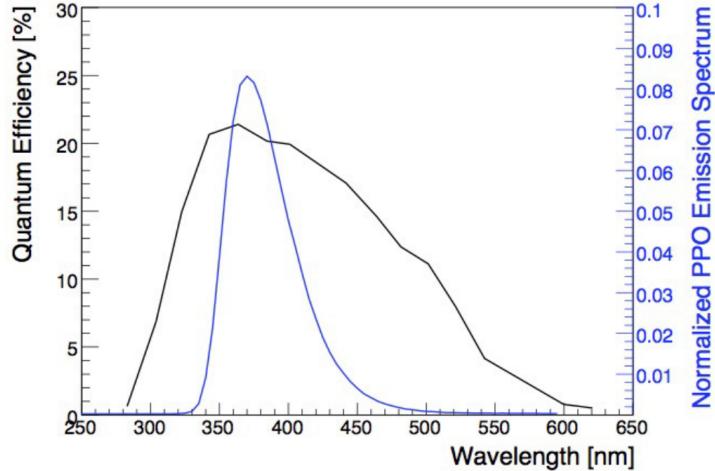


Figure 2.4: Quantum Efficiency of the KamLAND inner PMTs and PPO emission over wavelength. Figure taken from [26]

Next, is the 13m diameter outer balloon (OB). The OB is suspended in the center of the ID within the buffer oil, it is filled with one kiloton of highly purified organic liquid scintillator.

2.1.3 Liquid Scintillator

Liquid scintillator (LS) is the vital medium that sensitizes KamLAND to internal radioactivity. The KamLAND LS (KamLS), found in between the outer balloon and inner balloon, is composed of 80.2% of dodecane (D12), 1,2,4-trimethyl benzene, and 19.8% pseudocumene (PC). A wavelength shifter called 2,5-diphenyloxazole (PPO) is added to the LS at a concentration of 1.36 ± 0.03 g/L. KamLAND-Zen has achieved 5×10^{-18} g/g and 1.3×10^{-17} g/g contamination for ^{238}U and ^{232}Th , respectively.

The chemical composition of the KamLS can be found in Table 2.1

	D12	PC	PPO
Chemical Formula	C ₁₂ H ₂₆	C ₉ H ₁₂	C ₁₅ H ₁₁ NO
Density [g/cm ³]	0.7526	0.8796	-
Boiling Point [°C]	216	169	360
Melting Point [°C]	-10	-44	72
Flash Point [°C]	83	54	-

Table 2.1: Composition and properties of KamLAND Liquid Scintillator (KamLS)

2.1.4 KamLAND-ZEN and XeLS

At the center of KamLAND-ZEN lies the Xenon-loaded Liquid Scintillator (XeLS) contained in the 1.9m radius inner balloon (IB). The double-beta decaying isotope ^{136}Xe is thus placed in the cleanest, most sensitive part of the experiment. The Xenon gas is enriched to 90% ^{136}Xe and is dissolved into a modified version of KamLS. The PPO concentration was increased to 4g/L to boost the light yield. This increased PPO concentration compensates for the 10% reduction in emitted scintillation light when Xenon is mixed into the LS. The XeLS density is also tuned to match the surrounding KamLS. The chemical composition of the XeLS is shown in Table 2.2 in each of the different phases of the KamLAND-ZEN experiment.

Material	Decane (%)	PC (%)	PPO (%)	Xe (%)
Zen 400 Phase-1	82.3	17.7	2.7	2.44/2.48
Zen 400 Phase-2	80.7	19.3	2.29±0.03	2.91
Zen 800	82.4	17.6	2.38±0.02	3.13

Table 2.2: Composition of XeLS from three phases of KamLAND-ZEN

2.2 Chemical Handling Infrastructure

Background mitigation is crucial for $0\nu\beta\beta$. Maintaining the purity of the liquid volumes inside KamLAND is an important part of background mitigation in KamLAND-ZEN. In this section, we will briefly describe the systems that provided or maintain the purity of the LS and XeLS in KamLAND.

2.2.1 Water Extraction

The first purification is shown in Figure ???. Both the liquid scintillator and buffer oil are filtered in two stages with $1\mu\text{m}$ and $0.1\mu\text{m}$ pore sizes respectively. Next, the liquids are flushed with pure water in the water extraction tower where metals such as U, Th, and K, are absorbed by the water. Finally, the liquids are purged with ultra-pure nitrogen gas to remove gaseous contaminants like radon and oxygen.

2.2.2 Distillation

The next purification system utilizes the distillation system shown in Figure ???. LS from KamLAND is constantly cycled through the distillation system. There boiling is done to separate the individual chemical components of KamLS, namely Pseudocumene (PC) and PPO. Each component is individually distilled and purified. Then, the components are combined in the mixing tank to the original LS composition with an accuracy of 10^{-3}g/cm^3 . Finally high-purity nitrogen gas is used to purge the LS coming out of the mixing tank to eliminate any gaseous contaminants.

2.2.3 Xenon Handling

A schematic diagram of the XeLS handling system is shown in Figure 2.5. The system consists of the following components:

- A **1.1 m³ Main Tank** directly connected to KamLAND-ZEN’s inner balloon. The extracted XeLS first enters this tank.
- A **1.1 m³ Reservoir Tank** that is connected to the main tank via a vacuum pump and LS trap. It is refrigerated with liquid N₂ to -50°C, at which the LS gas is condensed and trapped. Only Xe gas is allowed to flow into the reservoir tank.
- A **25 m³ Storage Tank** is connected to the main tank. The degassed LS is poured into this tank for storage.
- A **1.1 m³ Sub-tank** is also connected to the main tank, the detector, the control tank, and the purified Xe gas system. The Xe gas is mixed into LS inside this tank. The density of chemical cocktails in the sub-tank is monitored and adjusted by the control tank. After mixing, the XeLS is filtered and fed back into the balloon.
- A **1.1 m³ Control Tank** is directly connected to the second purification area. The control tank controls the density in the sub-tank by adjusting the Decane percentage. The control tank is pressurized with Nitrogen gas.

2.3 Data Acquisition

2.3.1 KamLAND DAQ

KamLAND uses two data acquisition (DAQ) systems in parallel. The first is KamFEE (KamLAND Front End Electronics), which has been used since the start of

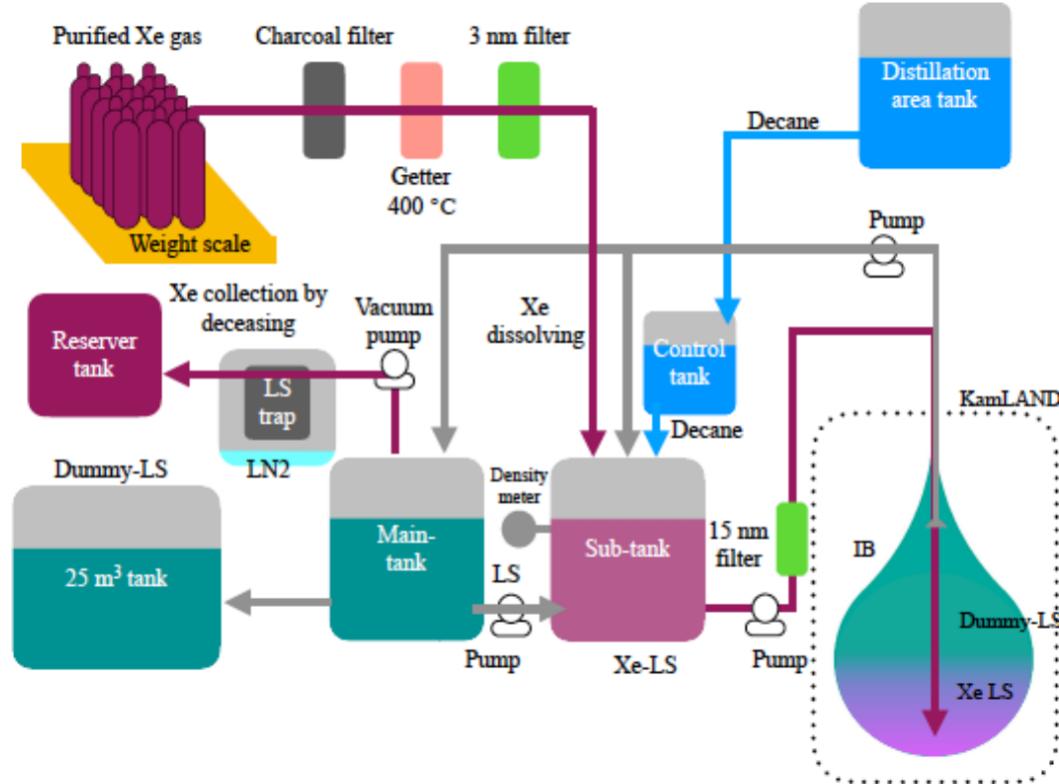


Figure 2·5: Flow diagram of the KLZ Xenon system. The purple lines denote the flow of Xe/XeLS, the blue line denotes the flow of decane, the grey line denotes the flow of LS. Figure from Reference

KamLAND physics data-taking. The other is MoGURA (Module for General-Use Rapid Application). MoGURA is a data acquisition system developed to eliminate the deadtime just after cosmic ray muon events. An overview of this dual scheme data acquisition system is shown in 2·6. What follows is a brief description of each DAQ system.

2.3.2 KamFEE DAQ

KamFEE are the front end electronics that read and control the KamLAND PMTs. The boards are of VME 9U form factor and are synchronized with a 40 MHz clock. The PMT signals are sent along two parallel channels. The first channel is sent to a

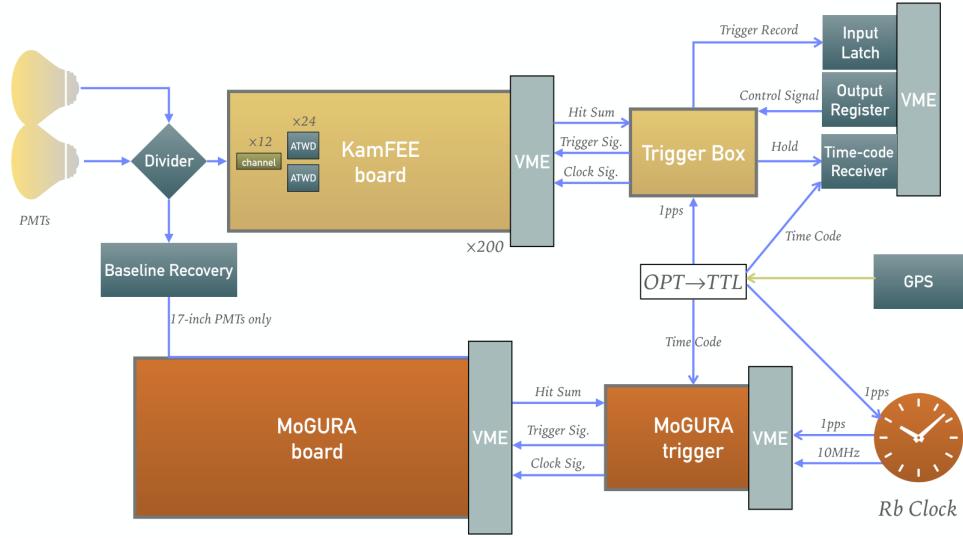


Figure 2.6: Flow diagram of the KamLAND data acquisition system, taken from [25]

discriminator which register a PMT hit if the voltage exceeds a predetermined value that corresponds to approximately 1/6th of a single photoelectron. The second channel, is delayed to give some time to process the discriminator signal and is fed into 3 amplifier stages (x20, x4, x0.5), this amplified signal is digitized by two analog Transient Waveform Digitizers (ATWDs). The ATWD is a 10-bit digitizer and samples every 1.5ns, 128 times per waveform. Each pulse takes 128 μ sec to digitize.

The KamFEE boards send a "hitsum" signal to the central KamFEE DAQ trigger, communicating a certain number of hits were received and can be digitized. The trigger board sends a signal back which issues the digitization command to the ATWDs. While the ATWD is digitizing, it cannot record further signals, therefore, two ATWDs are assigned to each channel to reduce deadtime.

2.3.3 MoGURA

MoGURA is the secondary data acquisition system in KamLAND; it is responsible for after pulses and dealing with PMT waveform overshoots caused cosmic muons.

KamLAND has a cosmic muon rate of 0.3 Hz, so it is important to compensate for the effects these high-energy events have on our detector. To accomplish this task, MoGDAQ has a few extra features over KamFEE.

- **Baseline Recovery:** After a high energy muon passes through the detector, the DAQ channels are saturated, which means the voltage exceeds the digitization window, so only the maximum value is read. Simultaneously, the voltage “overshoots” as it returns to normal and swings below the nominal value causing difficulties in digitizing signals that occur soon after these muons.
- **Adaptive mode:** Activates a special trigger mode after muon events to compensate for large after-pulses post-muon. This special trigger is based on differential PMT hits.

MoGURA data is used to tag neutrons created from muon spallation. These tagged spallation neutrons are vital in subsequent analyses to tag events that likely originated from these cosmic ray muons. The baseline restoration and neutron tagging will be further improved with the implementation of MoGURA2 trigger system. This is a planned replacement of the KamLAND data acquisition system (KamFEE and MoGDAQ both) for the KamLAND2-ZEN experiment, which is planned to begin physics data-taking in 2028.

2.4 KamLAND-ZEN Phases

The KamLAND-ZEN experiment has undergone multiple phases and renovations.

2.4.1 KamLAND-ZEN 400

The inner balloon and XeLS was added to the KamLAND experiment in 2011, starting the phase referred to as KamLAND-ZEN 400. This phase of the detector featured

a 3m diameter inner-balloon filled with liquid scintillator loaded with 3% Xenon by weight. The dissolved Xenon gas had 91% proportion of Xe^{136} .

The KamLAND-ZEN 400 data was split into two data-taking periods. Period-I data was contaminated with a high background of Ag^{110m} , the silver appeared to be leeching from the mini-balloon into the XeLS. The Ag^{110m} contamination on the inner balloon was likely due to nuclear fallout from the Fukushima reactor meltdown. The Fukushima meltdown occurred when the inner balloon was being manufactured and in the same geographical region of Japan. Period II started after the XeLS distillation suppressed the Ag^{110m} by a facator of 20. Period II continued data taking for 534.5 total livedays and the combined physics result of Periods I and II produced a $0\nu\beta\beta$ half-life limit of $T_{1/2}^{0\nu} > 1.07 \times 10^{25}$ years at 90% C.L. This half-life limit corresponds to an effective majorana mass limit of $m_{\beta\beta} < 61 - 165$ meV.

2.4.2 KamLAND-ZEN 800

KamLAND-ZEN 800 was the second phase of KamLAND-ZEN. KamLAND-ZEN took data from January 2019 to August 2024. Over 2kton·yrs of exposure was observed. KamLAND-ZEN 800 was decommission in Fall 2024, and is currently being disassembled.

Inner Balloon Manufacturing

KamLAND-ZEN 800 featured a larger, cleaner inner balloon which was fabricated at Tohoku University in a Class 1 cleanroom. The inner balloon is made from panels of 25 μm nylon-6. Innerballoon fabrication consisted of multiple steps some of these critical steps are listed here:

- **Washing** - the film is cleaned twice in an ultrasonic bathtub, then stored between cover films to prevent dust adhesion

- **Welding** - the cleaned balloon panels are welded with a semi-automatic welding machine. For delicate areas, such as the balloon neck, a hand welding machine was used. The average tensile strength on the balloon surface was 35 N/cm after welding.
- **He Leak Check** - Inevitably leaks will occur during the previous assembly procedures. Helium gas was pumped into the balloon to check for these leaks. The cover film of the balloon was peeled off before this leak check. Found leaks were repaired by patching the film. Over 900 leaks were found during the leak check.
- **Folding** - The inner balloon was folded into a cylinder shape and covered with sheath films to prevent contamination during transport. Teflon sheets and Vectran strings were used to tie the rolled balloon up for shipping.
- **Shipping** - The inner balloon was shipped within a silver gas bag. All corresponding tools were also shipped in airtight bags.

The inner balloon was installed on May 10, 2018. A rehearsal installation was performed in a swimming pool before the final deployment. In the final installation, the balloon is deployed through the 50cm port on the neck of the KamLAND detector. After filling the balloon with KamLS, the Teflon sheets, sheath films, and Vectran strings are pulled out of the detector. The whole operation was monitored in real-time via cameras and endoscope.

The top of the inner balloon is connected to a corrugated tube made from PEEK (poly-ether-ether-ketone). Twelve suspending belts support the inner balloon, wrapping around the full height of the balloon. The tension of each of these belts are monitored in real time to guarantee the position and stability of the balloon. A schematic of the balloon structure can be seen in Figure 2.7.

Contamination Control

Once deployed and exposed to the KamLAND scintillators, the inner balloon is very difficult to clean. Thus, maintaining balloon cleanliness is vital. After deployment, the IB was filled with distilled LS while the ^{232}Th level was measured at 10^{-15} g/g , exceeding the target background concentration. The PPO distillation tower was suspected to be a source of contamination and was investigated. ICP-MS and neutron activation analysis were used to measure ^{232}Th contamination at different locations along the distillation system. After meticulous washing and filter replacement, LS purification began to lower the ^{232}Th background. After two separate distillation campaigns, ^{238}U and ^{232}Th levels were reduced by a factor of 10 compared to KamLAND-ZEN 400. The contaminations can be estimated by performing a $^{214}\text{Bi}-^{214}\text{Po}$ and $^{212}\text{Bi}-^{212}\text{Po}$ coincidence analysis. The coincidence event rates plotted over time are shown in Figure 2.8 and listed in Table 2.3.

	^{238}U (10^{-17} g/g)	^{232}Th (10^{-17} g/g)
Zen 400 Phase-1	13 ± 2	190 ± 20
Zen 400 Phase-2	17 ± 1	5.5 ± 0.3
Zen 800	1.5 ± 0.4	30 ± 4

Table 2.3: Film Contamination three phases of KamLAND-ZEN. Values taken from [29]

KamLAND-ZEN 800 was decommissioned in 2024 after observing over 2 kiloton·yrs of exposure. The final half-life limit was reported as $T_{1/2}^{0\nu} > 3.8 \times 10^{26}$ years at 90% C.L. This half-life limit corresponds to an effective majorana mass limit range of 28–122 meV. As of Summer 2025, this is the world-leading limit on effective majorana mass from any double-beta decay isotope and is the only limit in the Inverted Mass Ordering region. The latest limits from KamLAND-ZEN800 are shown in Figure 2.9

2.4.3 KamLAND2-ZEN

KamLAND2 is the next generation of the KamLAND experiment, it will be built in the same detector cavern as KamLAND1. KamLAND2-ZEN will reach a goal limit of $T_{1/2}^{0\nu\beta\beta} > 2 \times 10^{27}$ yrs.

Most of the detector components will be replaced going from KamLAND to KamLAND2. Some of the more notable upgrades are:

- **Inner Detector PMTs** - All of the 1,879 inner PMTs will be replaced with modern low-TTS, high quantum efficiency (QE) phototubes.
- **Light Collecting Mirrors** - Light collecting winston cones will be attached to each of the PMTs to achieve virtually 100% photocoverage. These improvements will contribute to a goal energy resolution of 2%. This energy resolution will lead to a x100 reduction in the $2\nu\beta\beta$ background rate.
- **Improved Inner Balloon** - The new innerballon will be made up of PEN (polyethylenenaphthalate) which will scintillate from film radioactive backgrounds
- **MoGURA2** - Replace the 2 DAQ systems with MoGURA2, a newly developed, compact, dead-time free, RFSoC electronics.

KamLAND2-ZEN is scheduled to begin data-taking in 2028.

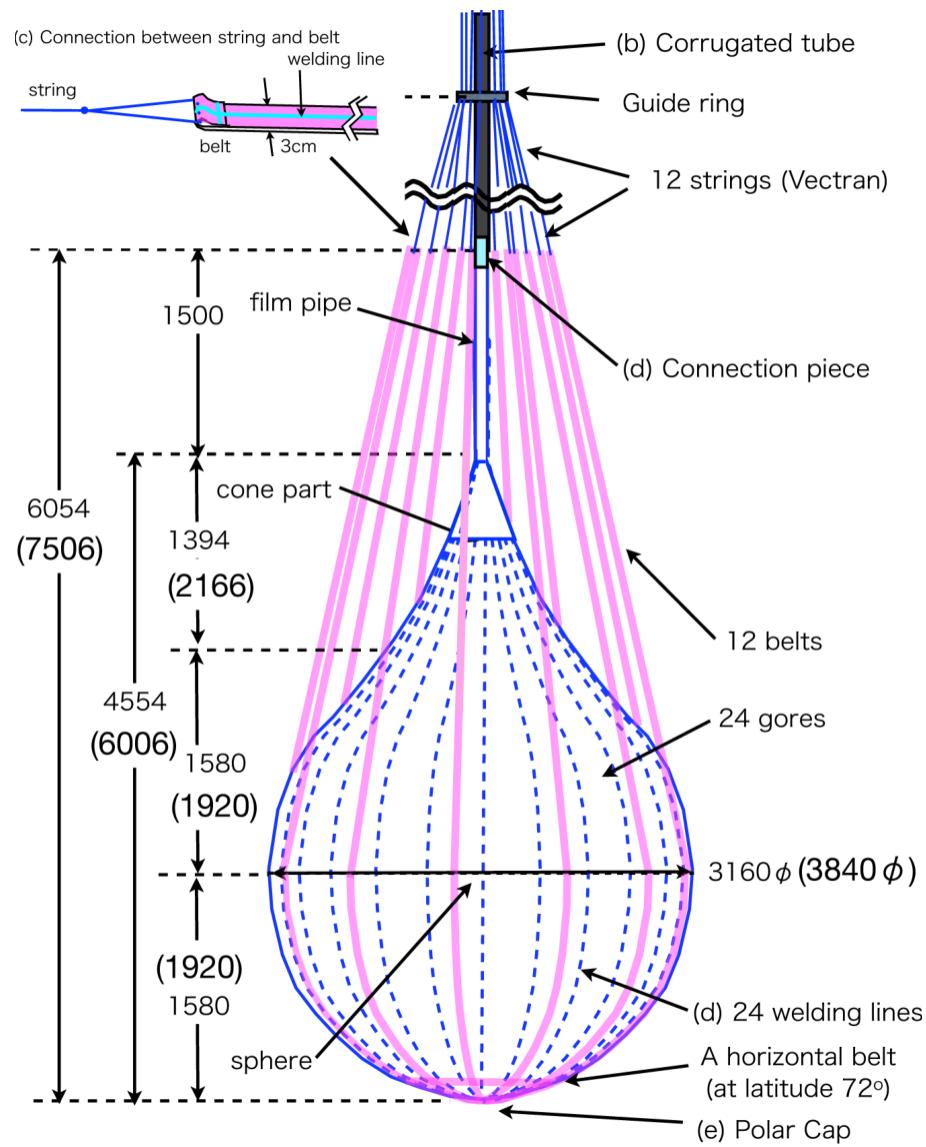


Figure 2·7: Inner balloon structure and measurements for KamLAND-ZEN 800 configuration, taken from [29]

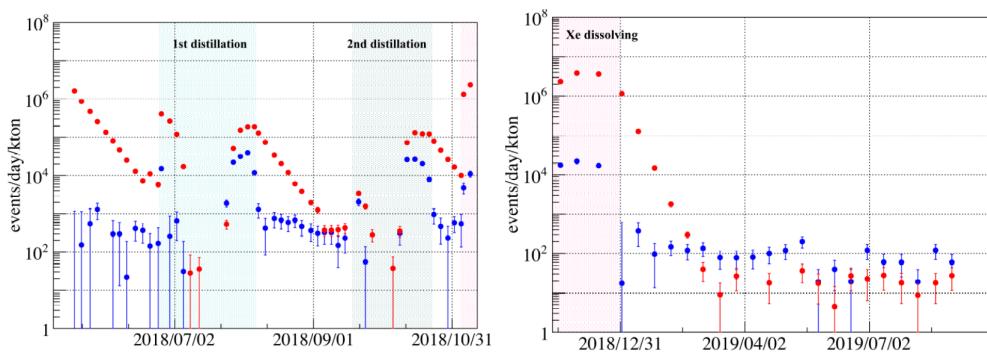


Figure 2·8: Coincidence event rate in KamLAND-ZEN 800 during the first distillation campaign, second distillation campaign, and Zenon loading phase. The red points denote ^{214}Bi and the blue points denote ^{212}Bi . Figure taken from [25].

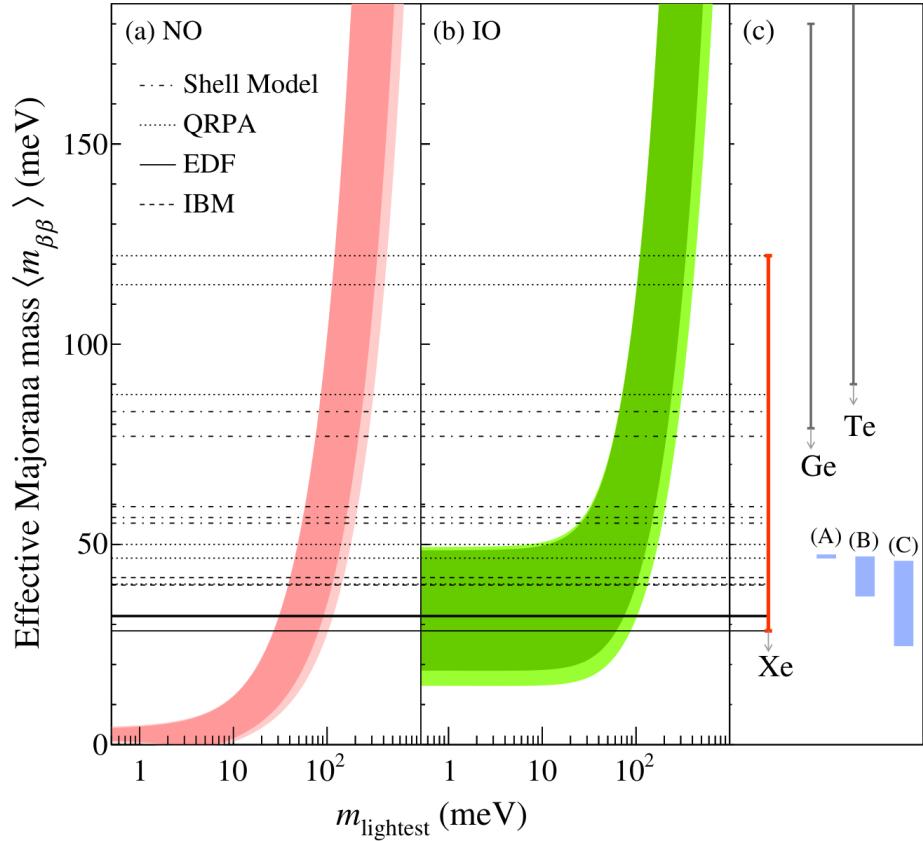


Figure 2.9: Effective Majorana neutrino mass $m_{\beta\beta}$ as a function of the lightest neutrino mass $m_{lightest}$. The dark shaded regions are based on the best-fit neutrino oscillation parameters, while the lighter regions indicate 3σ ranges calculated from oscillation parameter uncertainties [14] [1]. The horizontal lines indicate various 90% C.L. upper limits on $m_{\beta\beta}$ from KamLAND-ZEN's ^{136}Xe results and a few different NME calculations. The blue bars on the right indicate three different theoretical predictions in the IO region. [4]

Chapter 3

Event Reconstruction and Selection

KamLAND-ZEN uses detailed simulations defined in KLG4Sim, a GEANT4-based Monte Carlo (MC) simulation software. The MC simulated events are tuned with real calibration events to carefully match the real detector response. Simulated and physical events produce detector responses that are reconstructed to extract higher-level information such as energy and position. The reconstructed event information is used for data selection and spectrum fitting. This chapter discusses the MC simulation and event reconstruction procedures used in KamLAND-ZEN 800.

3.1 Analysis Framework

3.1.1 Data Flow

Figure 3.1 outlines the data flow in KamLAND-ZEN. PMT signals are digitized in either KamFEE or MoGURA, the two DAQ systems discussed in the previous chapter. The digitized signals are stored in Kinoko Data Format (KDF). KDF files contain trigger information and timestamped, digitized PMT waveforms. KDF files also store run condition information in the header. The EventBuilder collates the waveforms of a single event and stores them in a serial file. A waveform analyzer reconstructs hit time and charge (TQ) information for each of these waveforms. The RTQ files hold the Raw-TQ information for each PMT. Event vertices and visible energy are derived from the RTQ files through their respective reconstruction algorithms. There are secondary reconstructions that are also applied to the RTQ files, such as muon

track fitting, flasher vetoes, double pulse fit, and unphysical event selections. The general vector file (GVF) is used for the main physics analyses like the one presented in this thesis.

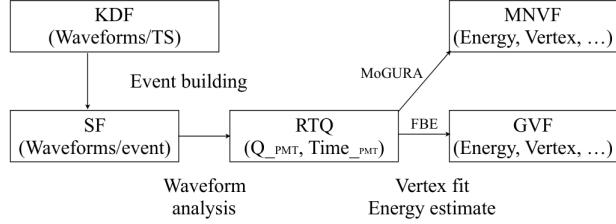


Figure 3·1: Data flow in KamLAND from raw waveforms to analysis variables such as energy, vertex, total hit PMTs, etc. [29]

GVF files contain the following information:

- **run number**
- **event number**
- **TimeStamp** based on DAQ clock time (25 ns for KamFEE, 20 ns for MoG-DAQ)
- **unixtime** is the number of seconds since January 1st, 1970 and is used for some run vetoes
- **trigger type** records which trigger was used
- **event vertex and badness** event vertices and a radius from the detector center are saved, along with a vertex fit quality parameter called badness
- **energy/energy17** visible energies given by the fitter; energy17 is the energy estimate using only 17-inch PMTs
- **TotalChargeID/17/OD** sum of all PMT charges of each PMT type
- **numhit/numhit17** the number of hit PMTs/17-inch PMTs in each event

- **NsumMax** the maximum number of hit PMTs in a single DAQ cycle within each event, a "peak" nhit of the event
- **N200OD** maximum number of simultaneous hit OD PMTs within 200 ns windows
- **muon entrance and direction** muon fitter results are recorded

Finally, MoGURA events are associated with muon events acquired in KamFEE DAQ (FBE) and stored in a Muon-Neutron Vector File (MNVF) to search for neutron capture events that occur shortly after muons.

3.2 Event Reconstruction

3.2.1 Waveform Analysis

Each digitized waveform has 128 samples with 1.5 ns sample intervals, corresponding to a waveform digitization window of 192 ns. The waveforms are processed and TQ values are reconstructed using the following procedure:

- **Smoothing** Each waveform is smoothed using a running-average first derivative.
- **Baseline adjustment** The baseline of each PMT is collected at the beginning of each run. This baseline is subtracted from each waveform.
- **Peak finding** Peaks are found with running-averaged 1st, 2nd, and 3rd derivatives.
- **Leading-edge and Trailing-edge tag** A leading-edge is stamped as 10 ns before the peak voltage. The trailing edge is stamped when the waveform returns to baseline. An example of this time-stamping is shown in Figure 3.2.

- **Waveform Sum calculation** The waveform is integrated from the leading-edge to the trailing-edge.

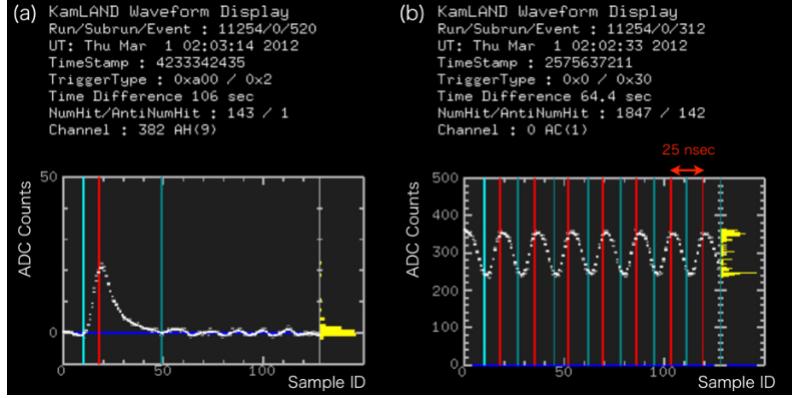


Figure 3.2: An example of waveform analysis from thesis [34]. (left) ADC counts of a real waveform after baseline subtraction. The left cyan line is the leading edge, the center red line is the peak position, and the right dark cyan line is a trailing-edge. (right) Clock calibration example on 25 nsec intervals.

When there are multiple hits in a single PMT waveform, the total charge of the hits and the earliest hit time are returned. This simplified information is used for vertex and energy reconstruction. The multi-photoelectron (multi-pe) information is used for double-pulse fitting and muon shower tagging.

3.2.2 PMT Corrections

Low Gain Problem and HV Reductions

Since approximately 2011, it has been observed that the gain of some 17-inch PMTs gradually decreased. As the gain of the PMTs fell, this compromised the signal-to-background ratio and PMT waveform quality. It was also observed that the PMTs entered a low impedance state before the gain dropped. An HV current and voltage monitor allows for real-time monitoring of this state. Usually, a simple HV power cycle could recover normal PMT behavior. Since 2016, an automatic HV power cycle mechanism has been implemented to mitigate the low gain problem, but the root

cause is still unknown.

Each time the PMTs enter the low impedance state, the HV on that channel was reduced in 50–100 V increments. Over time, some of the channels had their HV reduced by up to 450 V. Figure 3.3 shows the trend in low gain 17-inch PMTs.

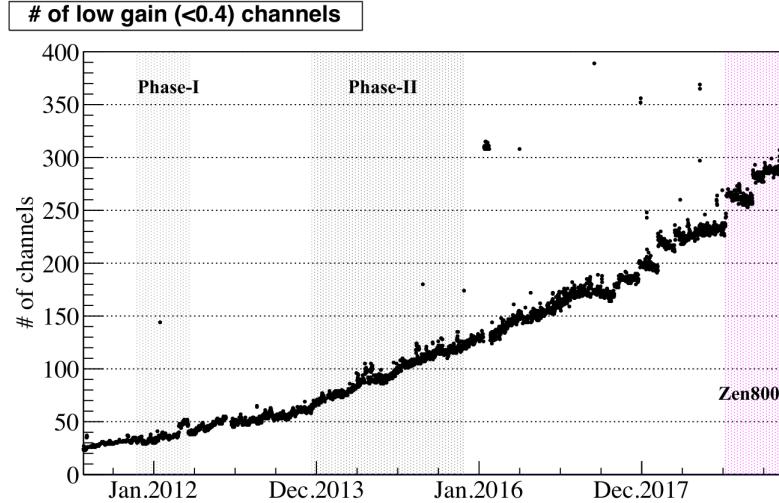


Figure 3.3: The trend in the number of low gain 17-inch PMTs, before ZEN-800. The number of low gain channels increased gradually, while the sudden increases are from HV reductions performed since 2017 [29].

Note about current low pmt gain analysis.

Bad Channel

A channel is considered bad if the PMT meets one or more of the following criteria:

- PMT pulses less than 0.6% of the time over all events
- PMT pulses below 0.48% for non-muon events
- PMT pulses less than 80% of the time for high-energy muon events
- PMT is missing a waveform more than 10% of the time
- Large discrepancy between the two ATWD hits

- High muon charge PMTs. A PMT may read much higher charge ($Q_{detected}$) than the average of its surrounding PMTs ($Q_{expected}$). A run is divided into 100 muon intervals; for each interval the criteria is defined as

$$\frac{1}{N_{interval}} \sum_{i=1}^{N_{interval}} \left(\frac{1}{N_{muon}} \sum_{j=1}^{N_{muon}} \frac{(Q_{expected} - Q_{detected})^2}{Q_{expected}} \right) > 1000 \text{ p.e.}$$

These bad channels are excluded from event reconstruction and physics analyses.

Dark Hit

Thermal fluctuations can emit electrons off the photocathode, leading to a PMT hit signal. These "dark hits" are an unavoidable hit-level background in PMT detectors; lowering the detector temperature reduces this effect. The dark hit rates are measured from run to run and are factored into our likelihood-maximizing reconstruction algorithms. The hit rate observed 50-100 ns before the PMT hit time rising edge is taken as the dark rate. Figure 3·4 shows the PMT hit time distribution and the dark rate window.

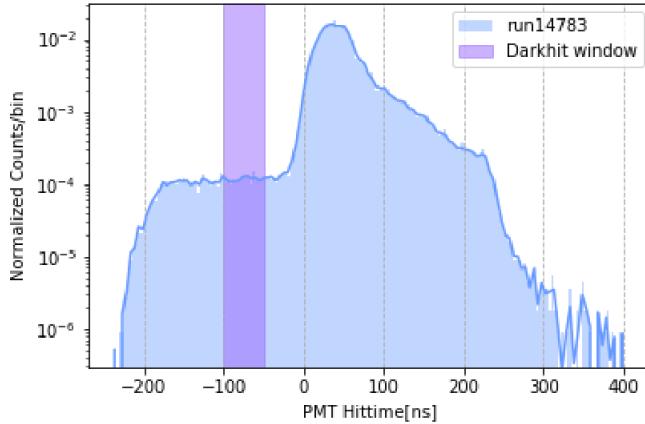


Figure 3·4: An example pmt hit time distribution from data run 14783, the 50-100 ns leading window is taken to measure the pmt dark hit rate. [25].

3.2.3 Primary Vertex Fitter

The primary vertex fitter provides a rough estimate of a scintillating event's location. This estimate serves as the input to a more thorough, but complex, secondary fitter. The fit works by constructing a hit time residual distribution:

$$T_i^{emit} = T_i - TOF_i = T_i - \frac{|R_i - r_{vertex}|}{c_{eff}} \quad (3.1)$$

Here T_i is the hit time of the i^{th} PMT, TOF_i is the time it takes for a scintillation photon to traverse from the vertex position to the i^{th} PMT position, R_i is the PMT position, r_{vertex} is the unknown vertex position to fit for, and c_{eff} is the speed of light in the given medium. By fitting T_i^{emit} to match the standard scintillation time profile, a primary r_{vertex} is produced by the fitter.

3.2.4 Secondary Fitter

The secondary V2 fitter uses the r_{vertex} given by the primary fitter to compute T_0 according to the equation 3.2

$$T_0 = \frac{\sum_i (T_i^{pmt} - TOF_i^{pmt}) \times Q_i}{\sum_i Q_i} - const. \quad (3.2)$$

This T_0 is the charge weighted sum of T_{emit} from 3.1. This T_0 serves as the universal start point of an event. From this time, each PMT hit time is

$$\tau(x, y, z, T_0) = T_i^{pmt} - TOF_i^{pmt} - T_0 \quad (3.3)$$

Finally, these time-of-flight corrected and centered hit time distributions are used to create probability distributions for the 17 and 20 inch PMTs respectively. These PDFs are shown in Figure 3.5. The likelihood function for an individual PMT is

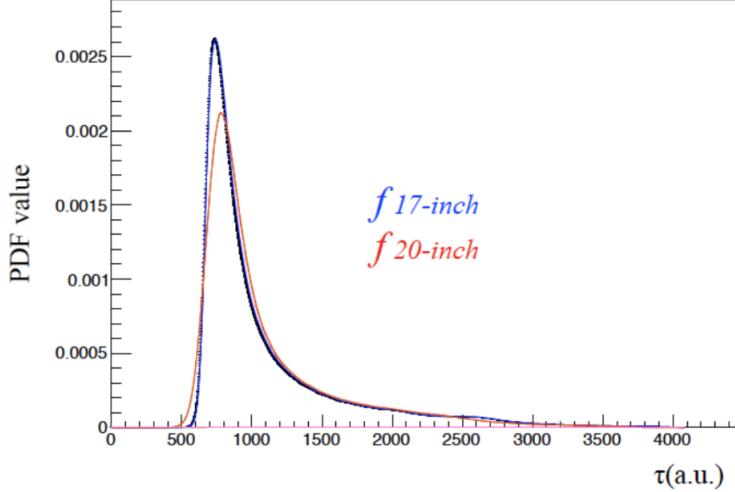


Figure 3.5: Probability density function of 17-inch and 20-inch PMT hit times calculated from calibration data. The plot is from [29] and originally from a 2005 calibration dataset.

defined as:

$$\phi_i = \frac{\mu \times f_i(\tau_i) + D_i}{\mu \times C_{17/20} + D_i} \quad (3.4)$$

Here, μ is the pulse shape determination factor, D_i is the dark hit rate for the i^{th} PMT and $C_{17/20}$ is the normalization constant for the 17 or 20 inch PMTs. The overall log-likelihood is given by the $\log(L) = \sum_i \log(\phi_i)$. The log-likelihood is maximized by the Newton-Raphson method, in which the x, y, z, T_0 are adjusted to the best-fit values, giving us the V2 reconstructed vertex.

3.2.5 Energy Reconstruction

Likelihood maximization is also used to reconstruct the energy of an event. A likelihood PDF is constructed using the number of hits, charge, and hit timing.

N_{hit} PDF

The expectation of the number of photons hitting PMT i , μ_i , is a function of the visible energy and dark charge.

$$\mu_i = a_i(x, y, z) \times E_{vis} + d_i \quad (3.5)$$

Here, $a_i(x, y, z)$ is a coefficient that converts the event energy to the number of photons, which is calibrated with neutron events. It is determined by the PMT position x, y, z . d_i is the dark noise charge of PMT i , which is electronically measured. The probability that μ_i photons hit the i th PMT j times, k_{ij} , is ideally expressed by the Poisson distribution:

$$k_{ij} = \frac{(\mu_i)^j}{j!} e^{-\mu_i} \quad (3.6)$$

However, in KamLAND waveform analysis, the 1 p.e. detection efficiency is reduced by the 0.3 p.e. software charge threshold. This threshold is set to reduce the acceptance of dark noise but also decreases hit detection efficiency. As a result, the PMT hit probability is reduced to:

$$P_{hit} = 1 - v_i e^{-\mu_i} \quad (3.7)$$

Hit Charge PDF

A Gaussian distribution is assumed for the hit charge PDF of each PMT:

$$f_{i,j(q_i)} = \frac{1}{\sqrt{2\pi j\sigma^2}} \exp\left(-\frac{(q_i - j)^2}{2j\sigma^2}\right) \quad (3.8)$$

q_i is the observed charge in p.e. units and σ is the charge resolution against 1 p.e. distribution.

Hit Time PDF

PMT hit timing factors into energy reconstruction by helping to discriminate hits unrelated to the physical event. The hit timing model is created using source calibration data.

$$P_{time,i} = \frac{\psi(t_i) a_i E_{vis} + d_i}{\mu_i} \quad (3.9)$$

The PDF is the sum of the signal hit distribution and the constant dark noise.

Energy Likelihood

The likelihood function to be maximized is constructed as

$$L = \prod_{Not\ hit\ PMTs} P_{no-hit,i} \prod_{Hit\ PMTs} \left[P_{hit,i} \left(\sum_{j=1}^{100} f_{i,j} \right) P_{time,i} \right] \quad (3.10)$$

The reconstructed energy is the one which maximizes this likelihood. The Newton-Raphson method is used to search for this energy. This process is implemented independently for the 17-inch PMTs and 20-inch PMTs, then the event energy is calculated with a weighting factor α :

$$E_{vis} = (1 - \alpha)E_{17inch} + \alpha E_{20inch} \quad (3.11)$$

The weighting factor $\alpha = 0.3$ was determined to maximize energy resolution.

Bad Channels in Energy Reconstruction

The increase in the number of low gain PMTs has lead to worsening energy resolution over time, as these PMTs are excluded from the typical energy reconstruction described above. In particular, some of the low gain PMTs still detect photons, but proper gain calibration is not possible. A method for utilizing the information from operational low gain PMTs was developed, and the basic strategy is as follows:

1. The change in gain causes the effect of the 0.3 p.e. threshold on hit probability to change. The no-hit probability was expanded as follows:

$$P'_{no-hit,i} = \left(1 + \epsilon_1 \mu_i + \epsilon_2 \frac{\mu_i^2}{2!} + \epsilon_3 \frac{\mu_i^3}{3!} \right) e^{-\lambda \mu_i} \quad (3.12)$$

This model was originally a simple expansion of P_{no-hit} , but in the end was adjusted phenomenologically to better reproduce real data. This adjustment is why an additional $e^{-\lambda \mu}$ appears in the model.

2. The parameters $\epsilon_1, \epsilon_2, \epsilon_3$, and λ are estimated with actual data. The events satisfying the following selections are collected and the no-hit probability is calculated for each expected charge. The expected charge of the i-th PMT μ_i is estimated using the vertex and total charge of the events that meet the following conditions.

- $r < 6m$
- Not muons or events within 2 ms after muons
- Events with more than 120 17-inch PMT hits
- PMT waveforms that contain only 1 peak

Figure 3.6 shows the result of fitting this adjusted no-hit probability model. The fitting is performed run-by-run and for each PMT independently.

3. Use the updated no-hit probability pdf in the event energy reconstruction in Equation 3.10.

Making use of the low-gain PMTs can improve energy resolution by up to 3% [23]. Further analysis in this work uses energy reconstructed from the combination of normal and low-gain PMTs.

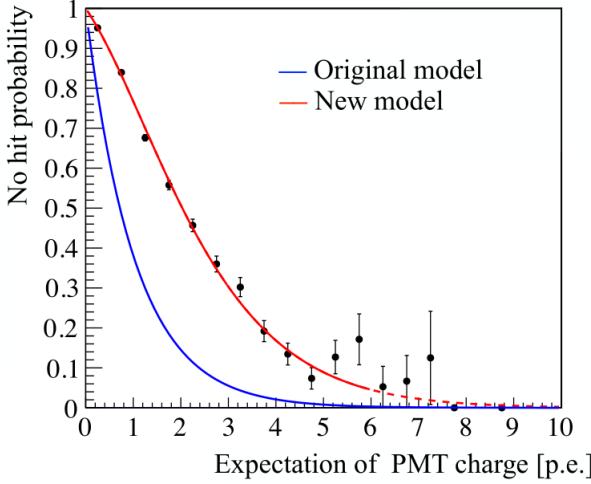


Figure 3.6: Fitting no hit probability to a low gain PMT against the expected charge μ . The original model is shown with the blue line while the red line is the new model which agrees better with low-gain PMT data.

3.2.6 Muon Reconstruction

The selection and understanding of muons and muon-correlated neutrons are essential to multiple background rejections. This section describes the special selection criteria and reconstruction methods used for muons and neutrons.

Muon Selection Criteria

The muon event selection criteria are as follows:

- Total charge of 17-inch PMTs, $Q_{17} \geq 10000$ p.e.
- $Q_{17} \geq 500$ p.e. and the number of hit OD PMTs ≥ 9 .

The former criterion selects muons which go through the scintillator volumes of the detector. A total charge of 10,000 p.e. roughly corresponds to an event energy of 30 MeV, which exceeds the energy range of most physical analyses in KamLAND-ZEN. The second selection is for muons that only deposit energy in the outer buffer oil (clipping muons). Muons passing through the buffer oil volumes do not scintillate; as

such, the 500 p.e. threshold in Cherenkov radiation roughly corresponds to about 40 MeV of energy deposition.

Cosmic Ray Muon Reconstruction

Cosmic ray muon events form tracks as opposed to the point-like events caused by single decay events. The process is shown diagrammatically in Figure ??

1. The ID PMT which detects the earliest light is identified. If the charge of this hit is low or isolated in time from the many other hits in the event, it is classed as a dark hit and ignored. A line is drawn from the earliest hit muon PMT and the center of the KamLAND detector. The intersection of this line and the outer balloon is marked as the temporary entrance point.
2. The PMT whose charge is the largest is identified. The brightest hit PMT should be hit later than the earliest PMT and the neighbors of the earliest PMTs. A line is drawn from the brightest hit PMT and the center of the KamLAND detector. The intersection of this line and the outer balloon is marked as the temporary exit.
3. The temporary track is defined as the line connecting the temporary entrance and exit. The temporary track is finally corrected by checking the correlation between the track length and the total charge.
4. The reconstruction quality is evaluated by checking the following:
 - Whether the earliest and the brightest PMTs can be identified
 - Whether the mean hit time of PMTs around the entrance is earlier than the around the exit.

A "badness" parameter value is assigned to the reconstruction according to this evaluation. With this evaluation, around 15% of muon candidates are

regarded as badly reconstructed though they can still be used in muon-neutron pairing. Bad muon reconstruction is caused by ringing in the PMT signals, muon bundles, and stopped muons.

The light yields in the muon events are estimated in [23]:

$$\langle dQ_C/dX \rangle = 28 \pm 5 \text{ p.e./cm (Cherenkov muons)} \quad (3.13)$$

$$\langle dQ_S/dX \rangle = 338 \pm 12 \text{ p.e./cm (Scintillation muons)} \quad (3.14)$$

3.2.7 MoGURA Neutron Reconstruction

Neutrons that are produced during cosmic ray spallation are best detected with the MoGURA DAQ due to the FBE's inability to handle the high after-pulse rate. After-pulsing is also present in MoGURA and needs to be rejected. An effective number of hits N_s was introduced. The neutron reconstruction procedure is as follows:

1. A 200 ns wide time window is opened. The vertex is reconstructed using LT Vertex with the hit information contained in this window.
2. The times of flight to each PMT are calculated assuming the reconstructed vertex. Then the ToF-subtracted hit timing distribution is obtained.
3. The obtained residual hit time distribution includes neutron capture 2.2 MeV gamma scintillation light and fake signals from after-pulses. To calculate the effective number of hits, N_{in} and N_{out} , the number of hits in a 30 ns wide "ontime" window and a 170 ns wide "offtime" window respectively are counted. N_s is then calculated as

$$N_s = N_{in} - N_{out} \times \frac{30 \text{ ns}}{170 \text{ ns}} \quad (3.15)$$

4. The ontime window is shifted by 20 ns, the clock time of MoGDAQ, and step 3 is repeated.
5. The 200 ns time window is shifted and steps 1-4 are repeated. The 200 ns window and 30 ns ontime window that maximize N_s are found. The vertex given by the N_s -maximizing time windows is taken as the reconstructed neutron capture event vertex.

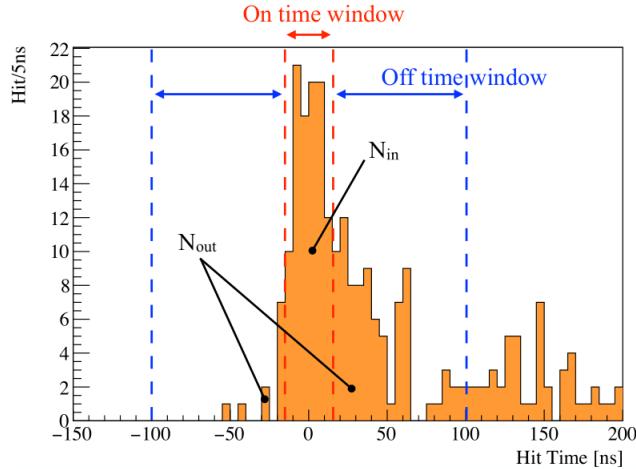


Figure 3.7: A neutron capture events hit times showing the contribution of fake after pulses and the time windows used to calculate N_s

3.2.8 Muon Neutron Correlation

The neutron selection process outlined above contains many noise events, thus the sample is only used in background discrimination when coincident with muons. In particular, MoGURA data neutrons are used to improve the rejection of xenon spallation products. The procedure for selecting muon-neutron pairs is:

1. Check the end unixtime of the previous KamDAQ run and the start unixtime of the current KamDAQ run.

2. Collect the MoGURA runs that collected data during this gap. Muon events collected by MoGURA are used in the gaps between KamDAQ runs; during KamDAQ runs, muons collected with FBE data are used.
3. The delayed coincidence analysis is done to select neutron candidate events in a short time period after muons. The first cuts applied are on $dT > 2500\mu s$ and $N_s = N_{in} - N_{out} < 100$, these events are first removed. The subsequent MoGURA neutron selection criteria are outlined below.

The neutron selection in MoGURA is outlined in Figure 3.8. Two quantities are used, dT , the time delay between the neutron event and the previous muon, and N_s . From the 2D distribution, one sees that the event rate is higher in the short dT region due to noise and after-pulses. The N_s values also tend to be small due to signal loss caused by baseline overshoot in the PMTs. The following criteria were chosen to select MoGURA neutrons:

- $N_{total} = N_{in} + N_{out} > 150$ (Number of hit requirement)
- $N_s > 50 \wedge 10 < dT < 1200\mu s$ (reject after-pulses and accidental events)
- $!((N_s < dT(\mu s) + 70 \wedge 10 < dT < 20\mu s) || N_s < -0.8 \times dT(\mu s) + 106 \wedge 20 < dT < 70\mu s)$

Figure 3.9 shows the dT distribution of the MoGURA neutrons collected with the above criteria. The histogram is fitted to an exponential between 500 and 1000 μs , and the fitted function is extrapolated to the rest of the data range. The inefficiency of the neutron tag in the shorter dT period can be seen as the distribution turns off at low dT .

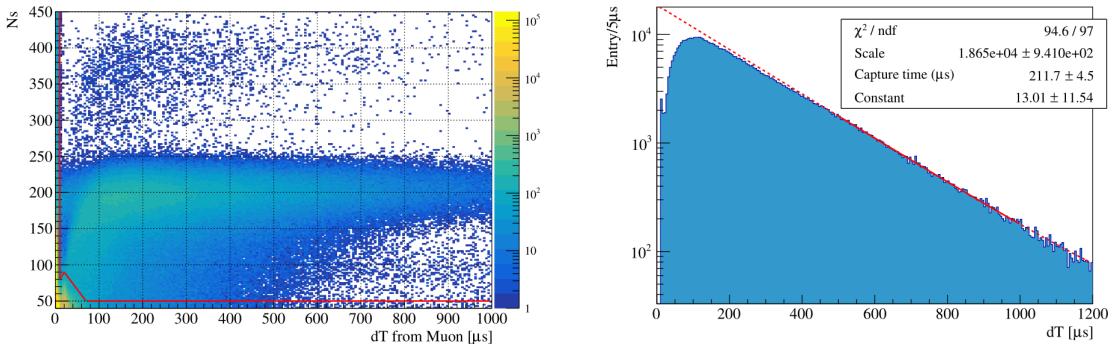


Figure 3.8: distribution showing the dT dependence of N_s . The events above the selected MoGURA neutrons. The fit to an exponential is performed between 500 and 1000 μs . [32]

Figure 3.9: The dT distribution of selected MoGURA neutrons. The fit to an exponential is performed between 500 and 1000 μs . [32]

3.3 Event Selection

Candidate $0\nu\beta\beta$ events must pass several event selections. The selections are separated into non-physical events and background cuts. In this section, we first describe the event selections used in this analysis. Then, the impact of these selections on signal inefficiency is discussed.

3.3.1 Unphysical and Bad Quality Event Rejection

Much of the data saved in the KamLAND DAQ systems includes "unphysical" events. Furthermore, many of the events associated with real physical processes are of poor quality. This section describes the criteria by which unphysical events and poor quality events are selected.

1. Flasher PMT

PMTs can occasionally emit light into the detector. These occurrences are called PMT flashers. There are multiple potential causes for a PMT to flash, such as the discharge of the dynodes and light emission from the epoxy around the breeder circuit. Figure 3.10 shows the typical event display of a flasher event. Such events have a distinct signature, as the PMT that flashes will have

exceptionally high charge and cause a huge deposition of charge in the nearest PMTs as well. The PMT flasher selection criteria are as follows:

- Total charge of ID PMTs > 2500 p.e.
- Maximum ID PMT charge/Total ID PMT Charge $> 60\%$
- Average charge of the neighboring PMTs > 20 p.e.

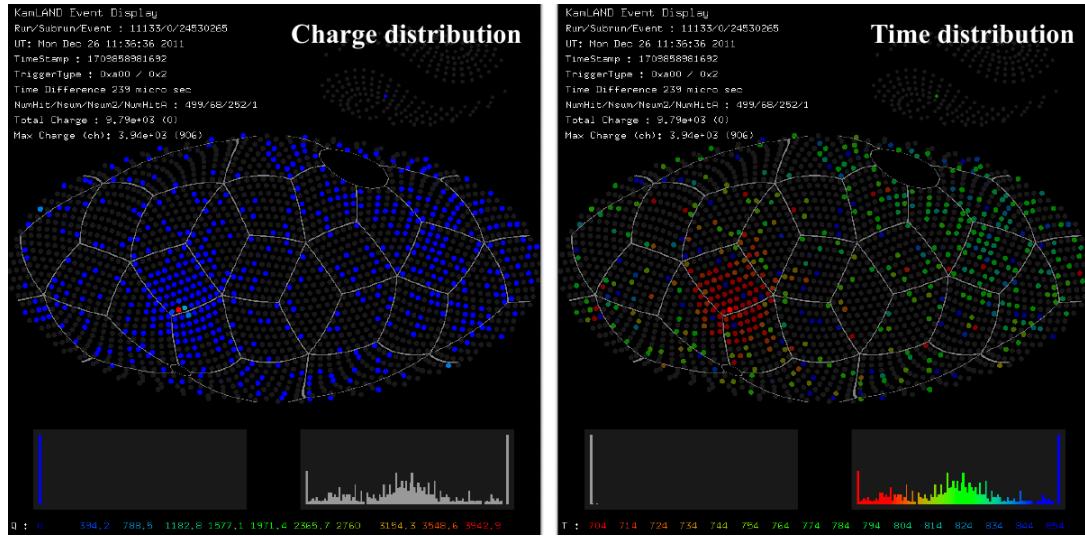


Figure 3.10: Event display of a flasher event. The left shows the charge distribution. One PMT has an exceptionally large charge. Right shows the time distribution. It is relatively flat since the source is not scintillator. The hit timing of the flasher PMTs and its neighbors are very early.

2. Post muon events

Cosmic ray muons deposit a large amount of energy into the detector. As a result, the detector behavior is unstable for a period afterwards. In particular, the detector suffers from a high fake event rate due to after-pulsing and the shift of baseline from overshoot. This instability causes not only a large amount of unphysical events, but also degrades the reconstructibility of real physical events. Thus, all events in the immediate 2 ms after cosmic ray muons are not

used for the excited state analysis. However, these events may be used for other analyses such as spallation background estimation.

3. Missing waveform events

High rate after-pulsing from cosmic ray muons can also cause the ATWD to be busy and the DAQ system to get stuck. When the DAQ electronics are in this state, event waveforms cannot be recorded. These are referred to as "missing waveform" events. In these situations, the number of hit 17-inch PMTs within 125 ns after a trigger issue is recorded as "NsumMax". In properly recorded events, NsumMax should be proportional to the total number of 17-inch PMT hits (Nhit17). So the missing waveform events are identified by the ratio between NsumMax and Nhit17; the distributions of these two quantities are shown in Figure 3.11. Events tagged by this selection are removed from the excited state physics analysis. The exact selection criteria are as follows:

- $Nhit17 < NsumMax \times 0.99 - 25$
- dT after muon events < 2 ms (if $NsumMax < 1200$)
- dT after muon events < 2 s (if $NsumMax > 1200$)

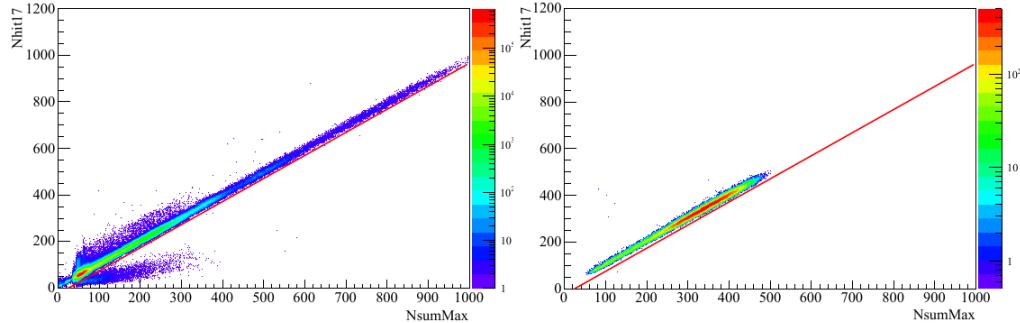


Figure 3.11: Nhit17 vs NHitSumMax distributions for all physics events (left) and Bi214-tagged events (right). The missing waveform cut inefficiency can be calculate from the Bi214-tagged events to be $< 0.01\%$

4. Post PPS trigger event

The PPS trigger is a forced trigger issued once a second used for constant diagnostic monitoring of the detector. However, the PPS trigger has been found to cause an increase in electronics noise and DAQ trigger rate. Thus, events within 100 μs from the last PPS trigger are removed from the analysis.

5. Badly reconstructed events

The fit quality of an event's vertex reconstruction is the event's "Badness". The quantity is calculated using nine parameters that describe the deviation of an event's PMT hit and charge distribution from the expectation. A detailed explanation of the Badness calculation can be found in section 3.8.3 of [?]. These poorly reconstructed events mostly consist of noise events and pileup. The events with large Badness are removed from the analysis by the following energy-dependent threshold:

$$\text{Badness} < 25.0 \times \exp(-4.5 \times E_{\text{vis}}[\text{MeV}]) + 3.1 \quad (3.16)$$

Figure 3.12 shows the Badness distribution of all physical events and the Badness of ^{214}Bi events selected by the delayed coincidence method.

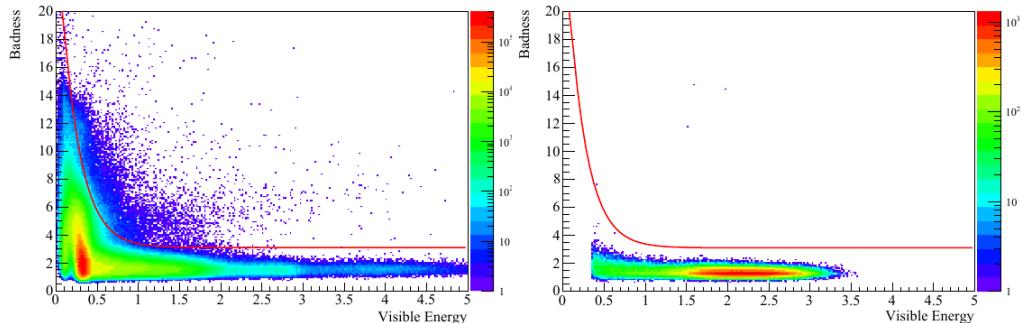


Figure 3.12: The badness distributions of all physics events (left) and Bi214-tagged events (right)

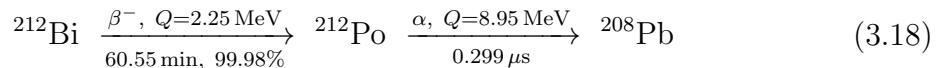
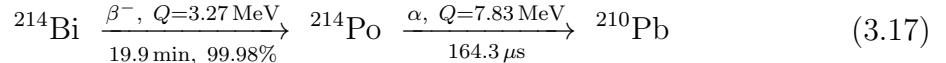
3.4 Background Rejection

3.4.1 Uranium/Thorium

^{214}Bi and ^{212}Bi are radioactive nuclei produced in the uranium and thorium decay series, respectively. They are among the dominant backgrounds in KamLAND-ZEN. These isotopes are introduced to the detector primarily by Uranium/Thorium contamination in the LS itself or on the surface of the inner balloon. There were also some ^{222}Rn introduced when the XeLS was filled, this decayed with a half-life of 3.8 days, as such the ^{222}Rn -related ^{214}Bi decayed away in the early stages of KamLAND-ZEN 800. This time-dependence of the Radon background is accounted for in the physics analysis. These Bismuth-decays are tagged in two ways: Delayed-coincidence veto and Double-pulse fitting.

Delayed Coincidence Veto

Both ^{214}Bi and ^{212}Bi decays are quickly followed by the decays of $^{214}\text{Po}/^{212}\text{Po}$:



These decays are correlated in space and time in KamLAND, they can be vetoed by searching for this correlation. The criteria of the Bi-Po delayed coincidence analysis used in the KamLAND-ZEN analysis is as follows:

- delayed energy : $0.2 < E_d < 1.3 \text{ MeV}$
- distance between prompt and delayed vertices : $dR < 170 \text{ cm}$
- timing delay between prompt and delayed vertices : $dT < 1.9 \text{ msec}$

Figure 3.13 shows the delayed-coincidence veto parameter distributions used in the ^{214}Bi selection. Coincident pairs within 10 μsec are excluded and set aside for the ^{212}Bi selection, as ^{212}Po has a much shorter half-life. The delayed energy deposition distribution, two peaks are found. The lower energy peak corresponds to polonium decays in which some energy is deposited not in the liquid scintillator but in the mini-balloon nylon film. Figure 3.14 shows the delayed-coincidence veto parameter

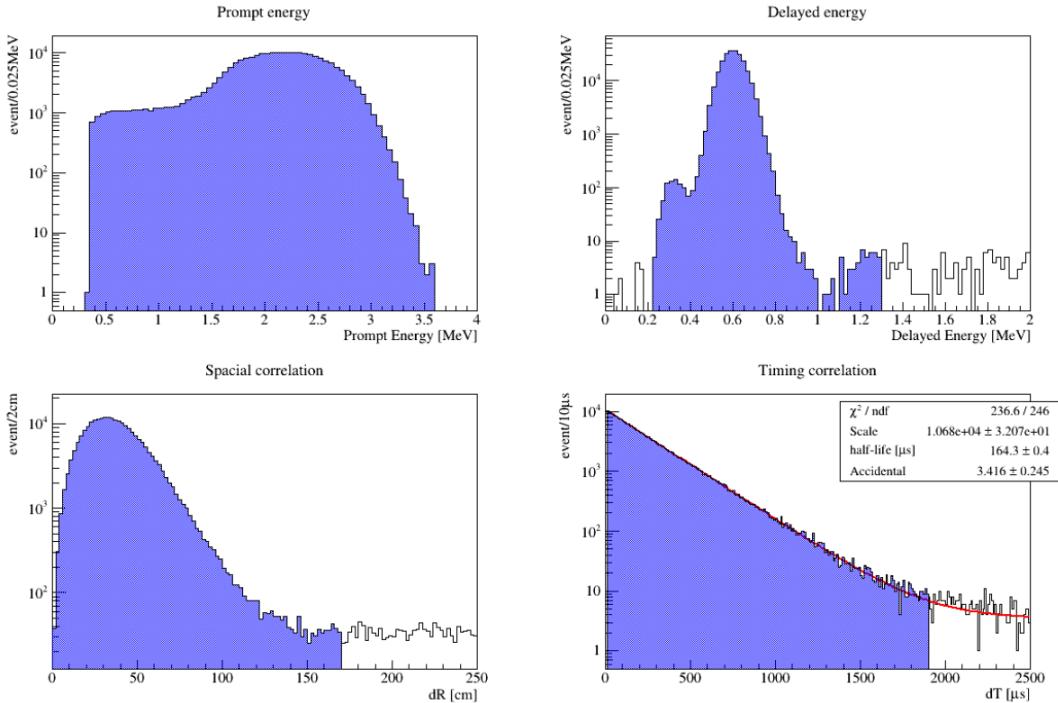


Figure 3.13: The delayed coincidence selection parameters for ^{214}Bi . The distributions of prompt energy, delayed energy, displacement, and delay time are shown. The blue shaded regions indicate the tagged events. Events with $dT < 10\mu\text{sec}$ are set aside for $^{212}\text{Bi-Po}$ selection.

distributions used in the ^{212}Bi selection. For this selection, the timing selection is $dT < 10\mu\text{sec}$. The veto efficiency of $^{214}\text{Bi-Po}$ decays in the XeLS is $99.89 \pm 0.03\%$. The veto efficiency of $^{214}\text{Bi-Po}$ decays in the balloon film is $48.9 \pm 9\%$. The lower veto efficiency is due to alpha decays depositing their energy in the film not the liquid scintillator. For ^{212}Po decays that occur immediately after the initial ^{212}Bi decay,

they can be tagged by the double pulse fitter, which the next section describes.

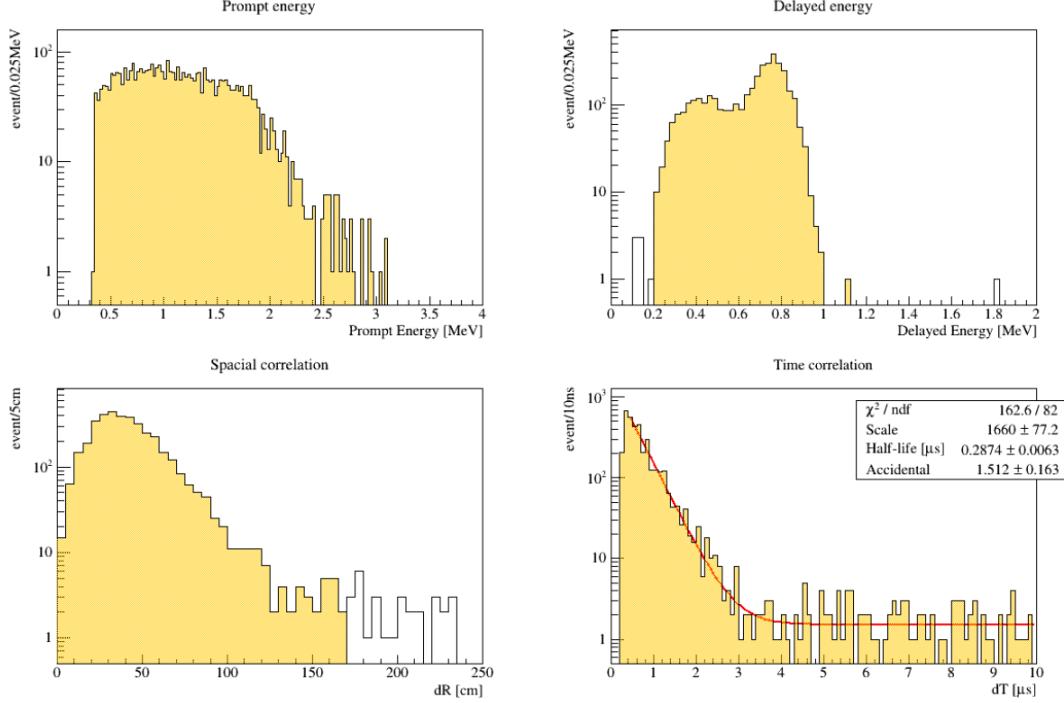


Figure 3.14: The delayed coincidence selection parameters for ^{212}Bi . The distributions of prompt energy, delayed energy, displacement, and delay time are shown. The yellow shaded regions indicate the tagged events. Only events with $dT < 10\mu\text{sec}$ are used for this selection.

Pileup Events

When the delay time, dT , between prompt and delayed events is small enough, Bi-Po sequential events can be stored as a single event in KamLAND's data acquisition window. In these cases, the delayed coincidence selection of two related events does not work. Such events are referred to as pile-up events. Since these pileup events contain the kinetic energy of the initial beta decay and the subsequent alpha decay, the combined deposited energy reaches beyond the $0\nu\beta\beta$ ROI and becomes an important background to reduce. The energy spectrum of these ^{212}Bi -Po pile-up events is shown in Figure ??.

A double pulse fit method has been developed to tag these pile-up events. The method simply searches for events with a hit-timing distribution indicative of two distinct energy depositions, or hit time peaks. The hit time distribution of an event is fitted with 2 reference waveforms by the following procedure:

1. Construct a reference time profile. A reference waveform is made from the hit time profile of $2\nu\beta\beta$ -decay candidates. The events are selected with $1.4 < E_{vis} < 1.6$ MeV and $radius < 157$ cm after $0\nu\beta\beta$ background vetoes.
2. Construct the hit timing profile of $0\nu\beta\beta$ decay candidates. The hit timing profile of the candidate events (events to be analyzed) is constructed. In the typical analyses and reconstructions, the time of the first hit on a PMT in an event is used. For this procedure, all hit times and hit charges (multi-hit) information is used to effectively separate the two peaks.
3. Fit the event's hit time profile The hit time profile is fitted by the reference waveform. The fit includes 4 parameters: E_p (prompt signal energy), T_p (prompt signal timing), E_d (delayed signal energy), ΔT (time delay between prompt and delayed signals). Then a maximum likelihood optimization is performed. χ^2 for the fit is defined as:

$$\chi^2 = \begin{cases} 2 \sum_i \left\{ -(x_i - f_i) + x_i \log \frac{x_i}{f_i} \right\} & (n_i > 0) \\ 2 \sum_i \{-(x_i - f_i)\} & (n_i = 0) \end{cases} \quad (5.27) \quad (3.19)$$

where i , x_i , and f_i denote the i -th bin, the number of hit PMTs in the i -th bin and the expectation of the number of hits in the i -th bin, respectively. The time bins are 1 ns wide. f_i can be calculated as the sum of a dark rate D and the reference waveform $R(i)$ as:

$$F_i = |E_p|R(i - T_p) + |E_d|R(i - T_p - \Delta T) + D \quad (3.20)$$

Here, the dark rate is a simple global dark rate taken from all the PMTs in the off-time period. The χ^2 minimization is performed with MINUIT in the ROOT analysis framework. For all the $(T_p, \Delta T)$ pairs, E_p and E_d are floated, and the optimal four parameters are found.

4. Correct the reconstructed energies E_p and E_d are used in the double-pulse fit to scale the reference waveform but they are not accurate individual pulse energy reconstructions. The energy reconstruction described in section 3.2.5 is more accurate. This "official" energy reconstruction is incorporated into the individual pulse energies by:

$$E_{p'} = E_{vis} \times \frac{E_p}{E_p + E_d} \quad (3.21)$$

$$E_{d'} = E_{vis} \times \frac{E_d}{E_p + E_d} \quad (3.22)$$

Thus, the double-pulse fit provides the fraction of the total event energy, E_{vis} , to assign to the prompt and delayed signals.

5. Candidate selection Finally, the pile-up tagged events are selected from the candidate events based on their ΔT and $E_{d'}$. The selection criteria are determined using MC simulated events while limiting the $0\nu\beta\beta$ inefficiency to about 0.1%. Figure 3.15 shows the selection criteria over the MC distributions. The remaining $^{212}\text{Bi-Po}$ events that pass pile-up are estimated to be $2.3 \pm 0.5\%$.

3.4.2 Antineutrinos

The original physics objective of the KamLAND experiment was to observe electron anti-neutrinos produced in nuclear reactors, among other sources. The signature of

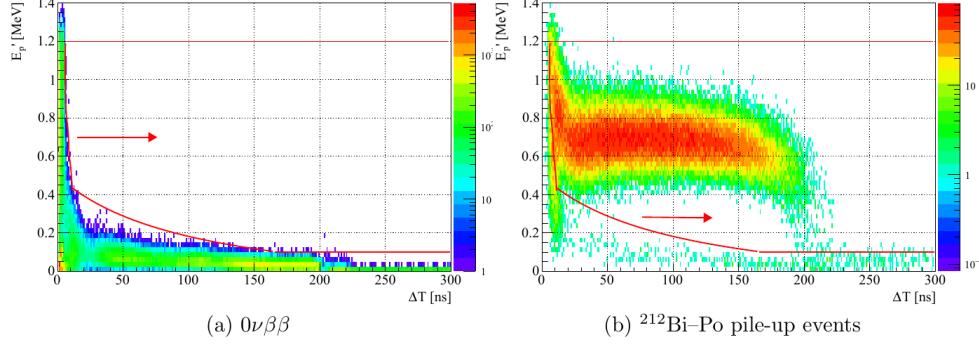


Figure 3.15: The selection criteria over E_d and ΔT used to tag pileup events. The distributions are of MC $0\nu\beta\beta$ (left) and $^{212}\text{Bi-Po}$ (right). The regions enclosed by the red lines are vetoed as pileup events.

anti-neutrinos in KamLAND and KamLAND-ZEN is inverse beta decay (IBD):

$$\bar{\nu}_e + p \rightarrow e^+ + n \quad (3.23)$$

IBD produces a neutron and a positron. The positron annihilates with an electron to produce gamma rays, 2×511 keV gammas. The neutron scatters in the detector until being captured by protons with an average capture time of $\tau = 207 \mu\text{s}$. This two-stage signal is ideal for tagging with the delayed coincidence method.

In the anti-neutrino analysis, IBD events were originally selected by a likelihood ratio selection; but in KLZ, a simple box cut analysis is applied. The IBD selection criteria are:

- delayed energy : $E_d > 1.5$ MeV
- distance between prompt and delayed vertices : $dR < 200$ cm
- timing correlation between prompt and delayed vertices : $dT < 1.0\text{msec}$

In the wake of the 2011 Tohoku earthquake and reactor meltdown, the Japanese nuclear power plants were turned off and the rate of anti-neutrino events are less than 0.2 event/day within $r < 550$ cm. The efficiency of the IBD box cuts are

99.14%. Thus, the remaining potential IBD background to the KLZ analyses are negligible.

3.4.3 Short-lived Spallation Products

High energy cosmic ray muons can break apart nuclei in the detector material into lighter nuclei and produce secondary particles. The spallation products of ^{12}C are one of the dominant backgrounds in the $2n\beta\beta^*$ search. Multiple tagging methods have been developed for identifying so-called short-lived spallation products.

^{12}B Veto

The ^{12}B β -decay has a large contribution to the background in the $0\nu\beta\beta$ ROI. The rate of muons is ≈ 3 Hz in the KamLAND detector thus ^{12}B can be removed with a veto after muons. In this analysis, a 150 msec window, corresponding to 5 times the livetime of ^{12}B , is vetoed and counted as detector deadtime.

MoGURA Neutron Veto

Neutrons are also ejected during the muon spallation process. These neutrons are correlated with the spallation products. The MoGURA DAQ system is used to observe neutron captures that occur shortly after cosmic-ray muons. The correlation with these MoGURA neutrons can be used to tag other short-lived spallation products, mainly ^{10}C , ^6He , and ^8Li . The selection of the MoGURA neutron veto is as follows:

- distance between candidate decay and spallation neutron : $dR < 160$ cm
- timing correlation : $dT < 180$ s (about 5 times the lifetime of ^{10}C)

^{137}Xe Veto

Neutrons capturing onto ^{136}Xe nuclei form ^{137}Xe . The Q-value of ^{137}Xe β^- -decay is 4.2 MeV with a half-life of 3.82 minutes. This decay can be tagged by the triple

coincidence of a muon, the neutron capture, and the beta decay itself. The selection criteria is as follows:

- distance between candidate decay and spallation neutron : $dR < 160$ cm
- timing correlation : $dT < 1,620$ sec

Since the neutron capture gamma on ^{137}Xe has a gamma energy about 4 MeV, higher than captures on protons, the neutron selection criteria is adjusted slightly. The ^{137}Xe neutrons are required to have N_s values above 240. A schematic of spallation veto of Carbon and Xenon is shown in Figure 3.16.

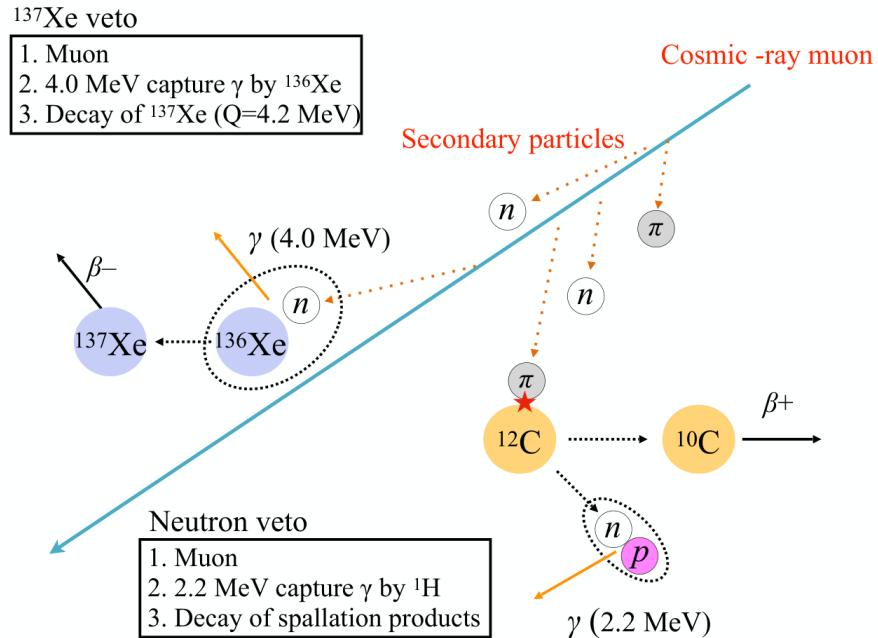


Figure 3.16: A schematic of spallation veto with MoGURA neutrons

3.4.4 Shower Veto

As a cosmic-ray muon passes through the detector, it does not interact with uniform probability along its path. There is a point where it deposits the most energy and

spallates the most nuclei. Secondary decay products are correlated with this position. The shower veto identifies this location of high energy deposition and correlates background with this position.

PDF($dE/dX, dL$)

dE/dX , the distribution of energy deposition along muon tracks, and dL , the distance from the muon track to the candidate event, are correlated to the decay candidates. A two dimensional PDF($dE/dX, dL$) is constructed from muon data by the following procedure:

1. The cosmic ray muons are selected and their tracks reconstructed.
2. The time when the muon entered the ID T_0 is calculated.
3. The distance between the muon ID entrance and the generated point L is calculated for each photon. Figure 3.17 shows the schematic of photon generation from cosmic muons.

$$x_2^2 = r^2 + s_1^2 - 2x_1r \cos \theta \quad (3.24)$$

$$x_1 + nx_2 = c(t - t_0) \quad (3.25)$$

Here, n is the refractive index of the liquid scintillator. These equations are solved for x_1 , the distance L can be obtained. For general analysis and reconstruction, only the PMT hit times of the first photons are used. However, for this calculation, multiple photons for each PMT are considered, referred to as multiTQ analysis. L is calculated for each incident photon on each PMT.

^{12}B is used for estimating the PDF($dE/dX, dL$) as it can be easily tagged by the dT selection after muon events. Figure 3.18 shows an example of a dE/dX calculation result. The accidental event likelihood can also be calculated using the off-time events. The spallation backgrounds are rejected by calculating a likelihood

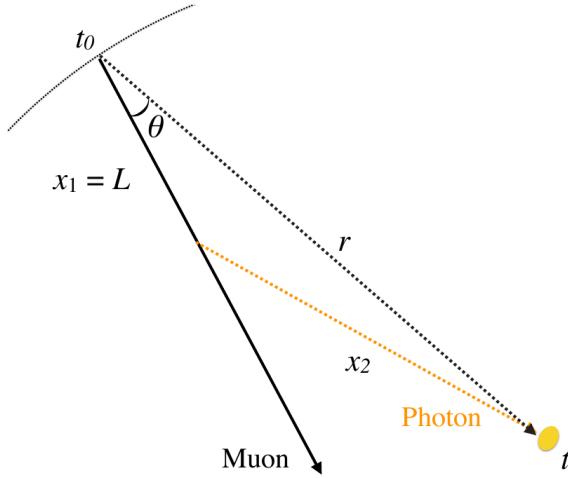


Figure 3·17: dE/dx reconstruction.

ratio value of spallation vs accidental. The log-likelihood ratio threshold used is -1.8, events with spallation-accidental logarithmic ratios below this value are classified as spallation backgrounds and rejected.

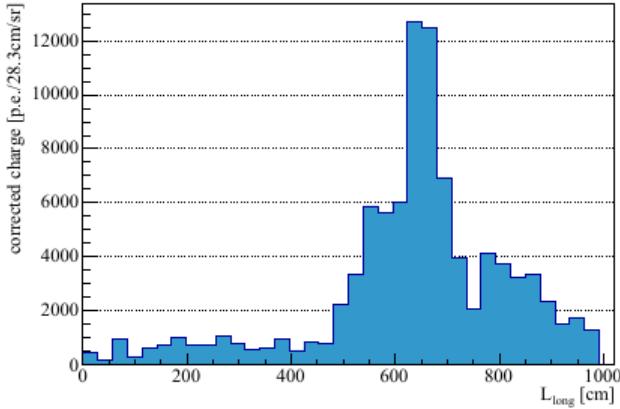


Figure 3·18: An example of a calculated dE/dx . The muon's largest energy deposit can be seen at $L_{long} = 600$ cm.

3.4.5 Xenon Spallation Products

The spallation products of Xenon are an important background to the $0\nu\beta\beta$ search. For the $2\nu\beta\beta^*$ search, they obscure the endpoint of the $2\nu\beta\beta$ spectrum. Rejecting

this background is important to both double-beta physics searches. However, these heavier nuclei can have half-lives of hours or longer, much longer than their Carbon-spallation counterparts; therefore, the MoGURA neutron veto is ineffective against these.

For these backgrounds, a likelihood selection has been developed specifically for these "long-lived" spallation products. The method involves constructing PDFs of dT (time since muon), dR (spatial distance from the nearest neutron created by each muon), and ENN (Effective Number of Neutrons).

^{136}Xe spallation is characterized by the production of many free neutrons; these post-muon neutron captures are useful in identifying likely long-lived spallation isotopes. However, there is a high rate of accidental neutrons and unphysical detector noise that can be attributed to neutrons. The ENN , Effective Number of Neutrons, was developed to define a weighted counting of neutrons by who likely they are to be related to a given event. Each neutron following a muon is assigned a weight based on the spatial distributions of neutron captures from spallation products and accidentals. Figure 3.19 shows the weight over dR .

$$ENN = \sum_{neutrons} \frac{PDF_{spl.}(dR)}{PDF_{spl.}(dR) + PDF_{acc.}(dR)} \quad (3.26)$$

The PDFs are the probability distributions of dR which is the spatial distance between a candidate event and a neutron event. Spallation products and neutrons that originate from the same muon have a spatial correlation. The PDFs are shown in Figure 3.19a. $PDF_{spl.}(dR)$ is modeled with an exponentially modified Gaussian distribution, while $PDF_{acc.}(dR)$ is simply quadratic, assuming uniform distribution in space of uncorrelated events. The exponentially modified Gaussian function features

3 free parameters:

$$f(x; \mu, \sigma, \lambda) = \frac{\lambda}{2} \exp\left(\frac{\lambda}{2}(\mu + \lambda\sigma^2 - 2x)\right) \operatorname{erfc}\left(\frac{\mu + \lambda\sigma^2 - x}{\sqrt{2}\sigma}\right) \quad (3.27)$$

$\operatorname{erfc}(x)$ is the complementary error function defined as $\operatorname{erfc}(x) = 1 - \operatorname{erf}(x)$. The free parameters are determined using ^{10}C data. The sum in equation 3.26 is over all the neutrons in a short window after a muon, it is a quantity assigned to each muon.

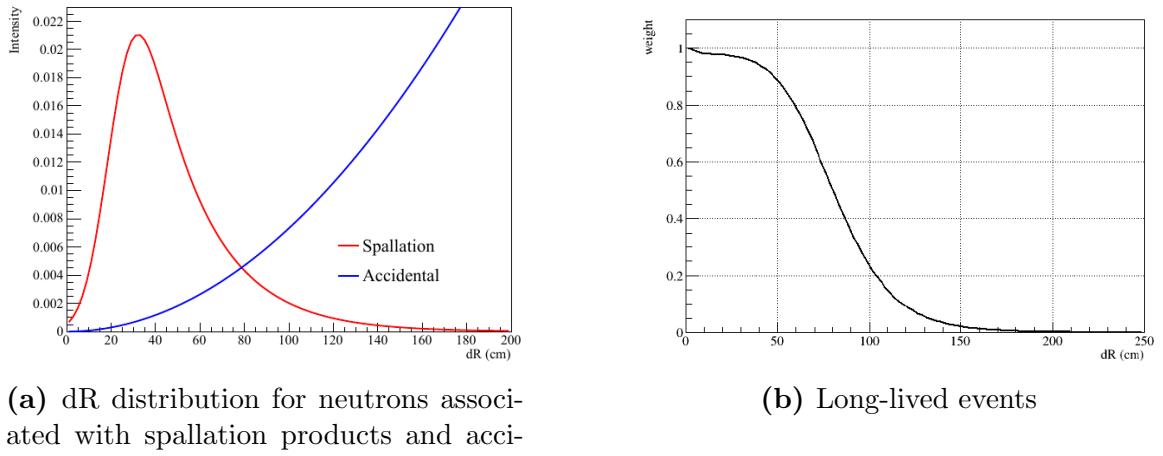


Figure 3.19: Weighting factor function for ENN.

Long-Lived Spallation Likelihood

Long-lived spallation backgrounds are handled not by rejecting them from the analysis outright, but by separating long-lived spallation candidates into a separate spectrum to be fitted alongside the residual events. The long-lived data (LD) and the singles data (SD) are separated by calculating a likelihood ratio threshold. The likelihood ratio is defined as:

$$R_L = \frac{L_{spl.}}{L_{acc.} + L_{spl.}} \quad (3.28)$$

where $L_{acc.}$ and $L_{spl.}$ are the likelihood functions of accidental events and long-lived spallation backgrounds.

The spallation product likelihood is constructed from:

$$L_{spl.}(dR_{near}, ENN, dT) = \sum_{spl.products} PDF(dT) \times PDF(dR_{near}, ENN) \quad (3.29)$$

where the sum is calculated for all spallation isotopes listed in Table ???. There is an implicit assumption that the time-component of the likelihood and the $PDF(dR, ENN)$ are independent. L_{acc} is assumed to be uniform in time and is defined as:

$$L_{acc.}(dR, ENN, dT) = PDF(dR, ENN) \quad (3.30)$$

The likelihoods are constructed from FLUKA simulations and real muon data in KamLAND-ZEN. The long-lived likelihood uses FLUKA simulations of spallation product production and neutron ejection. The accidental likelihood uses events that occur after muons to get a data-informed dR and ENN distribution. Figure 3·20 shows the 2D profiles of the two likelihood functions. The differences are clear, in particular that the spallation products are more likely to have higher ENN and lower dR . In order to avoid dividing by a joint 0 likelihood in the likelihood ratio, bin-smoothing is done to both likelihoods to extend them into the full range.

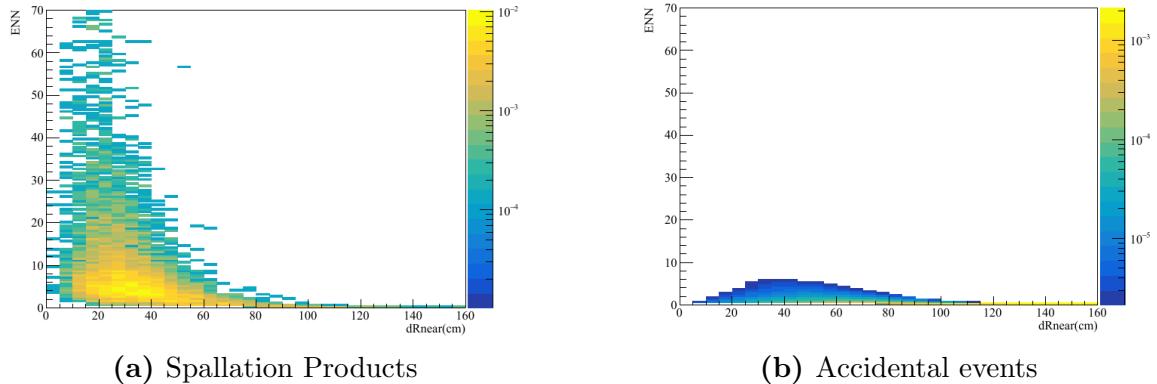


Figure 3·20: Weighting factor function for ENN.

Figure 3·21 shows the distributions of log-likelihood ratios, calculated from our PDFs from toy-MC trials. 10^6 events are generated for each PDF. The log-likelihood

ratio is $\log_{10} \left(1 - \frac{L_{acc}}{L_{acc} + L_{spl}} \right)$, the logarithm is taken to bring all events into a similar range. With this definition, a smaller likelihood ratio or LHR means a higher likelihood of being a long-lived spallation product and a larger LHR indicates a higher likelihood of being an accidental event.

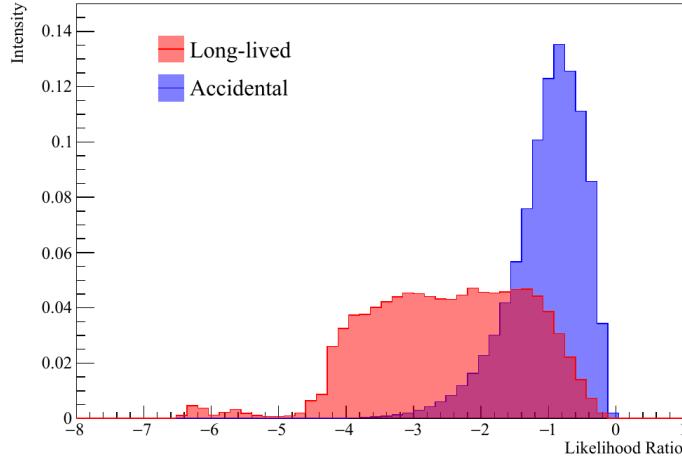


Figure 3.21: Log-Likelihood ratio distributions generated from the PDFs by a ToyMC study. A clear separation between the distributions can be seen.

Figure of Merit

To separate the data events into SD/LD datasets a threshold on the LHR variable must be determined. This threshold is determined by a Figure of Merit calculation (FOM).

$$FOM = \frac{S(t)}{\sqrt{s(t) + B(t)}} \quad (3.31)$$

$S(t)$ and $B(t)$ are the integrated LHR distributions above threshold, t , of signal and background generated by the toyMC study above. Due to inconsistent run conditions, including MoGURA livetime and efficiency, the datasets are separated into 3 time periods and a threshold is independently determined for each time period.

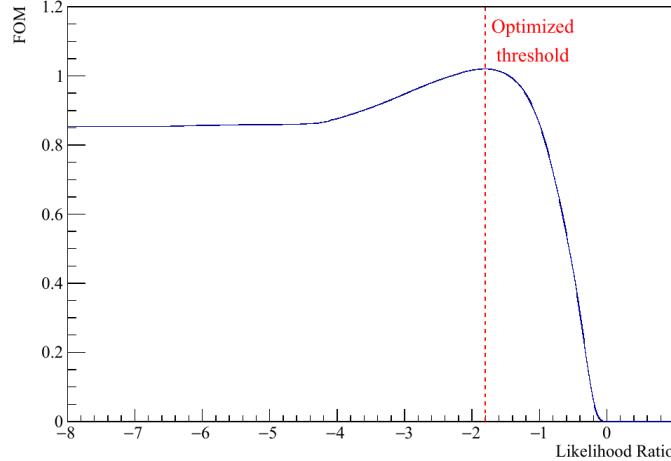


Figure 3.22: Long-lived spallation veto Figure of Merit

Veto Efficiency

The veto efficiency of the long-lived spallation veto is estimated for each spallation background in Table ?? using ToyMC informed by FLUKA simulations. FLUKA simulated isotope production and neutron correlation is convolved with our measured KamLAND-ZEN energy and vertex resolution. The tagging procedure using the above PDFs and likelihood ratio is applied to estimate the veto efficiency.

Furthermore, some of the other background rejection methods will simultaneously help reject some of the long-lived spallation backgrounds. Namely, the pileup veto and MoGURA neutron veto reject some spallation backgrounds; the effects of those vetoes are described as:

- Pileup veto: The double pulse fitter for pileup veto is sensitive to the o-Ps (ortho-positronium decays) of β^+ decaying isotopes. The efficiency of the double-pulse fitter is estimated for each isotope using the lifetime and production rate of o-Ps in [18]. Averaging over the isotopes weighted by production, the efficiency is 4.01%.
- MoGURA neutron veto: Long-lived spallation products that happen to decay

in the 160 s time window of the MoGURA neutron veto are tagged. FLUKA and GEANT4 simulations inform an averaged efficiency of 6.6%.

Uncertainties

Table 3.1 lists the estimated systematic errors of the FLUKA simulation of long-lived spallation isotope production. The most significant of these systematic errors is the uncertainty in the FLUKA spallation simulation. In the absence of dedicated cosmic-ray muon induced xenon-spallation measurements, checking the validity of FLUKA's spallation simulation is difficult. The results of 2 beam experiments are taken into account. The first is an experiment where a 490 GeV μ^+ beam on gaseous xenon reports the production of charged hadrons [11]. Test FLUKA simulations can reproduce their measurements.

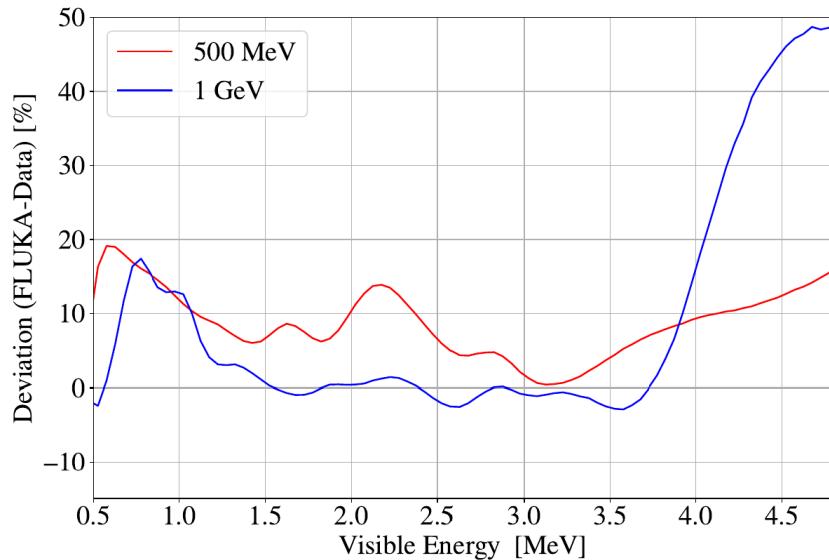


Figure 3.23: The comparison between FLUKA simulation and Xenon beam experiment data. Red line shows the difference from [16]. Blue line shows the difference from [28]. The red line is adopted as the error and considered in the spectrum fit since the deviation in $0\nu\beta\beta$ ROI is larger

Another experiment measured the cross section of a ^{136}Xe beam on a 1 cm^3 liquid-hydrogen target. The incident energy per nucleon used was 500 MeV [16] and 1 GeV

[28]. The comparison of our FLUKA derived long-lived spallation decay spectrum and these beam measurements are shown in Figure 3.23.

	Error
Time-bin dependence	2.9%
Neutron detection efficiency	2.73%
Comparison between FLUKA and beam experiments	7.5%
Energy resolution of MoGURA	5.67%

Table 3.1: Errors of FLUKA

Spectrum Distortion

The discrepancy shown in Figure 3.23 indicates a potential mismodeling of the long-lived spallation background energy distribution. This uncertainty is implemented in the spectral fit, by introducing a distortion parameter that varies the model of the long-lived spallation background, based on this discrepancy with experiment.

3.4.6 Signal Inefficiency

The effect of all these background vetoes on the $0\nu\beta\beta$ signal needs to be understood. This signal inefficiency is determined by calculating the livetime of the analysis.

The livetime calculation is done by applying the same event selections to toy MC events distributed uniformly in time and space. Real detector data is used for the Muon-neutron pairs, delayed coincidence analysis, 1PPS trigger event, and missing waveform events. Livetime is the fraction of runtime leftover after event selection.

$$\text{Livetime} = \frac{\# \text{ of Toy MC events after event selection}}{\# \text{ of generated Toy MC events}} \times \text{Runtime} \quad (3.32)$$

The $2\nu\beta\beta^*$ spectral fit is performed over long-lived spallation enriched and depleted events simultaneously. A later section describes this selection. For proper relative normalization, the livetime is calculated for both long-lived enriched and depleted samples. The deadtime of the KLZ physics analysis is listed in Table 3.2.

Table 3.2: Summary of the deadtime

Event selection	Deadtime ratio [%]
Spallation veto	14.64
MoGURA neutron veto	4.91
${}^8\text{Xe}$ veto	1.33
Shower veto	7.37
${}^{12}\text{B}$ veto	3.11
Xe spallation veto	8.56
Detector deadtime veto (post PPS, after muons and missing waveforms)	9.47
Hardware related	0.0078
Delayed coincidence Ra veto	0.0013
Delayed coincidence Reactor veto	0.0010
Total	29.52

The signal inefficiency of the double-pulse fitter and vertex Badness are omitted from Table 3.2. This is due to the Toy MC livetime study not being done at the PMT hit level. Sections 3.4.1 & 3.3.1 show that the signal inefficiency from these selections is negligible.

The signal inefficiency of the double-pulse fitter and vertex Badness are omitted from table 3.2. This is due to the Toy MC livetime study not being done at the PMT hit level. Sections 3.4.1 & 3.3.1 show that the signal inefficiency from these selections are negligible.

Chapter 4

Detector Calibration and MC Tuning

Accurate modeling of physics events and detector response are essential for correct interpretations of KamLAND-ZEN experimental data. This chapter outlines the detector calibration and Monte-Carlo (MC) tuning methods used. Since the commissioning of KamLAND-ZEN 800, no deployed laser or radioactive source calibration was done. This was to avoid any radioactive contamination from inserting these components into the detector. Thus, known backgrounds are the primary tools for detector calibration. [4]

4.1 Detector Calibration

The KamLAND detector has taken data for over 20 years. The energy scale, non-linearity, bias, resolution, and vertex bias and resolutions have been well calibrated and studied. However, it is important to understand the variation of the detector performance over time. Electronics issues, such as HV reduction, channel loss, and detector work can affect our reconstructions.

4.1.1 Variation of Energy Scale Over Time

As PMT channels are lost or deteriorate into bad channels, or have their gains adjusted, the energy scale of the detector can vary over time. Variation from the beginning of the analysis period in 2019 and until the end of KLZ-800 data-taking in 2024, the energy scale varied by 3%.

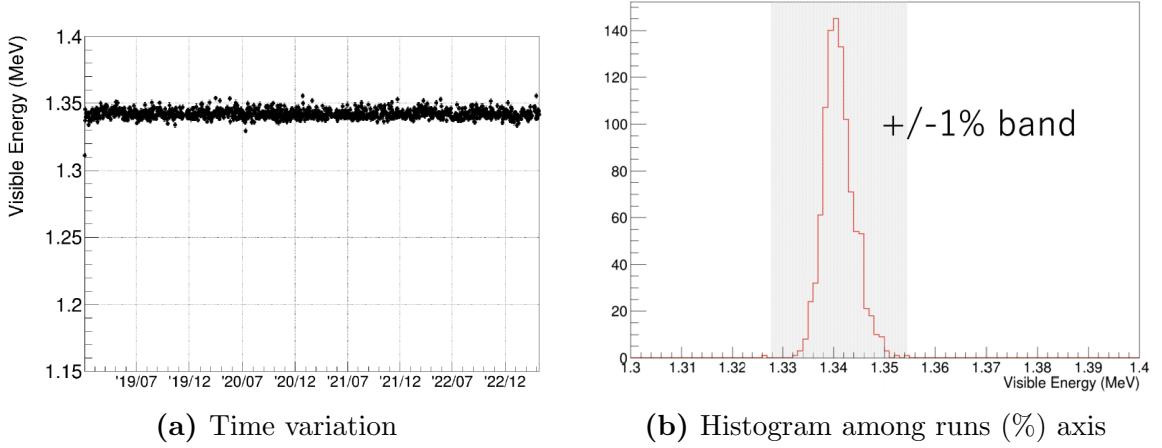


Figure 4.1: Time variation of ^{40}K peak after correction. (A) Time variation of energy scale is corrected using ^{40}K and this figure is a check using ^{40}K itself. (B) Fluctuations among runs are within 1% (gray band).

^{40}K PEEK Gammas

Reconstructing the $^{40}\text{K}-\gamma$ peak from balloon PEEK material can help calibrate the energy scale over time. The PEEK material is located 550cm above the center of the detector and is a consistent source of ^{40}K radioactive decays. The decay energy of the ^{40}K electron-capture decay to ^{40}Ar has an energy of $Q_{EC} = 1504$ keV. However, as the energy scale of the detector decreases as you move from the center of the detector. This EC- γ peak is observed at around $E_{vis} = 1.35$ MeV in KamLAND-ZEN. These ^{40}K PEEK events are selected by the following simple selection:

- Passes Flasher Veto
- Passes Muon Veto
- Passes 2msec veto after muons
- cylindrical volume selection around PEEK material ($450 < z < 600, \rho < 250$ cm)

Neutron Capture Gammas

The KamLAND energy scale is primarily set by neutron captures on Hydrogen. Figure 4.2 shows the variation in neutron capture visible energy over time in XeLS and KamLS. Events are taken simply in a time window following muons. Due to post-muon instability, such as high after-pulsing, PMT ringing, and baseline shifts, the time directly after muons is excluded. An on-off time analysis is performed to subtract any incidental backgrounds and resolve the neutron capture energy distribution.

- On-time window : $400 < dT < 1500 \mu\text{sec}$
- Off-time window : $2800 < dT < 4000 \mu\text{sec}$

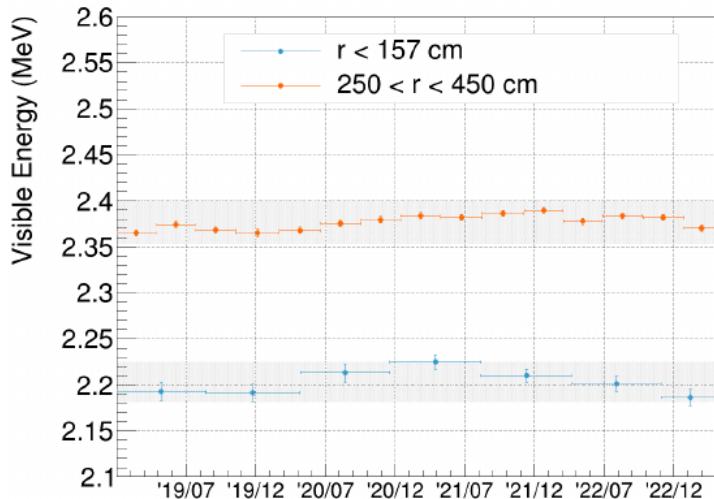


Figure 4.2: Neutron capture energy over KLZ-800 data-taking. The blue and orange points correspond to XeLS and KamLS respectively. Gray bands show $\pm 1\%$ deviation from the average. Note that the energy scale is 7% higher in KamLS due to the higher scintillator light-yield.

$2\nu\beta\beta$ Rate

The tail of the $2\nu\beta\beta$ decay spectrum is another useful handle on variations in energy scale over time. In the absence of any XeLS leakage out of the inner balloon, the rate

of $2\nu\beta\beta$ events in an energy range can be used to verify the energy scale. We apply all the $0\nu\beta\beta$ analysis event selections and a further $1.85 < E_{vis} < 2.35$ MeV energy selection to select the $2\nu\beta\beta$ -dominant region. Figure 4·3 shows minor fluctuations, but no clear trend upward or downwards.

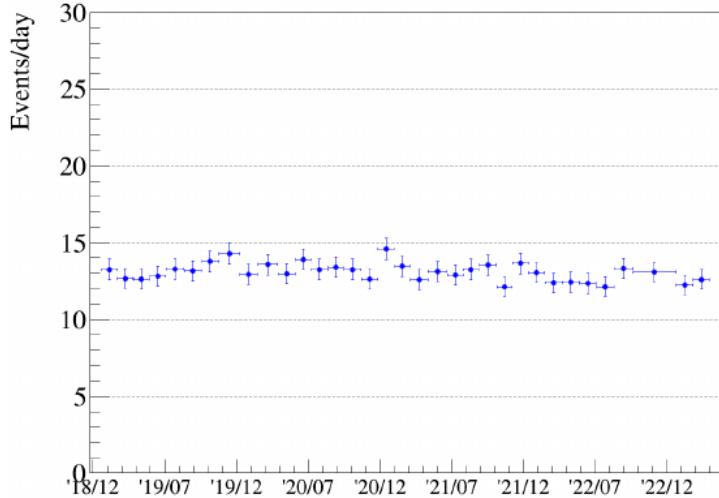


Figure 4·3: The event rate in the $2\nu\beta\beta$ dominant energy region over KLZ-800 data-taking.

4.1.2 MoGURA Stability

Cosmic ray muon induced spallation reactions are a constant source of well understood background. MoGURA’s dead-time-free electronics allow it to observe neutron capture’s closer in time to the original muons. This higher tagging efficiency than KAMFEE provides more data that can be used for calibration.

The MoGURA stability performance over time is marked by the neutron capture rate and distributions. Figure 4·2 shows the variation over time of MoGURA’s neutron tagging performance. The neutron selection in MoGURA was outlined in section 3.2.7.

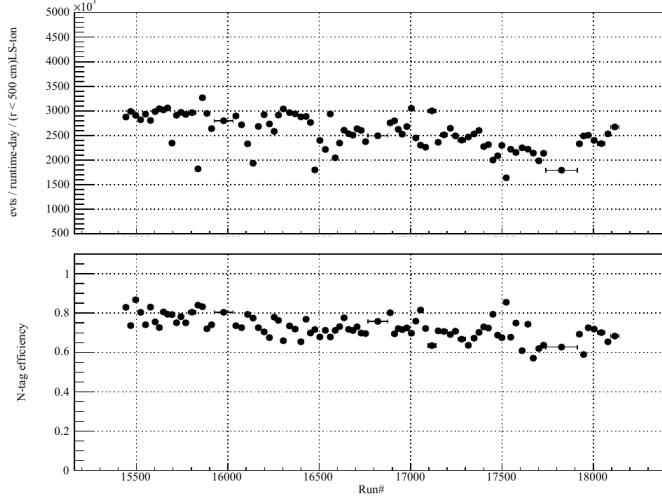


Figure 4.4: MoGURA’s neutron capture rate and neutron tagging efficiency over KLZ-800 data-taking.

^{10}C tagging Stability

^{10}C is an easily isolated, well-understood background that can be further used to monitor detector stability. ^{10}C tagging via triple coincidence was described in section 3.4.3. Note that for this study, the ^{10}C selection was adjusted from the $0\nu\beta\beta$ analysis for higher signal purity.

- Select events in KamLS volume ($250 < r < 400\text{cm}$) and veto the corrugated tube ($r > 250\text{cm} \& z > 0$)
- $2.0 < E_{vis} < 5.0 \text{ MeV}$
- On-time window: $10 < dT < 90 \text{ sec}$
- Off-time window: $300 < dT < 1000 \text{ sec}$

The on-time window begins at 10 seconds to exclude the ^6He spallation background with a 1.16 second lifetime and $Q_\beta = 3.5 \text{ MeV}$. Figure 4.5 shows the characteristic distributions that identify the dataset as ^{10}C . The rate is estimated by fitting an exponential plus constant background to the dT distribution. The dR , distance to

nearest neutron, distribution is modeled by an *exGaussian*, exponentially modified Gaussian. The variation in ^{10}C rate and mean of the exGaussian function are shown in Figure 4.6

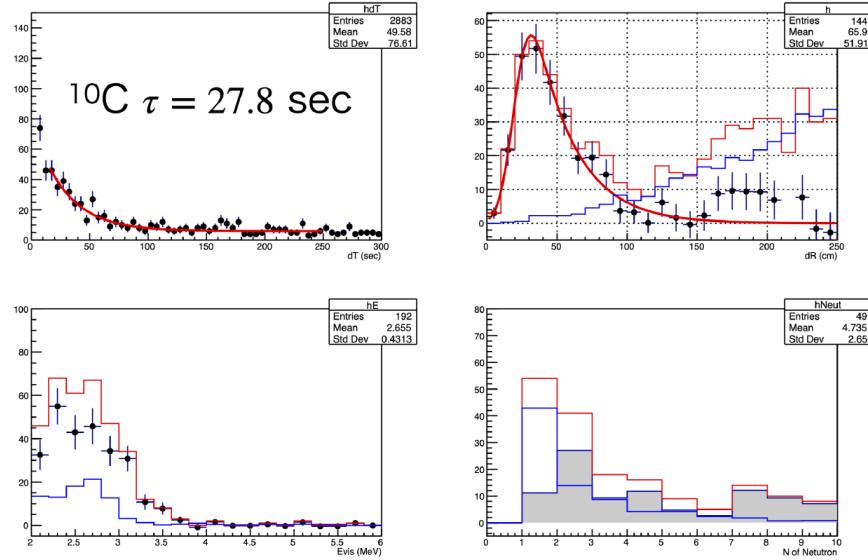


Figure 4.5: Characteristic distributions of ^{10}C decays. Red and blue histograms show on-time and off-time events respectively, and the black markers or grey histograms show the subtracted distributions (on-time - off-time).

4.2 MC Tuning

KamLAND physics simulation is built on two simulation tools: GEANT4 and FLUKA. GEANT4 is used to simulate the distributions of signals, backgrounds decays, and scintillation light propagation in KamLAND detector media. KamLAND's GEANT4-based simulation tool chain is called KLG4Sim. FLUKA is used to simulate cosmic-ray muon induced spallation. Namely for neutron multiplicity and topology and spallation isotope production.

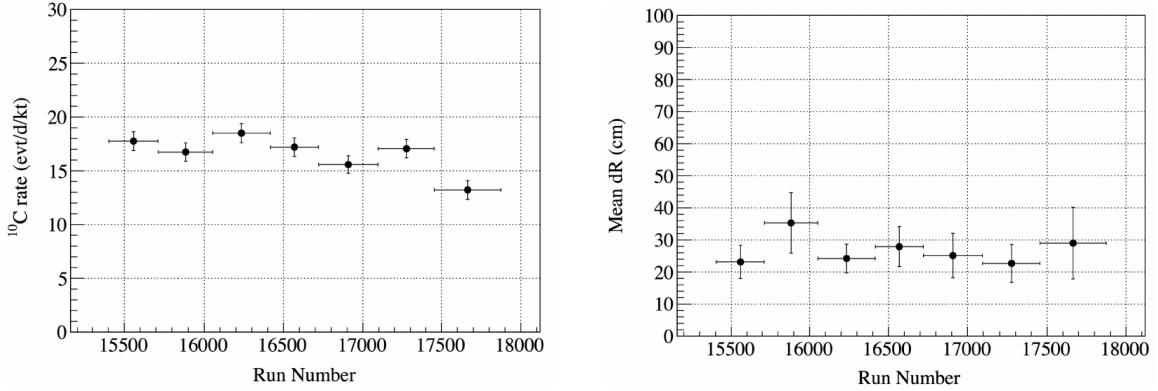


Figure 4.6: Time variation of ^{10}C rate and dR distribution shape over KLZ-800 data-taking.

4.2.1 Geant4 (KLG4)

KLG4 simulations used in this thesis analysis were tuned in [29] and [32]. This section describes their prior work in tuning KLG4 parameters.

KamLS Tuning

KamLS properties, the outer scintillator volume without dissolved xenon, are tuned using source calibration data taken on January 16, 2018. The calibration deployment involved moving a composite radioactive source between -550 and 550 cm in 50cm intervals. With 20 minutes of data-taking at each position. Table 4.1 describes the source composition.

Table 4.1: Summary of radioactive source. Estimated intensities are as of January 17, 2018 on which the calibration DAQ was taken.

Construction date	Aug. 24, 2015		
DAQ date	Jan. 16, 2018		
Source ID	Kam-41 (composite source)		
Particle	^{137}Cs	^{68}Ge	^{60}Co
Energy (keV)	1 γ	2 γ	2 γ
Initial Intensity (Bq)	661.7	511.0	1173.2, 1332.5
Estimated Intensity (Bq)	181	419	322
	180	356	234

Figure 4.7 shows the N_{hit} and total charge spectra of the composite source, with

clearly visible gamma peaks. The gamma peaks are used to calibrate the nonlinearity of KamLS energy scale. The figure also shows the tuned KLG4 spectra that agrees well with data after tuning.

The energy scale is also tracked through position, via calibration source deployment. The deployment data was used to tune material properties like attenuation length, re-emission probabilities, and scattering probabilities. Figure 4.8 shows the position dependence of total charge for each source isotope. The variability and simulation reproducibility with tuning is deteriorates as we move from the center of the detector. The physics analysis presented in this thesis focuses on data within 250cm. In this region, the deviation is within 2%.

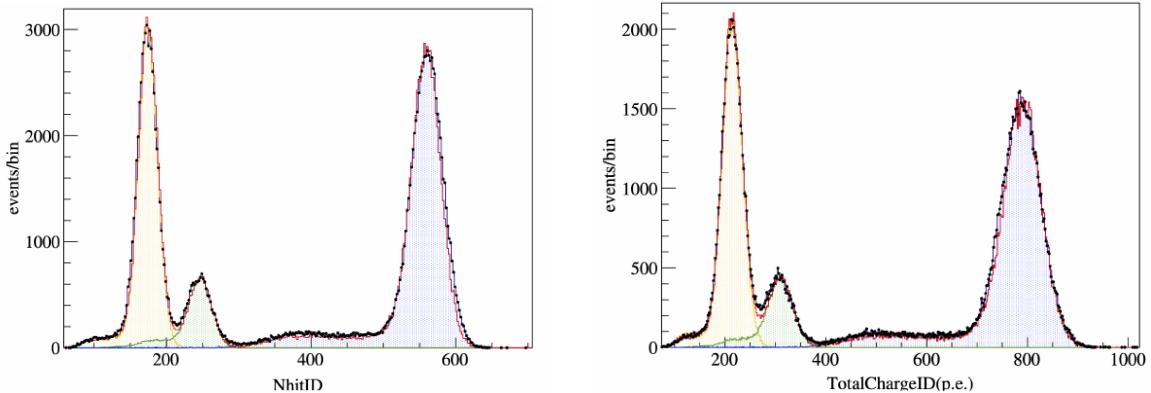


Figure 4.7: N_{hit} and total charge distribution of source calibration. Black plots show data and colored histograms (orange: 137 Cs, green: 68Ge, blue: 60 Co) show MC simulation. MC spectra are well tuned to data in both N_{hit} and total charge. Figures from [29]

XeLS Tuning

There are no source calibration located in XeLS. Alternatively, some background sources are available to calibrate the detector. ^{222}Rn is mixed in XeLS by emanation from pipeline or buffer tanks during xenon resolving work. A sequential decay of daughter isotopes $^{214}\text{Bi-Po}$ can be tagged using delayed coincidence and they exists

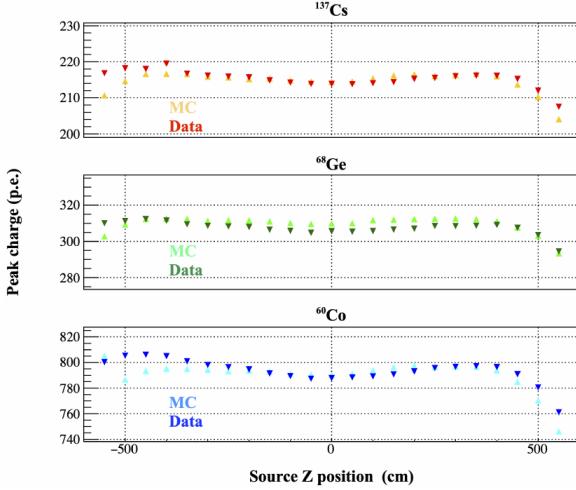


Figure 4.8: Position dependence of total charge peak for each calibration source isotope [29]

only in XeLS. The half life of ^{222}Rn is 3.8 days and after completion of xenon resolving work, ^{222}Rn does not supplied. Thus $^{214}\text{Bi-Po}$ as high statistic calibration source is available only in first several months of KamLAND-Zen 800 observation. Birk's constant, attenuation length, scattering probability, LS time properties, and re-emission for XeLS are tuned using $^{214}\text{Bi-Po}$.

Position-dependent Energy Correction

Position dependence, over radius and θ , of visible energy in XeLS is observed using the ^{214}Po *alpha* decay peak. The deviation from the center of the detector is reproduced in KLG4 as shown in Figure 4.9. The MC correction factors were tuned to ensure that the MC $0\nu\beta\beta$ decay peak in XeLS does not have a position dependence.

Energy Non-Linearity

The visible energy and the energy deposited by charged particles have a nonlinear relation due to the scintillation quenching and the contribution of Cherenkov light.

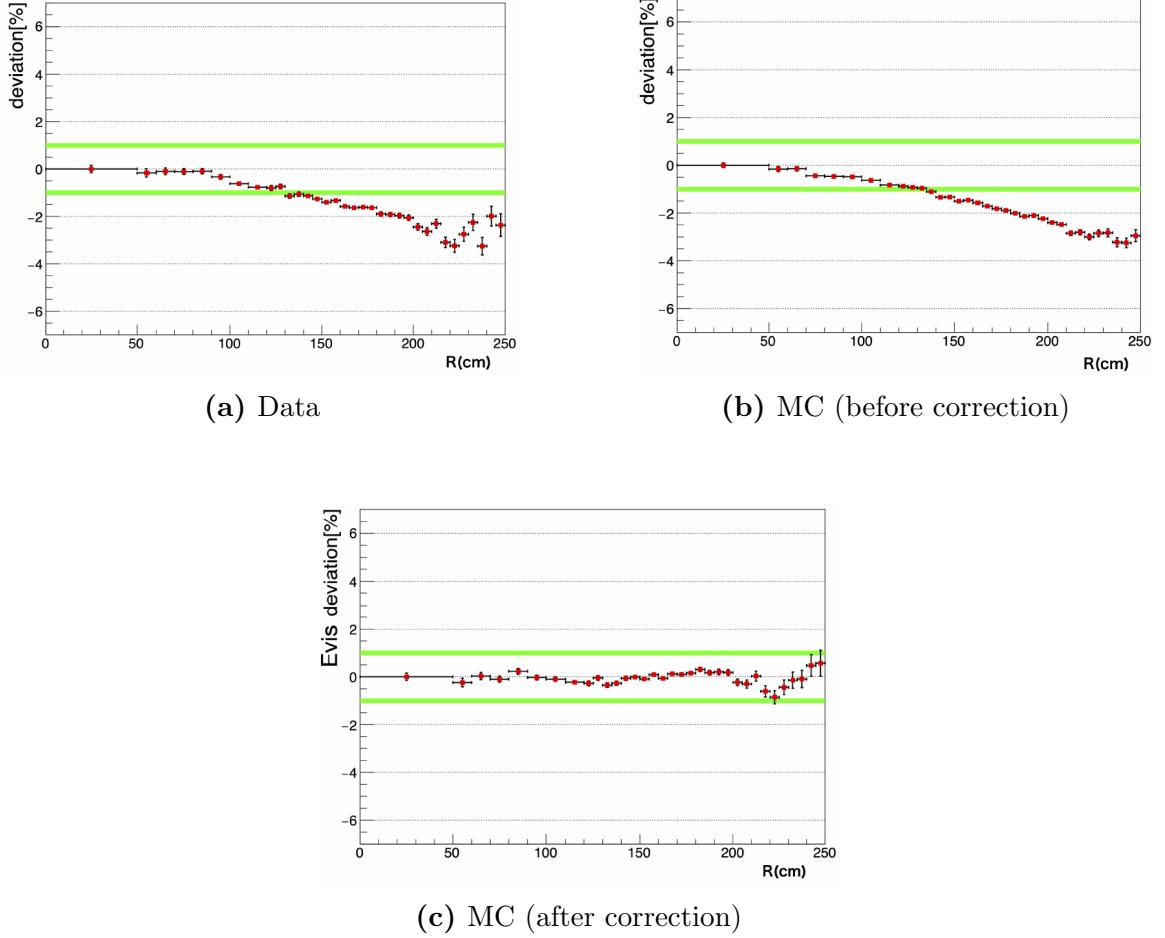


Figure 4.9: Radius dependence of total charge of ^{214}Po . Figures from [29].

The following model is well known as Birks formula:

$$\frac{dL}{dx} \propto \frac{dE/dx}{1 + kB \cdot dE/dx'} \quad (4.1)$$

where dL/dx is light yield per unit length along particle track, dE/dx is energy deposited per unit length, and kB is the Birks' constant which is material dependent. Charged particles also emit cherenkov light, the proportion of the light yield attributed to cherenkov radiation is denoted by the chrenkov-scintillation ratio, R . Tagged ^{214}Bi data is used to tune kB and R . The tagged ^{214}Bi data in XeLS is primarily from the early ^{222}Rn -rich period. The tuning analysis was performed in

[29] and [32]. Figure 4.10 shows a $\Delta\chi^2$ scan over kB and R and the best fit of $(kB, R) = (0.31, 0.01)$. These are the values used in KLG4 for background and signal simulation. Figure 4.11 shows the result of XeLS tuning. The BiPo decay energies are matched to data and the spatial correlation between the coincident decays agree.

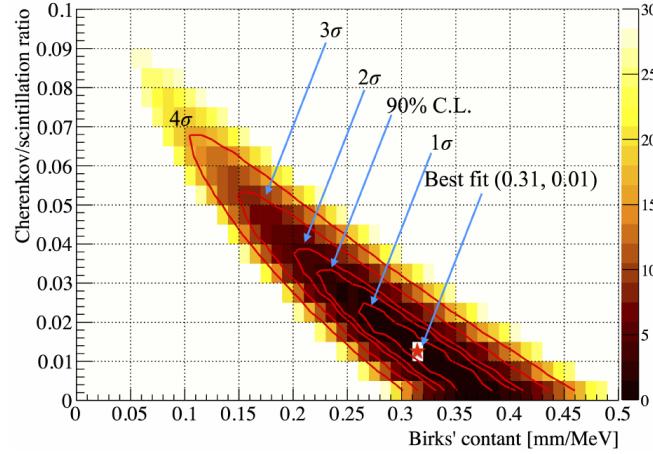


Figure 4.10: $\Delta\chi^2$ scan over kB and R

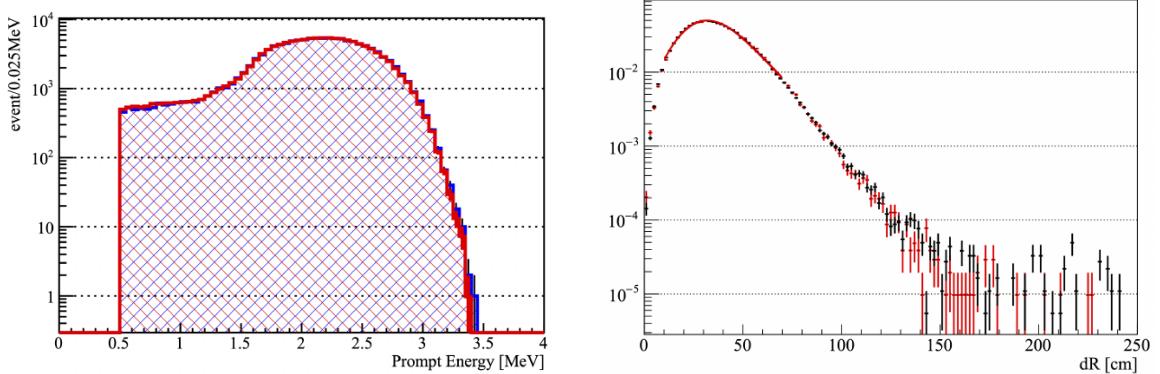


Figure 4.11: Tuned ^{214}Bi - β decay energy spectrum and spatial correlation of delayed-coincidence Bi-Po decays. Figures from [32]

Energy Scale

The overall energy scale of KamLS and XeLS are tuned by the neutron capture gamma peak of 2.2 MeV. XeLS introduces extra quenching by the xenon which reduces the

light yield in XeLS slightly. Figure 4.2 shows the peak energies used. This is the same dataset used for the energy scale time variation check.

4.2.2 FLUKA

FLUKA simulation software is used to predict cosmic muon spallation isotope yields and neutron production. The FLUKA version used in this modeling is FLUKA 2011.08.patch. Simulations and the results are described in [5]. Studies and measurements performed in KamLS are outlined in [6].

Simulation Configuration

The FLUKA physics process packages used in these spallation studies are listed in Table 4.2. FLUKA is only used to generate the production of spallation isotopes and neutrons, their decays and isomer production are disabled. The subsequent decays and neutron capture gammas are simulated in GEANT4.

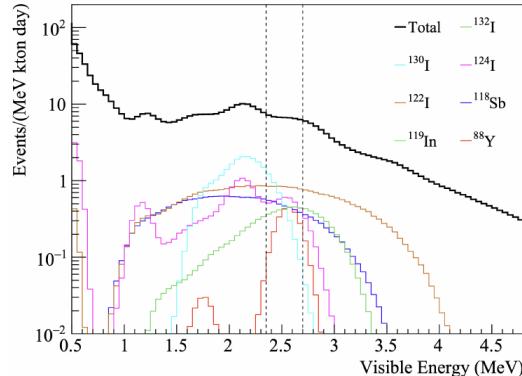
Cosmic ray muon spallation is simulated by injecting muons into a cylindrical XeLS volume of 10 m radius and 40 m height. The inner balloon radius is only 2m. The volume within 10 m from the side and 5m from the exit is excluded from the analysis to avoid boundary effect. The MUSIC package is used to generate the cosmic ray muon energy distribution[8]. MUSIC takes in the detailed geometric description of the Kamioka mine where KamLAND is located. The generated energy distribution is fed into FLUKA and fired into the simulation’s XeLS volume. The mean simulated muon energy is 260 ± 1 GeV. The simulation yields a neutron capture time of $\tau = 207.0 \pm 0.3\mu\text{sec}$ which is consistent with the previously measured value. The muon charge ratio is taken to be $\mu^+/\mu^- = 1.3$ in this simulation[22].

Table 4.2: FLUKA physics processes. From Ref.[5].

card	Physics	Status
DEFAULTS	A set of physics models	PRECISIO(n)
PHOTONNUC(lear)	Gamma interactions with nuclei	Activated
MUPHOTON	Muon photonuclear interaction	Activated
PHYSICS	Emission of light fragments	Activated by COALESCE(nse)
PHYSICS	Emission of heavy fragments	Activated by EVAPORAT(ion)
PHYSICS	Ion electromagnetic dissociation	Activated by EM-DISSO(ciation)
PHYSICS	Decay and isomer production	Activated by RADDECAY

Radioactive Decays

As previously described, FLUKA is used only for the direct spallation isotope production and neutron captures. The subsequent radioactive decays are simulated in the "Radioactive Decay" package in Geant4. The GEANT4 version used is Geant4.10.6.p01 with G4ENSDFSTATE2.2 for the Evaluated Nuclear Structure Data File (ENSDF) [10]. Table 4.3 lists the xenon spallation products considered in this study. In total, 32 isotopes are selected that have production rates exceeding 0.01/day/XeLS-kton in the Region of Interest (ROI). Figure ?? shows the simulated energy spectra.

**Figure 4.12:** Simulated energy spectra of ^{136}Xe spallation products including their decay chain.

Tuning With ^{10}C

FLUKA simulations of radioactive decays and neutron capture gamma do not include detector effects and reconstruction performance. The information given by

the FLUKA simulation includes the capture points of neutron captures but not the reconstructed vertices.

To approximate the effect of event reconstruction, the true neutron capture positions from FLUKA are convolved with a Gaussian resolution distribution. The neutron detection efficiency is also empirically modeled by:

$$\epsilon(\log_1 0Q_\mu) = \epsilon \left(1 - \frac{1}{1 + e^{-\sigma(\log_1 0Q_\mu - a)}} + b \right) \quad (4.2)$$

The neutron detection efficiency is known to be particularly sensitive to baseline fluctuations in the immediate aftermath of a muon. Since, the baseline recovery time depends on the muon charge, the neutron detection efficiency, ϵ , is assumed to depend on the charge.

$(1 + e^{-\sigma x})^{-1}$ is a sigmoid function which mimics the error function and Q_μ is muon charge. σ controls the steepness of the sigmoid function's transition. Free parameters, σ, a, b are tuned to reproduce the dR and ENN distributions of ^{10}C as shown in Figure 4.13. dR is the spatial distance to the nearest neutron of a given shower, while ENN is the "effective number of neutrons". Vertex resolution affect both of these variables, while the neutron tagging efficiency primarily affects ENN .

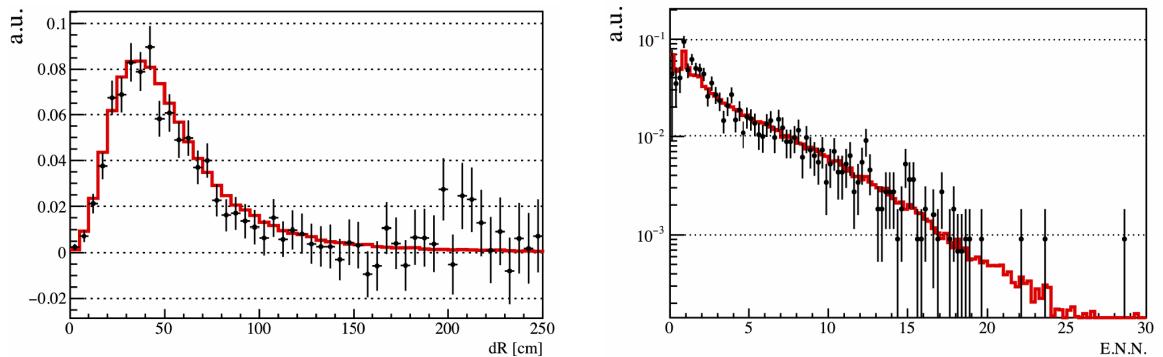


Figure 4.13: Tuned ^{10}C dR (left) and ENN (right) distributions from FLUKA (red curve) and data (black dots) Figures from [27]

Table 4.3: Breakdown of ^{136}Xe spallation products. Isotopes with production rates exceeding 0.01 /day/XeLS-kton in the Region of Interest (ROI) were considered and included in the background model.

isotope	decay mode	Q-value (MeV)	half-life (s)	ROI (day-kton) $^{-1}$	Total (day-kton) $^{-1}$
^{88}Y	EC/ β^+/γ	3.62	9.212×10^6	0.110	0.136
^{90m}Zr	IT	2.31	8.092×10^{-1}	0.012	0.093
^{90}Y	EC/ β^+/γ	6.11	9.212×10^5	0.024	0.095
^{96}Tc	EC/ β^+/γ	2.97	3.698×10^5	0.012	0.059
^{98}Rh	EC/ β^+/γ	5.06	5.232×10^2	0.011	0.076
^{98}Rh	EC/ β^+/γ	3.63	7.488×10^4	0.088	0.234
^{103}Ag	EC/ β^+/γ	4.28	4.152×10^3	0.012	0.160
^{104m}Ag	EC/ β^+/γ	4.28	2.010×10^3	0.018	0.111
^{107}Cd	EC/ β^+/γ	3.43	1.944×10^3	0.019	0.135
^{108}In	EC/ β^+/γ	5.16	3.480×10^3	0.089	0.194
^{110}In	EC/ β^+/γ	3.89	1.771×10^4	0.053	0.236
^{110m}In	EC/ β^+/γ	3.89	4.146×10^3	0.066	0.351
^{110}Sn	EC/ β^+/γ	3.85	1.080×10^3	0.027	0.122
^{113}Sb	EC/ β^+/γ	3.92	4.002×10^2	0.036	0.231
^{114}Sb	EC/ β^+/γ	5.88	2.094×10^2	0.020	0.297
^{115}Sb	EC/ β^+/γ	3.03	1.926×10^3	0.031	0.839
^{116}Sb	EC/ β^+/γ	4.71	9.480×10^2	0.071	0.939
^{118}Sb	EC/ β^+/γ	3.66	2.160×10^2	0.165	1.288
^{116}Te	EC/ β^+/γ	2.90	5.201×10^6	0.016	0.054
^{115}Te	EC/ β^+/γ	4.64	3.489×10^2	0.012	0.124
^{117}Te	EC/ β^+/γ	3.54	3.720×10^3	0.052	0.584
^{119}I	EC/ β^+/γ	3.51	1.146×10^3	0.053	0.533
^{120}I	EC/ β^+/γ	5.62	4.896×10^3	0.091	0.953
^{122}I	EC/ β^+/γ	4.23	2.178×10^2	0.289	1.965
^{124}I	EC/ β^+/γ	3.16	3.608×10^5	0.190	1.654
^{108}I	β^-/γ	2.95	4.450×10^4	0.195	1.188
^{132}I	β^-/γ	3.58	8.262×10^3	0.148	0.427
^{134}I	β^-/γ	4.18	3.150×10^3	0.043	0.183
^{121}Xe	EC/ β^+/γ	3.75	2.406×10^3	0.100	0.540
^{125}Cs	EC/ β^+/γ	3.09	2.802×10^3	0.012	0.266
^{126}Cs	EC/ β^+/γ	4.82	9.840×10^1	0.011	0.080
^{128}Cs	EC/ β^+/γ	3.93	2.196×10^2	0.031	0.229

Chapter 5

Conclusions

5.1 Summary of the thesis

Time to get philosophical and wordy.

Important: In the list of references at the end of thesis, abbreviated journal and conference titles aren't allowed. Either you must put the full title in each item, or create a List of Abbreviations at the beginning of the references, with the abbreviations in one column on the left (arranged in alphabetical order), and the corresponding full title in a second column on the right. Some abbreviations, such as IEEE, SIGMOD, ACM, have become standardized and accepted by librarians, so those should not be spelled out in full.

Appendix A

Proof of xyz

This is the appendix.

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Selected Publications

- "Search for Majorana Neutrinos with the Complete KamLAND-Zen Dataset" KamLAND-Zen Collaboration, arXiv:2406.11438 [hep-ex] (2024)
- "Eos: conceptual design for a demonstrator of hybrid optical detector technology" T. Anderson et al. JINST 18 P02009 (2023)
- "KamNet: An integrated spatiotemporal deep neural network for rare event searches in KamLAND-Zen" A. Li, et al. Phys. Rev. C 107, 014323 (2023)
- "RFSoC-based front-end electronics for pulse detection" S.N. Axani et al. 2024 JINST 19 P03013 (2024)
- "Search for the Majorana Nature of Neutrinos in the Inverted Mass Ordering Region with KamLAND-Zen" KamLAND-Zen Collaboration, Phys. Rev. Lett. 130, 051801 (2023)

Scientific Collaborations

- EoS Collaboration 2023–Present
- NuDOT Collaboration 2022–Present
- KamLAND Collaboration 2020–Present
- NIM+ 2020–2021
- Mu2E Collaboration 2018–2019

Conferences and Presentations

- ”Getting Excited About Double Beta Decay in KamLAND-Zen”, APS DNP, Talk, Boston, MA, 2024.
- ”Understanding KamNet Performance in KamLAND-ZEN with ML Interpretability”, SLAC Summer Institute, Poster, SLAC, 2023.
- ”KamLAND-Zen’s New ML Tricks”, Neutrino Physics and Machine Learning, Talk, Northeastern University, 2023.
- ”Rejecting Spallation Backgrounds in KamLAND-ZEN with KamNet”, Neutrino, Poster, Seoul, Korea, 2022.
- ”Rejecting Spallation Backgrounds in KamLAND-ZEN with KamNet”, TAUP, Poster, Valenica, Spain, 2021.
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